# COMMUTATION METHODS FOR JACOBI OPERATORS

F. GESZTESY AND G. TESCHL

Abstract. We offer two methods of inserting eigenvalues into spectral gaps of a given background Jacobi operator: The single commutation method which introduces eigenvalues into the lowest spectral gap of a given semi-bounded background Jacobi operator and the double commutation method which inserts eigenvalues into arbitrary spectral gaps. Moreover, we prove unitary equivalence of the commuted operators, restricted to the orthogonal complement of the eigenspace corresponding to the newly inserted eigenvalues, with the original background operator. In addition we compute the (matrix-valued) Weyl $m$-functions of the commuted operator in terms of the background Weyl $m$-functions. Finally we show how to iterate the above methods and give explicit formulas for various quantities (such as eigenfunctions and spectra) of the iterated operators in terms of the corresponding background quantities and scattering matrix. Concrete applications include an explicit realization of the isospectral torus for algebro-geometric finite-gap Jacobi operators and the $N$-soliton solutions of the Toda and Kac-van Moerbeke lattice equations with respect to arbitrary background solutions.

## 1. Introduction

For a variety of reasons, techniques to insert and remove eigenvalues in spectral gaps of a given one-dimensional second-order differential (i.e., Sturm-Liouville) respectively difference (i.e., Jacobi) operator have recently attracted great interest. In fact, these techniques are vital in diverse fields such as the inverse scattering approach used by Deift and Trubowitz [16], supersymmetric quantum mechanics (cf. the literature cited, e.g., in [34]), level comparison theorems (see, e.g., [4]), in the construction of soliton solutions of the Korteweg-de Vries (KdV) and Toda hierarchies relative to general KdV and Toda background solutions (see, e.g., [6], [7], [14], [16], [17], Ch. 4, [23], [26], [30], [34], [38]-[40], [41], Sect. 6.6, [45]–[48]), and in connection with Bäcklund transformations for the KdV and Toda hierarchies (cf., e.g., [7], [18], [20], [24], [30], [32], [34], [42], [43], [53]).

Historically, methods of inserting eigenvalues in the case of differential operators go back to Jacobi [37], Darboux [13], Crum [12], Gel'fand and Levitan [27], Schmincke [46], and especially Deift [14]. Two particular such methods, the so called single commutation or Crum-Darboux method and the double commutation method, shortly to be described below, turned out to be of particular importance. The operator theoretic approach developed in [14] applies to the single commutation method and has been used in [14] to give a complete spectral characterization in the differential operator case. The double commutation method on the other hand required entirely different methods and was only recently solved in the differential operator case. A solution based on ODE techniques was given in [28] and most recently, a more general and at the same time greatly simplifying operator theoretic approach to a spectral characterization of the double commutation method appeared in [31].

Surprisingly, a complete spectral characterization of both the single and double commutation methods in the difference operator context is lacking in the literature thus far. Although special cases of the single commutation method with constant or algebro-geometric backgrounds have been discussed in [7], [15], [52], no treatment of general backgrounds is known to us. Moreover, with the exception of reference [52], where an eigenvalue is inserted into the spectral gap of a two-band periodic Jacobi operator with period 2, no general formulation of the double commutation

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method for finite difference operators seems to be available in the literature. The present paper fills these gaps and provides a complete spectral characterization of the single commutation method (based on Deift's operator theoretic approach) in Sections 2 and 3 and develops the corresponding results for the double commutation method in Sections 4-6. Section 7 gives three applications of our results. The discrete analog of the FIT formula for the isospectral torus of periodic Schrödinger operators, thereby deriving an explicit realization of the isospectral torus of all algebro-geometric quasi-periodic finite-gap Jacobi operators, and the $N$-soliton solutions of the Toda and Kac-van Moerbeke equations on an arbitrary background solution using the single and double commutation methods. Section 8 collects various appendices on the Weyl-Titchmarsh theory for second-order difference operators.

In the remainder of this introduction we provide an informal discussion of commutation methods and restrict ourselves to the case of the whole line and bounded Jacobi operators (so we don't have to bother with domain considerations). Throughout this paper we denote by $\ell(I) = \ell((M,N))$, $I = \{n \in \mathbb{Z} | M < n < N\}$, $M, N \in \mathbb{Z} \cup \{\pm\infty\}$ the set of complex-valued sequences $\{u(n)\}_{n\in I}$ and by $\ell^p(I)$, $1 \le p \le \infty$ the sequences $u \in \ell(I)$ such that $|u|^p$ is summable. Furthermore, $\ell_0(I)$ denotes the set of sequences with only finitely-many values being nonzero. The scalar product in the Hilbert space $\ell^2(I)$ will be denoted by

$$\langle u, v\rangle = \sum_{n\in I} \overline{u(n)} v(n), \quad u, v \in \ell^2(I). \tag{1.1}$$

For brevity we focus in the following on the case $I = \mathbb{Z}$.

We first review the single commutation method [35]: Let $a, b \in \ell(\mathbb{Z})$ be two bounded, real-valued sequences satisfying

$$a(n) < 0, \qquad b(n) \in \mathbb{R}, \tag{1.2}$$

and introduce the corresponding Jacobi operator $H$ in $\ell^2(\mathbb{Z})$

$$(Hf)(n) = a(n)f(n+1) + a(n-1)f(n-1) - b(n)f(n), \quad u \in \ell^2(\mathbb{Z}). \tag{1.3}$$

Next (cf. Lemma 2.3), assume the existence of two weak positive solutions $u_\pm(\lambda_1, n)$ of

$$Hu_\pm = \lambda_1 u_\pm, \qquad u_\pm(\lambda_1, n) > 0, \quad u_\pm(\lambda_1, n) \in \ell^2(\pm\mathbb{N}) \tag{1.4}$$

(implying $b(n) + \lambda_1 < 0$, i.e., $H - \lambda_1 \ge 0$). $u_\pm$ are the principal solutions as used, e.g., in [33]. Any positive solution can then be written as

$$u_{\sigma_1}(\lambda_1, n) = \frac{1+\sigma_1}{2} u_+(\lambda_1, n) + \frac{1-\sigma_1}{2} u_-(\lambda_1, n), \quad \sigma_1 \in [-1, 1]. \tag{1.5}$$

Now define the operator $A_{\sigma_1}$ in $\ell^2(\mathbb{Z})$ by

$$(A_{\sigma_1} f)(n) = \rho_{o,\sigma_1}(n) f(n+1) + \rho_{e,\sigma_1}(n) f(n), \quad f \in \ell^2(\mathbb{Z}), \tag{1.6}$$

where

$$\rho_{o,\sigma_1}(n) = -\sqrt{-\frac{a(n)u_{\sigma_1}(\lambda_1, n)}{u_{\sigma_1}(\lambda_1, n+1)}}, \quad \rho_{e,\sigma_1}(n) = \sqrt{-\frac{a(n)u_{\sigma_1}(\lambda_1, n+1)}{u_{\sigma_1}(\lambda_1, n)}}. \tag{1.7}$$

We will always take the positive branch of all square roots involved. We note that $\rho_{o,\sigma_1}$ and $\rho_{e,\sigma_1}$ are bounded sequences as can be seen from

$$|\frac{a(n)u_{\sigma_1}(\lambda_1, n+1)}{u^1_{\sigma_1}(\lambda_1, n)}| + |\frac{a(n-1)u_{\sigma_1}(\lambda_1, n-1)}{u_{\sigma_1}(\lambda_1, n)}| = |b(n) + \lambda_1|. \tag{1.8}$$

The adjoint operator $A^*_{\sigma_1}$ of $A_{\sigma_1}$ is given by

$$(A^*_{\sigma_1} f)(n) = \rho_{o,\sigma_1}(n-1) f(n-1) + \rho_{e,\sigma_1}(n) f(n), \quad f \in \ell^2(\mathbb{Z}), \tag{1.9}$$

and for the (positive self-adjoint) operator $A^*_{\sigma_1} A_{\sigma_1}$ one infers

$$A^*_{\sigma_1} A_{\sigma_1} = H - \lambda_1. \tag{1.10}$$

This shows that $(H - \lambda_1) \ge 0$ is a necessary condition for the existence of a positive solution of (1.4). We remark that this condition is also sufficient (see, e.g., [33], Theorem 2.8). Commuting

$A^*_{\sigma_1}$ and $A_{\sigma_1}$ (observing $(A^*_{\sigma_1})^* = A_{\sigma_1}$) yields a second positive self-adjoint bounded operator $A_{\sigma_1} A^*_{\sigma_1}$ and further the commuted operator

$$H_{\sigma_1} = A_{\sigma_1} A^*_{\sigma_1} + \lambda_1. \tag{1.11}$$

A straightforward calculation shows

$$(H_{\sigma_1} f)(n) = a_{\sigma_1}(n) f(n+1) + a_{\sigma_1}(n-1) f(n-1) - b_{\sigma_1}(n) f(n), \tag{1.12}$$

with

$$a_{\sigma_1}(n) = -\frac{\sqrt{a(n)a(n+1)u_{\sigma_1}(\lambda_1,n)u_{\sigma_1}(\lambda_1,n+2)}}{u_{\sigma_1}(\lambda_1,n+1)}, \tag{1.13}$$

$$b_{\sigma_1}(n) = a(n)\Big(\frac{u_{\sigma_1}(\lambda_1,n)}{u_{\sigma_1}(\lambda_1,n+1)} + \frac{u_{\sigma_1}(\lambda_1,n+1)}{u_{\sigma_1}(\lambda_1,n)}\Big) - \lambda_1. \tag{1.14}$$

As proven by Deift [14], the operators $H - \lambda_1$ and $H_{\sigma_1} - \lambda_1$, restricted to the orthogonal complements of their respective null-spaces, are unitarily equivalent. Specifically, we have

$$\begin{aligned} \sigma(H_{\sigma_1}) &= \left\{ \begin{array}{cc} \sigma(H) \cup \{\lambda_1\}, & \sigma_1 \in (-1,1) \\ \sigma(H), & \sigma_1 \in \{-1,1\} \end{array} \right., & \sigma_{ac}(H_{\sigma_1}) &= \sigma_{ac}(H), \\ \sigma_p(H_{\sigma_1}) &= \left\{ \begin{array}{cc} \sigma_p(H) \cup \{\lambda_1\}, & \sigma_1 \in (-1,1) \\ \sigma_p(H), & \sigma_1 \in \{-1,1\} \end{array} \right., & \sigma_{sc}(H_{\sigma_1}) &= \sigma_{sc}(H). \end{aligned} \tag{1.15}$$

Here $\sigma_p(.), \sigma_{ac}(.)$, and $\sigma_{sc}(.)$ denote the the point spectrum (i.e., the set of eigenvalues), absolutely, and singularly continuous spectrum, respectively.

This method is known as the single commutation method [35] and we will give a complete spectral characterization of it in Sections 2 and 3.

Our next aim is to remove the condition that $H$ is bounded from below and thereby introduce the double commutation method. Fix $\gamma_\pm > 0$ and define

$$\rho_{o,\gamma_\pm}(n) = \rho_{e,\pm 1}(n+1)\sqrt{\frac{c_{\gamma_\pm}(\lambda_1,n)}{c_{\gamma_\pm}(\lambda_1,n+1)}}, \tag{1.16}$$

$$\rho_{e,\gamma_\pm}(n) = \rho_{o,\pm 1}(n)\sqrt{\frac{c_{\gamma_\pm}(\lambda_1,n+1)}{c_{\gamma_\pm}(\lambda_1,n)}}, \tag{1.17}$$

where

$$c_{\gamma_\pm}(\lambda_1,n) = 1 + \gamma_\pm \sum_{j=\pm\infty}^{\substack{n+1\\ n}} u_\pm(\lambda_1,j)^2, \tag{1.18}$$

and introduce corresponding operators $A_{\gamma_\pm}, A^*_{\gamma_\pm}$ in $\ell^2(\mathbb{Z})$ by

$$(A_{\gamma_\pm} f)(n) = \rho_{o,\gamma_\pm}(n) f(n+1) + \rho_{e,\gamma_\pm}(n) f(n), \tag{1.19}$$

$$(A^*_{\gamma_\pm} f)(n) = \rho_{o,\gamma_\pm}(n-1) f(n-1) + \rho_{e,\gamma_\pm}(n) f(n). \tag{1.20}$$

A simple calculation shows that $A^*_{\gamma_\pm} A_{\gamma_\pm} = A_{\pm 1} A^*_{\pm 1}$ and hence

$$H_{\pm 1} = A^*_{\gamma_\pm} A_{\gamma_\pm} + \lambda_1. \tag{1.21}$$

Performing a second commutation yields the doubly commuted operator

$$H_{\gamma_\pm} = A_{\gamma_\pm} A^*_{\gamma_\pm} + \lambda_1. \tag{1.22}$$

Explicitly, one verifies

$$(H_{\gamma_\pm} f)(n) = a_{\gamma_\pm}(n) f(n+1) + a_{\gamma_\pm}(n-1) f(n-1) - b_{\gamma_\pm}(n) f(n), \tag{1.23}$$

with

$$a_{\gamma_\pm}(n) = a(n+1)\frac{\sqrt{c_{\gamma_\pm}(\lambda_1,n)c_{\gamma_\pm}(\lambda_1,n+2)}}{c_{\gamma_\pm}(\lambda_1,n+1)}, \tag{1.24}$$

$$\begin{aligned} b_{\gamma_\pm}(n) &= b(n+1) \pm \gamma_\pm\Big(\frac{a(n)u_\pm(\lambda_1,n)u_\pm(\lambda_1,n+1)}{c_{\gamma_\pm}(\lambda_1,n)} \\ &\quad - \frac{a(n+1)u_\pm(\lambda_1,n+1)u_\pm(\lambda_1,n+2)}{c_{\gamma_\pm}(\lambda_1,n+1)}\Big). \end{aligned} \tag{1.25}$$

Now observe that $H_{\gamma_\pm}$ remains well-defined even if $u_\pm$ is no longer positive. This applies, in particular, in the case where $u_\pm(\lambda_1)$ has zeros and hence all intermediate operators $A_{\pm 1}, A_{\gamma_\pm}, H_{\pm 1}$, etc., become ill-defined. Thus to define $H_{\gamma_\pm}$ it suffices to assume the existence of a solution $u_\pm(\lambda_1)$ which is square summable near $\pm\infty$. This condition is much less restrictive than the existence of a positive solution (e.g., $\sigma(H) \neq \mathbb{R}$, i.e., the existence of a spectral gap for $H$ around $\lambda_1$ is sufficient in this context).

One expects that formulas analogous to (1.15) will carry over to this more general setup. That this is actually the case will be shown in our principal Theorem 4.4 of Section 4. Hence the double commutation method (contrary to the single commutation method) enables one to insert eigenvalues not only below the spectrum of $H$ but into arbitrary spectral gaps of $H$.

## 2. The single commutation method

In this section we intend to give a detailed investigation of the single commutation method. We will need the following condition on $a, b$ which will be used throughout Sections 2 and 3.

**Hypothesis (H.2.1).** Suppose

$$a(n) < 0, \quad b(n) \in \mathbb{R}, \qquad b(n) \geq c, \quad c \in \mathbb{R},\ n \in \mathbb{Z}. \tag{2.1}$$

We shall consider (self-adjoint) Jacobi operators $H$ associated with the difference expression

$$(\tau f)(n) = a(n)f(n+1) + a(n-1)f(n-1) - b(n)f(n), \tag{2.2}$$

in the Hilbert space $\ell^2(\mathbb{Z})$. We remark that the case $a(n) \neq 0$ can be reduced to the case $a(n) > 0$ or $a(n) < 0$ (cf., e.g., [19], p. 141). In fact one has

**Lemma 2.2.** *Assume (H.2.1) and let $H$ be a Jacobi operator associated with the difference expression (2.2). Introduce $a_\varepsilon$ by*

$$a_\varepsilon(n) = \varepsilon(n)a(n),\ \varepsilon(n) \in \{+1,-1\}, \quad n \in \mathbb{Z} \tag{2.3}$$

*and the unitary operator $U_\varepsilon$ by*

$$U_\varepsilon = \{\tilde\varepsilon(n)\delta_{m,n}\}_{m,n\in\mathbb{Z}}, \quad \tilde\varepsilon(n) \in \{+1,-1\},\ \tilde\varepsilon(n)\tilde\varepsilon(n+1) = \varepsilon(n). \tag{2.4}$$

*Then $H_\varepsilon$ defined as*

$$H_\varepsilon = U_\varepsilon^{-1} H U_\varepsilon, \tag{2.5}$$

*is associated with the difference expression*

$$(\tau_\varepsilon f)(n) = a_\varepsilon(n)f(n+1) + a_\varepsilon(n-1)f(n-1) - b_\varepsilon(n)f(n). \tag{2.6}$$

*In particular, $H_\varepsilon$ is unitarily equivalent to $H$.*

As a preparation we prove

**Lemma 2.3.** *Assume (H.2.1). Let $H$ be a given Jacobi operator in $\ell^2(\mathbb{Z})$ and let $\lambda < \inf(\sigma(H))$ ((H.2.1) implies that $H$ is semi-bounded, cf. [33]). Then there exist unique positive solutions $u_\pm(\lambda,n)$ of $\tau u = \lambda u$ (up to constant multiples) which are square summable near $\pm\infty$. (They are sometimes called principal solutions of $(H-z)u = 0$ near $\pm\infty$.)*

*Proof.* For the existence of square summable sequences $u_+(\lambda)$ near $\infty$ consider the sequence $((H-\lambda)^{-1}\delta_0)(n)$ for $n>0$ and extend it to a solution of $(\tau-\lambda)u=0$ for all $n\in\mathbb{Z}$. Let $H_{+,n}$ be the restriction of $H$ to $\ell^2((n,\infty))$ with a Dirichlet boundary condition at $n$. From $(H-\lambda)>0$ one infers $(H_{+,n}-\lambda)>0$ and hence

$$0<\langle\delta_{n+1},(H_{+,n}-\lambda)^{-1}\delta_{n+1}\rangle=\frac{u_+(\lambda,n+1)}{-a(n)u_+(\lambda,n)} \tag{2.7}$$

which shows that $u_+(\lambda)$ can be chosen to be positive. The existence of $u_-$ is proven similarly. □

We start with operators associated with the difference expression (2.2) on the half axis $\pm\mathbb{N}$. For simplicity we will do most calculations only for $\ell^2(\mathbb{N})$. Let $u(\lambda_1)$ be a positive solution of $\tau u=\lambda_1 u$ and define

$$\rho_{o,+}(n) = -\sqrt{-\frac{a(n)u(\lambda_1,n+1)}{u(\lambda_1,n)}}, \tag{2.8}$$

$$\rho_{e,+}(n) = \sqrt{-\frac{a(n-1)u(\lambda_1,n-1)}{u(\lambda_1,n)}}, \quad n>0. \tag{2.9}$$

Define the operator $\dot{A}_+$ on $\ell_0(\mathbb{N})$

$$(\dot{A}_+f)(n)=\rho_{o,+}(n)f(n+1)+\rho_{e,+}(n)f(n), \quad f\in\ell_0(\mathbb{N}) \tag{2.10}$$

and denote its operator closure (in $\ell^2(\mathbb{N})$) by $A_+$. One verifies,

$$\mathfrak{D}(A_+)\subseteq\{f\in\ell^2(\mathbb{N})|\rho_{o,+}(n)f(n+1)+\rho_{e,+}(n)f(n)\in\ell^2(\mathbb{N})\}. \tag{2.11}$$

The adjoint $A_+^*$ of $A_+$ is then given by

$$\begin{gathered}(A_+^*f)(n)=\rho_{o,+}(n-1)f(n-1)+\rho_{e,+}(n)f(n),\\ \mathfrak{D}(A_+^*)=\{f\in\ell^2(\mathbb{N})|f(0)=0;\rho_{o,+}(n-1)f(n-1)+\rho_{e,+}(n)f(n)\in\ell^2(\mathbb{N})\}.\end{gathered} \tag{2.12}$$

(The boundary condition $f(0)=0$ is only introduced so that we don't have to specify $(A_+^*f)(1)$ separately.) Due to a well known result of von Neumann (see, e.g., [54], Theorem 5.39) the operator $A_+A_+^*$ is a positive self-adjoint operator when defined naturally

$$\mathfrak{D}(A_+A_+^*)=\{f\in\mathfrak{D}(A_+^*)|A_+^*f\in\mathfrak{D}(A_+)\}. \tag{2.13}$$

A simple calculation shows $A_+A_+^*f=(\tau-\lambda_1)f$ and hence we may define

$$H_+=A_+A_+^*+\lambda_1, \quad \mathfrak{D}(H_+)\subseteq\{f\in\ell^2(\mathbb{N})|f(0)=0,\ \tau f\in\ell^2(\mathbb{N})\}, \tag{2.14}$$

where equality in the last relation is equivalent to $\tau$ being limit point (*l.p.*) at $+\infty$. Similarly one defines for $n<0$

$$\rho_{o,-}(n)=-\sqrt{-\frac{a(n)u(\lambda_1,n)}{u(\lambda_1,n+1)}}, \quad \rho_{e,-}(n)=\sqrt{-\frac{a(n)u(\lambda_1,n+1)}{u(\lambda_1,n)}} \tag{2.15}$$

and operators $A_-$, and $A_-^*$ in $\ell^2(-\mathbb{N})$ which satisfy $H_-=A_-^*A_-+\lambda_1$.

Commuting $A_\pm^*$ and $A_\pm$ yields a second positive self-adjoint operator $A_-A_-^*$, respectively $A_+^*A_+$, and further the commuted operators

$$H_{+,1}=A_+^*A_++\lambda_1, \qquad H_{-,1}=A_-A_-^*+\lambda_1. \tag{2.16}$$

The next theorem characterizes $H_{\pm,1}$ in terms of $H_\pm$, but first we need to introduce

**Hypothesis (H.2.4).** Suppose $H_\pm$ satisfies one of the following spectral conditions.

(i). $\sigma_{ess}(H_\pm)\neq\emptyset$.

(ii). $\sigma(H_\pm)=\sigma_{\rm d}(H_\pm)=\{\lambda_{\pm,j}\}_{j\in J_\pm}$ with $\sum_{j\in J_\pm}(1+\lambda_{\pm,j}^2)^{-1}=\infty$.

Hypothesis (H.2.4) is satisfied if $a, b$ are bounded near $\pm\infty$.

Either one of the conditions (i), (ii) implies that $\tau$ is *l.p.* at $\pm\infty$. This follows since otherwise the resolvent of $H_\pm$ would be a Hilbert-Schmidt operator contradicting (i), (ii). This further implies that the domain of $H_\pm$ is given by

$$\mathfrak{D}(H_\pm) = \{f \in \ell^2(\pm\mathbb{N}) | f(0) = 0,\ \tau f \in \ell^2(\pm\mathbb{N})\}. \tag{2.17}$$

**Theorem 2.5.** *Assume (H.2.1) and (H.2.4). Then the operators $H_{\pm,1}$ constructed above satisfy (H.2.1) and (H.2.4) and are given by*

$$\begin{aligned} (H_{\pm,1} f)(n) &= (\tau_{\pm,1} f)(n) \\ &= a_{\pm,1}(n) f(n+1) + a_{\pm,1}(n-1) f(n-1) - b_{\pm,1}(n) f(n), \\ \mathfrak{D}(H_{\pm,1}) &= \{f \in \ell^2(\pm\mathbb{N}) | f(0) = 0,\ \tau_{\pm,1} f \in \ell^2(\pm\mathbb{N})\}, \end{aligned} \tag{2.18}$$

*with*

$$a_{+,1}(n) = -\frac{\sqrt{a(n-1)a(n)u(\lambda_1,n-1)u(\lambda_1,n+1)}}{u(\lambda_1,n)}, \quad n > 0, \tag{2.19}$$

$$b_{+,1}(n) = a(n-1)\Big(\frac{u(\lambda_1,n)}{u(\lambda_1,n-1)} + \frac{u(\lambda_1,n-1)}{u(\lambda_1,n)}\Big) - \lambda_1, \quad n > 1,$$

$$b_{+,1}(1) = a(0)\frac{u(\lambda_1,0)}{u(\lambda_1,1)} - \lambda_1, \tag{2.20}$$

*and*

$$a_{-,1}(n) = -\frac{\sqrt{a(n)a(n+1)u(\lambda_1,n)u(\lambda_1,n+2)}}{u(\lambda_1,n+1)}, \quad n < -1, \tag{2.21}$$

$$b_{-,1}(n) = a(n)\Big(\frac{u(\lambda_1,n)}{u(\lambda_1,n+1)} + \frac{u(\lambda_1,n+1)}{u(\lambda_1,n)}\Big) - \lambda_1, \quad n < -1,$$

$$b_{-,1}(-1) = a(-1)\frac{u(\lambda_1,0)}{u(\lambda_1,-1)} - \lambda_1. \tag{2.22}$$

*Moreover, $H_\pm - \lambda_1$ and $H_{\pm,1} - \lambda_1$ restricted to the orthogonal complements of their null-spaces are unitarily equivalent and hence*

$$\begin{aligned} \sigma(H_{\pm,1})\backslash\{\lambda_1\} &= \sigma(H_\pm)\backslash\{\lambda_1\}, \quad & \sigma_{ac}(H_{\pm,1}) &= \sigma_{ac}(H_\pm), \\ \sigma_p(H_{\pm,1})\backslash\{\lambda_1\} &= \sigma_p(H_\pm)\backslash\{\lambda_1\}, \quad & \sigma_{sc}(H_{\pm,1}) &= \sigma_{sc}(H_\pm). \end{aligned} \tag{2.23}$$

*Proof.* The unitary equivalence follows from [14], Theorem 1 and clearly settles the spectral claims. Thus both $H_\pm$ and $H_{\pm,1}$ satisfy (H.2.4) and hence $\tau_\pm$ and $\tau_{\pm,1}$ are *l.p.* at $\pm\infty$. The rest are straightforward calculations. □

Next we turn to the case of the whole lattice $\ell^2(\mathbb{Z})$. We pick $\sigma_1 \in [-1,1]$ and $\lambda_1 < \inf(\sigma(H))$. Further denote by $u_\pm(\lambda,n)$ (for $\lambda < \inf(\sigma(H))$) the solutions constructed in Lemma 2.3 and set

$$u_{\sigma_1}(\lambda_1,n) = \frac{1+\sigma_1}{2} u_+(\lambda_1,n) + \frac{1-\sigma_1}{2} u_-(\lambda_1,n). \tag{2.24}$$

Now define sequences

$$\rho_{o,\sigma_1}(n) = -\sqrt{-\frac{a(n)u_{\sigma_1}(\lambda_1,n)}{u_{\sigma_1}(\lambda_1,n+1)}}, \quad \rho_{e,\sigma_1}(n) = \sqrt{-\frac{a(n)u_{\sigma_1}(\lambda_1,n+1)}{u_{\sigma_1}(\lambda_1,n)}}, \tag{2.25}$$

and the corresponding operator $A_{\sigma_1}$ (first on $\ell_0(\mathbb{Z})$ and then take the closure in $\ell^2(\mathbb{Z})$ as before) together with its adjoint $A^*_{\sigma_1}$,

$$\begin{aligned} (A_{\sigma_1} f)(n) &= \rho_{o,\sigma_1}(n) f(n+1) + \rho_{e,\sigma_1}(n) f(n), \\ \mathfrak{D}(A_{\sigma_1}) &\subseteq \{f \in \ell^2(\mathbb{Z}) | \rho_{o,\sigma_1}(n) f(n+1) + \rho_{e,\sigma_1}(n) f(n) \in \ell^2(\mathbb{Z})\}, \end{aligned} \tag{2.26}$$

$$\begin{aligned} (A^*_{\sigma_1} f)(n) &= \rho_{o,\sigma_1}(n-1) f(n-1) + \rho_{e,\sigma_1}(n) f(n), \\ \mathfrak{D}(A^*_{\sigma_1}) &= \{f \in \ell^2(\mathbb{Z}) | \rho_{o,\sigma_1}(n-1) f(n-1) + \rho_{e,\sigma_1}(n) f(n) \in \ell^2(\mathbb{Z})\}. \end{aligned} \tag{2.27}$$

Again by von Neumann's result $A_{\sigma_1}^* A_{\sigma_1}$ is a positive self-adjoint operator when defined naturally by

$$\mathfrak{D}(A_{\sigma_1}^* A_{\sigma_1}) = \{f \in \mathfrak{D}(A_{\sigma_1}) | A_{\sigma_1} f \in \mathfrak{D}(A_{\sigma_1}^*)\}. \tag{2.28}$$

A simple calculation shows $A_{\sigma_1}^* A_{\sigma_1} = \tau - \lambda_1$ and we hence may define

$$H = A_{\sigma_1}^* A_{\sigma_1} + \lambda_1, \qquad \mathfrak{D}(H) \subseteq \{f \in \ell^2(\mathbb{Z}) | \tau f \in \ell^2(\mathbb{Z})\}. \tag{2.29}$$

Commuting $A_{\sigma_1}^*$ and $A_{\sigma_1}$ yields a second positive self-adjoint operator $A_{\sigma_1} A_{\sigma_1}^*$ and further the commuted operator

$$H_{\sigma_1} = A_{\sigma_1} A_{\sigma_1}^* + \lambda_1, \qquad \mathfrak{D}(H_{\sigma_1}) \subseteq \{f \in \ell^2(\mathbb{Z}) | \tau_{\sigma_1} f \in \ell^2(\mathbb{Z})\}, \tag{2.30}$$

where $\tau_{\sigma_1}$ is the difference expression corresponding to $H_{\sigma_1}$. The next theorem characterizes $H_{\sigma_1}$ under Assumption (H.2.2) for $H_+$ and $H_-$ implying that $\tau$ is *l.p.* at $\pm\infty$ and hence that

$$\mathfrak{D}(H) = \{f \in \ell^2(\mathbb{Z}) | \tau f \in \ell^2(\mathbb{Z})\}. \tag{2.31}$$

**Theorem 2.6.** *Assume (H.2.1) and (H.2.4). Then the operator $H_{\sigma_1}$,*

$$\begin{aligned} (H_{\sigma_1} f)(n) &= (\tau_{\sigma_1} f)(n) \\ &= a_{\sigma_1}(n) f(n+1) + a_{\sigma_1}(n-1) f(n-1) - b_{\sigma_1}(n) f(n), \\ \mathfrak{D}(H_{\sigma_1}) &= \{f \in \ell^2(\mathbb{Z}) | \tau_{\sigma_1} f \in \ell^2(\mathbb{Z})\}, \end{aligned} \tag{2.32}$$

*is self-adjoint. Moreover,*

$$a_{\sigma_1}(n) = -\frac{\sqrt{a(n)a(n+1) u_{\sigma_1}(\lambda_1, n) u_{\sigma_1}(\lambda_1, n+2)}}{u_{\sigma_1}(\lambda_1, n+1)}, \tag{2.33}$$

$$b_{\sigma_1}(n) = a(n)\Big(\frac{u_{\sigma_1}(\lambda_1, n)}{u_{\sigma_1}(\lambda_1, n+1)} + \frac{u_{\sigma_1}(\lambda_1, n+1)}{u_{\sigma_1}(\lambda_1, n)}\Big) - \lambda_1 \tag{2.34}$$

*and $a_{\sigma_1}$, $b_{\sigma_1}$ satisfy (H.2.1). The equation $\tau_{\sigma_1} v = \lambda_1 v$ has the positive solution*

$$v_{\sigma_1}(\lambda_1, n) = \frac{1}{\sqrt{-a(n) u_{\sigma_1}(\lambda_1, n) u_{\sigma_1}(\lambda_1, n+1)}} \tag{2.35}$$

*which is an eigenfunction of $H_{\sigma_1}$ if and only if $\sigma_1 \in (-1, 1)$. $H - \lambda_1$ and $H_{\sigma_1} - \lambda_1$ restricted to the orthogonal complements of their corresponding one-dimensional null-spaces are unitarily equivalent and hence*

$$\begin{aligned} \sigma(H_{\sigma_1}) &= \begin{cases} \sigma(H) \cup \{\lambda_1\}, & \sigma_1 \in (-1,1) \\ \sigma(H), & \sigma_1 \in \{-1,1\} \end{cases}, & \sigma_{ac}(H_{\sigma_1}) &= \sigma_{ac}(H), \\ \sigma_p(H_{\sigma_1}) &= \begin{cases} \sigma_p(H) \cup \{\lambda_1\}, & \sigma_1 \in (-1,1) \\ \sigma_p(H), & \sigma_1 \in \{-1,1\} \end{cases}, & \sigma_{sc}(H_{\sigma_1}) &= \sigma_{sc}(H). \end{aligned} \tag{2.36}$$

*In addition, the sequence*

$$(A_{\sigma_1} u)(z, n) = \frac{W_n(u_{\sigma_1}(\lambda_1), u(z))}{\sqrt{-a(n) u_{\sigma_1}(\lambda_1, n) u_{\sigma_1}(\lambda_1, n+1)}} \tag{2.37}$$

*solves $\tau_{\sigma_1} u = zu$ if $u(z)$ solves $\tau u = zu$ for some $z \in \mathbb{C}$, where $W_n(u, v) = a(n)(u(n)v(n+1) - u(n+1)v(n))$ denotes the modified Wronskian. Moreover, one obtains*

$$W_{\sigma_1, n}(A_{\sigma_1} u(z), A_{\sigma_1} v(z)) = (\lambda_1 - z) W_n(u(z), v(z)) \tag{2.38}$$

*for solutions $u, v$ of $\tau u = zu$, where $W_{\sigma_1, n}(u, v) = a_{\sigma_1}(n)(u(n)v(n+1) - u(n+1)v(n))$. The resolvents of $H, H_{\sigma_1}$ for $z \in \mathbb{C} \backslash (\sigma(H) \cup \{\lambda_1\})$ are related via*

$$(H_{\sigma_1} - z)^{-1} = \frac{1}{z - \lambda_1}\Big(A_{\sigma_1} (H - z)^{-1} A_{\sigma_1}^* - 1\Big) \tag{2.39}$$

*or, in terms of Green's functions for* $n \geq m$, $z \in \mathbb{C}\backslash(\sigma(H) \cup \{\lambda_1\})$,

$$G(z,n,m) = \frac{u_+(z,n)u_-(z,m)}{W_n(u_+(z),u_-(z))}$$

$$\text{implies} \quad G_{\sigma_1}(z,n,m) = \frac{(A_{\sigma_1}u_+)(z,n)(-A_{\sigma_1}u_-)(z,m)}{(z-\lambda_1)W(u_+(z),u_-(z))}. \tag{2.40}$$

*Furthermore,* $u_{\sigma_1,\pm}(z,n)$*, the principal solutions of* $(H_{\sigma_1} - z)u = 0$ *for* $z < \lambda_1$*, are given by*

$$u_{\sigma_1,\pm}(z,n) = \pm A_{\sigma_1}u_\pm(z,n) = \frac{\mp W_n(u_{\sigma_1}(\lambda_1),u_\pm(z))}{\sqrt{-a(n)u_{\sigma_1}(\lambda_1,n)u_{\sigma_1}(\lambda_1,n+1)}}. \tag{2.41}$$

*In addition, we have*

$$\sum_{n\in\mathbb{Z}} v_{\sigma_1}(\lambda_1,n)^2 = \frac{4}{1-\sigma_1^2}W(u_-(\lambda_1),u_+(\lambda_1))^{-1}, \quad \sigma_1 \in (-1,1) \tag{2.42}$$

*and, if* $\tau u(\lambda) = \lambda u(\lambda)$, $u(\lambda,.) \in \ell^2(\mathbb{Z})$,

$$\sum_{n\in\mathbb{Z}} (A_{\sigma_1}u)(\lambda,n)^2 = (\lambda - \lambda_1)\sum_{n\in\mathbb{Z}} u(\lambda,n)^2. \tag{2.43}$$

*Proof.* The unitary equivalence together with equation (2.39) follow from [14], Theorem 1. That $H_{\sigma_1}$ is *l.p.* at $\pm\infty$ follows upon looking at the restrictions $H_\pm$, $H_{\pm,1}$ and using Theorem 2.5. Equation (2.39) together with (2.38) imply (2.40). The facts concerning the point spectrum follow since $G_{\sigma_1}(z,n,n)$ has a pole at $z = \lambda_1$ if and only if $\sigma_1 \in (-1,1)$. (2.42) can be obtained by investigating the residue of $G_{\sigma_1}(z,n,n)$ at $z = \lambda_1$. The rest are straightforward calculations. □

*Remark* 2.7. (i). Hypothesis (H.2.4) is only needed in Theorem 2.6 to characterize the domains of $H$ and $H_{\sigma_1}$ explicitly.
(ii). Multiplying $u_{\sigma_1}$ with a positive constant leaves all formulas and, in particular, $H_{\sigma_1}$ invariant.
(iii). If $H$ is bounded from above we can insert eigenvalues into the highest spectral gap, i.e., above the spectrum of $H$, upon considering $-H$. Then $\lambda > \sup(\sigma(H))$ implies that we don't have positive but rather alternating solutions and all our previous calculations carry over with minor changes.
(iv). We can weaken (H.2.1) by requiring $a(n) \neq 0$ instead of $a(n) < 0$. Everything stays the same with the only difference that $u_\pm$ are not positive but change sign in such a way that (2.7) stays positive. Moreover, the signs of $a_{\sigma_1}(n)$ can also be prescribed arbitrarily by altering the signs of $\rho_{o,\sigma_1}$ and $\rho_{e,\sigma_1}$.
(v). The fact that $v_{\sigma_1} \in \ell^2(\mathbb{Z})$ if and only if $\sigma_1 \in (-1,1)$ gives an alternate proof of

$$\sum_{n=0}^{\pm\infty} \frac{1}{-a(n)u_{\sigma_1}(\lambda_1,n)u_{\sigma_1}(\lambda_1,n+1)} < \infty \text{ if and only if } \sigma_1 \in \begin{matrix} [-1,1) \\ (-1,1] \end{matrix} \tag{2.44}$$

(cf. [44] and [33], Lemma 2.10, Remark 2.11).

At the end of this section we will show some connections between the single commutation method and some other theories. We start with the Weyl-Titchmarsh theory and freely use the definitions of Appendices B and C.

**Lemma 2.8.** *Assume (H.2.1). The Weyl* $\tilde{m}$*-functions* $\tilde{m}_{\pm,\sigma_1}(z)$ *of* $H_{\sigma_1}$, $\sigma_1 \in [-1,1]$ *in terms of* $\tilde{m}_\pm(z)$*, the ones of* $H$*, read*

$$\tilde{m}_{\pm,\sigma_1}(z) = \frac{-u_{\sigma_1}(\lambda_1,1)}{a(1)u_{\sigma_1}(\lambda_1,2)}\Big(1 + \frac{(z-\lambda_1)\tilde{m}_\pm(z)}{1 + \frac{a(0)u_{\sigma_1}(\lambda_1,0)}{u_{\sigma_1}(\lambda_1,1)}\tilde{m}_\pm(z)}\Big). \tag{2.45}$$

*Proof.* The above formulas are straightforward calculations using (2.40) and (C.20), (C.21). □

Finally we turn to scattering theory. In order to facilitate comparison with the standard literature on (inverse) scattering theory for second-order difference operators (cf. [9], [10], [21], [29], [51]) we now assume

$$a(n) > 0,\ b(n) \in \mathbb{R}, \qquad n|1-2a(n)|, nb(n) \in \ell^1(\mathbb{Z}) \tag{2.46}$$

(cf. Remark 2.7). This implies

$$\sigma_{ac}(H) = [-1,1], \quad \sigma_{sc}(H) = \emptyset, \quad \sigma_p(H) = \{\lambda_j\}_{j\in J} \subseteq \mathbb{R}\backslash[-1,1], \tag{2.47}$$

where $J \subseteq \mathbb{N}$ is a suitable (finite) index set, and the existence of the so called Jost solutions $f_\pm(k,n)$,

$$\Big(\tau - \frac{k+k^{-1}}{2}\Big) f_\pm(k,n) = 0, \quad \lim_{n\to\pm\infty} k^{\mp n} f_\pm(k,n) = 1, \quad |k| \le 1. \tag{2.48}$$

Transmission $T(k)$ and reflection $R_\pm(k)$ coefficients are then defined via

$$T(k) f_\mp(k,n) = f_\pm(k^{-1},n) + R_\pm(k) f_\pm(k,n), \quad |k| = 1, \tag{2.49}$$

and the norming constants $\gamma_{\pm,j}$ corresponding to $\lambda_j \in \sigma_p(H)$ are given by

$$\gamma_{\pm,j}^{-1} = \sum_{n\in\mathbb{Z}} |f_\pm(k_j,n)|^2, \quad k_j = \lambda_j + \sqrt{\lambda_j^2 - 1} \in (-1,0),\ j \in J. \tag{2.50}$$

**Lemma 2.9.** *Suppose $H$ satisfies (2.46) and let $H_{\sigma_1}$ be constructed as in Theorem 2.6 with*

$$u_{\sigma_1}(\lambda_1,n) = \frac{1+\sigma_1}{2} f_+(k_1,n) + \frac{1-\sigma_1}{2} f_-(k_1,n). \tag{2.51}$$

*Then the transmission $T_{\sigma_1}(k)$ and reflection coefficients $R_{\pm,\sigma_1}(k)$ of $H_{\sigma_1}$ in terms of the corresponding scattering data $T(k), R_\pm(k)$ of $H$ are given by*

$$T_{\sigma_1}(k) = \frac{1-k\,k_1}{k-k_1} T(k), \quad R_{\pm,\sigma_1}(k) = k^{\pm1}\frac{k-k_1}{1-k\,k_1} R_\pm(k),\ \sigma_1 \in (-1,1), \tag{2.52}$$

$$T_{\sigma_1}(k) = T(k), \quad R_{\pm,\sigma_1}(k) = \frac{k_1^{\sigma_1} - k^{\mp1}}{k_1^{\sigma_1} - k^{\pm1}} R_\pm(k), \quad \sigma_1 \in \{-1,1\}, \tag{2.53}$$

*where $k_1 = \lambda_1 + \sqrt{\lambda_1^2-1} \in (-1,0)$. Moreover, the norming constants $\gamma_{\sigma_1,\pm,j}$ associated with $\lambda_j \in \sigma_p(H_{\sigma_1})$ in terms of $\gamma_{\pm,j}$ corresponding to $H$ read*

$$\begin{aligned} \gamma_{\sigma_1,\pm,j} &= |k_j|^{\pm1}\frac{1-k_jk_1}{(k_j-k_1)}\gamma_{\pm,j}, \quad j \in J,\ \sigma_1 \in (-1,1), \\ \gamma_{\sigma_1,\pm,1} &= \left(\frac{1-\sigma_1}{1+\sigma_1}\right)^{\pm1} |1-k_1^{\mp2}|\,T(k_1), \quad \sigma_1 \in (-1,1), \end{aligned} \tag{2.54}$$

$$\gamma_{\sigma_1,\pm,j} = |k_1^{\sigma_1} - k_j^{\mp1}|\gamma_{\pm,j}, \quad j \in J,\ \sigma_1 \in \{-1,1\}. \tag{2.55}$$

*Proof.* The claims follow easily after observing that up to normalization the Jost solutions of $H_{\sigma_1}$ are given by $A_{\sigma_1} f_\pm(k,n)$ (compare (2.40)). □

## 3. Iteration of the single commutation method

By choosing $\lambda_2 < \lambda_1$ and $\sigma_2 \in [-1,1]$ we can define

$$u_{\sigma_1,\sigma_2}(\lambda_2,n) = \frac{1+\sigma_2}{2} u_{\sigma_1,+}(\lambda_2,n) + \frac{1-\sigma_2}{2} u_{\sigma_1,-}(\lambda_2,n) \tag{3.1}$$

and repeat the process of the previous section by defining $\rho_{o,\sigma_1,\sigma_2}$, $\rho_{e,\sigma_1,\sigma_2}$ and corresponding operators $A_{\sigma_1,\sigma_2}$, $A^*_{\sigma_1,\sigma_2}$ which satisfy

$$H_{\sigma_1} = A^*_{\sigma_1,\sigma_2} A_{\sigma_1,\sigma_2} - \lambda_2. \tag{3.2}$$

A further commutation then yields the operator

$$H_{\sigma_1,\sigma_2} = A_{\sigma_1,\sigma_2} A^*_{\sigma_1,\sigma_2} - \lambda_2 \tag{3.3}$$

associated with sequences $a_{\sigma_1,\sigma_2}$, $b_{\sigma_1,\sigma_2}$. The result after $N$ steps is summarized in

**Theorem 3.1.** *Assume (H.2.1) and (H.2.4). Let $H$ be as in Section 2 and choose*

$$\lambda_N < \cdots < \lambda_2 < \lambda_1 < \inf(\sigma(H)), \quad \sigma_\ell \in [-1,1], \ 1 \le \ell \le N, \ N \in \mathbb{N}. \tag{3.4}$$

*Then we have*

$$a_{\sigma_1,\dots,\sigma_N}(n) = -\sqrt{a(n)a(n+N)}\frac{\sqrt{C_n(u^1_{\sigma_1},\dots,u^N_{\sigma_N})C_{n+2}(u^1_{\sigma_1},\dots,u^N_{\sigma_N})}}{C_{n+1}(u^1_{\sigma_1},\dots,u^N_{\sigma_N})}, \tag{3.5}$$

$$\begin{aligned} b_{\sigma_1,\dots,\sigma_N}(n) &= -\lambda_N + a(n)\frac{C_{n+2}(u^1_{\sigma_1},\dots,u^{N-1}_{\sigma_{N-1}})C_n(u^1_{\sigma_1},\dots,u^N_{\sigma_N})}{C_{n+1}(u^1_{\sigma_1},\dots,u^{N-1}_{\sigma_{N-1}})C_{n+1}(u^1_{\sigma_1},\dots,u^N_{\sigma_N})} \\ &\quad + a(n+N-1)\frac{C_n(u^1_{\sigma_1},\dots,u^{N-1}_{\sigma_{N-1}})C_{n+1}(u^1_{\sigma_1},\dots,u^N_{\sigma_N})}{C_{n+1}(u^1_{\sigma_1},\dots,u^{N-1}_{\sigma_{N-1}})C_n(u^1_{\sigma_1},\dots,u^N_{\sigma_N})}, \end{aligned} \tag{3.6}$$

*where*

$$u^\ell_{\sigma_\ell}(n) = \frac{1+\sigma_\ell}{2}u_+(\lambda_\ell,n) + (-1)^{\ell+1}\frac{1-\sigma_\ell}{2}u_-(\lambda_\ell,n), \tag{3.7}$$

*and $C_n$ denotes the $n$-dimensional Casoratian*

$$C_n(u_1,\dots,u_N) = \det\{u_i(n+j-1)\}_{1\le i,j\le N}. \tag{3.8}$$

*Moreover, for $1 \le \ell \le N$, $\lambda < \lambda_\ell$*

$$u_{\sigma_1,\dots,\sigma_\ell,\pm}(\lambda,n) = \frac{\pm\sqrt{\prod_{j=0}^{\ell-1}(-a(n+j))}C_n(u^1_{\sigma_1},\dots,u^\ell_{\sigma_\ell},u_\pm(\lambda))}{\sqrt{C_n(u^1_{\sigma_1},\dots,u^\ell_{\sigma_\ell})C_{n+1}(u^1_{\sigma_1},\dots,u^\ell_{\sigma_\ell})}}, \tag{3.9}$$

*are the principal solutions of $\tau_{\sigma_1,\dots,\sigma_\ell}u = \lambda u$ and*

$$u_{\sigma_1,\dots,\sigma_\ell}(\lambda_\ell,n) = \frac{1+\sigma_\ell}{2}u_{\sigma_1,\dots,\sigma_{\ell-1},+}(\lambda_\ell,n) + \frac{1-\sigma_\ell}{2}u_{\sigma_1,\dots,\sigma_{\ell-1},-}(\lambda_\ell,n) \tag{3.10}$$

*is used to define $H_{\sigma_1,\dots,\sigma_\ell}$. We also have*

$$\rho_{o,\sigma_1,\dots,\sigma_N}(n) = -\sqrt{-a(n)\frac{C_{n+2}(u^1_{\sigma_1},\dots,u^{N-1}_{\sigma_{N-1}})C_n(u^1_{\sigma_1},\dots,u^N_{\sigma_N})}{C_{n+1}(u^1_{\sigma_1},\dots,u^{N-1}_{\sigma_{N-1}})C_{n+1}(u^1_{\sigma_1},\dots,u^N_{\sigma_N})}}, \tag{3.11}$$

$$\rho_{e,\sigma_1,\dots,\sigma_N}(n) = \sqrt{-a(n+N-1)\frac{C_n(u^1_{\sigma_1},\dots,u^{N-1}_{\sigma_{N-1}})C_{n+1}(u^1_{\sigma_1},\dots,u^N_{\sigma_N})}{C_{n+1}(u^1_{\sigma_1},\dots,u^{N-1}_{\sigma_{N-1}})C_n(u^1_{\sigma_1},\dots,u^N_{\sigma_N})}}. \tag{3.12}$$

*The spectrum of $H_{\sigma_1,\dots,\sigma_N}$ is given by*

$$\sigma(H_{\sigma_1,\dots,\sigma_N}) = \sigma(H) \cup \{\lambda_\ell \mid \sigma_\ell \in (-1,1), \ 1 \le \ell \le N\}. \tag{3.13}$$

*Proof.* It is enough to prove the formulas for $a_{\sigma_1,\dots,\sigma_N}(n)$ and $u_{\sigma_1,\dots,\sigma_N}(n)$, the remaining assertions then follow easily. We will use a proof by induction on $N$. They are valid for $N = 1$ and we need to show

$$u_{\sigma_1,\dots,\sigma_{N+1},\pm}(\lambda,n) = \frac{\sqrt{-a_{\sigma_1,\dots,\sigma_N}(n)}C_n(u_{\sigma_1,\dots,\sigma_N}(\lambda_N),u_{\sigma_1,\dots,\sigma_N,\pm 1}(\lambda))}{\pm\sqrt{u_{\sigma_1,\dots,\sigma_N}(\lambda_N,n)u_{\sigma_1,\dots,\sigma_N}(\lambda_N,n+1)}}, \tag{3.14}$$

$$\begin{aligned} a_{\sigma_1,\dots,\sigma_{N+1}}(n) &= \sqrt{a_{\sigma_1,\dots,\sigma_N}(n)a_{\sigma_1,\dots,\sigma_N}(n+1)} \times \\ &\quad \frac{\sqrt{u_{\sigma_1,\dots,\sigma_N}(\lambda_N,n)u_{\sigma_1,\dots,\sigma_N}(\lambda_N,n+1)}}{u_{\sigma_1,\dots,\sigma_N}(\lambda_N,n+1)}. \end{aligned} \tag{3.15}$$

The first relation follows after a straightforward calculation using Sylvester's determinant identity (cf. [25], Sect. II.3)

$$\begin{aligned} & C_n(u^1_{\sigma_1},\dots,u^N_{\sigma_N},u_\pm(\lambda))C_{n+1}(u^1_{\sigma_1},\dots,u^{N+1}_{\sigma_{N+1}}) \\ & - C_{n+1}(u^1_{\sigma_1},\dots,u^N_{\sigma_N},u_\pm(\lambda))C_n(u^1_{\sigma_1},\dots,u^{N+1}_{\sigma_{N+1}}) \\ & = C_{n+1}(u^1_{\sigma_1},\dots,u^N_{\sigma_N})C_n(u^1_{\sigma_1},\dots,u^{N+1}_{\sigma_{N+1}},u_\pm(\lambda)), \end{aligned} \tag{3.16}$$

and the second is a simple calculation. □

*Remark* 3.2. If $u(z,n)$ is any solution of $\tau u = zu$, $z\in\mathbb{C}$ define $u_{\sigma_1,\dots,\sigma_N}(z,n)$ as in (3.9) but with $\ell = N$ and $u_\pm(\lambda,n)$ replaced by $u(z,n)$. Then $u_{\sigma_1,\dots,\sigma_N}(z,n)$ solves $\tau_{\sigma_1,\dots,\sigma_N}u = zu$.

Finally we extend Lemma 2.9 and assume for brevity $\sigma_\ell\in(-1,1)$.

**Lemma 3.3.** *Suppose $H$ satisfies* (2.46) *and let $H_{\sigma_1,\dots,\sigma_N}$, $\sigma_\ell\in(-1,1,)$, $1\le\ell\le N$ be constructed as in Theorem 3.1 with*

$$u^\ell_{\sigma_\ell}(n) = \frac{1+\sigma_\ell}{2}f_+(k_\ell,n) + (-1)^{\ell+1}\frac{1-\sigma_\ell}{2}f_-(k_\ell,n). \tag{3.17}$$

*Then the transmission $T_{\sigma_1,\dots,\sigma_N}(k)$ and reflection coefficients $R_{\pm,\sigma_1,\dots,\sigma_N}(k)$ of the operator $H_{\sigma_1,\dots,\sigma_N}$ in terms of the corresponding scattering data $T(k), R_\pm(k)$ of $H$ are given by*

$$T_{\sigma_1,\dots,\sigma_N}(k) = \left(\prod_{\ell=1}^N \frac{1-k\,k_\ell}{k-k_\ell}\right)T(k), \tag{3.18}$$

$$R_{\pm,\sigma_1,\dots,\sigma_N}(k) = k^{\pm N}\left(\prod_{\ell=1}^N \frac{k-k_\ell}{1-k\,k_\ell}\right)R_\pm(k), \tag{3.19}$$

*where $k_\ell = \lambda_\ell + \sqrt{\lambda_\ell^2-1}\in(-1,0)$, $1\le\ell\le N$. Moreover, the norming constants $\gamma_{\sigma_1,\dots,\sigma_N,\pm,j}$ associated with $\lambda_j\in\sigma_p(H_{\sigma_1,\dots,\sigma_N})$ in terms of $\gamma_{\pm,j}$ corresponding to $H$ read*

$$\begin{aligned} \gamma_{\sigma_1,\dots,\sigma_N,\pm,j} &= \left(\tfrac{1-\sigma_j}{1+\sigma_j}\right)^{\pm1}|k_j|^{-2\mp(N-1)}\frac{\prod_{\ell=1}^N|1-k_jk_\ell|}{\prod_{\substack{\ell=1\\ \ell\ne j}}^N|k_j-k_l|}T(k_j), \quad 1\le j\le N, \\ \gamma_{\sigma_1,\dots,\sigma_N,\pm,j} &= |k_j|^{\pm N}\prod_{\ell=1}^N\frac{1-k_jk_\ell}{|k_j-k_\ell|}\gamma_{\pm,j}, \quad j\in J. \end{aligned} \tag{3.20}$$

*Proof.* Observe that

$$\begin{aligned} u_{\sigma_1,\sigma_2}(\lambda_2,n) &= \frac{1+\sigma_2}{2}A_{\sigma_1}f_+(k_2,n) + \frac{1-\sigma_2}{2}A_{\sigma_1}f_-(k_2,n) \\ &= c\Big(\frac{1+\hat\sigma_2}{2}f_{\sigma_1,+}(k_2,n) + \frac{1-\hat\sigma_2}{2}f_{\sigma_1,-}(k_2,n)\Big), \end{aligned} \tag{3.21}$$

where $c>0$ and $\sigma_2,\hat\sigma_2$ are related via

$$\frac{1+\hat\sigma_2}{1-\hat\sigma_2} = \frac{1}{k_2}\frac{1+\sigma_1}{1-\sigma_1}. \tag{3.22}$$

The claims now follow from Lemma 2.9 after extending this result by induction. □

## 4. The double commutation method

In this section we provide a complete characterization of the double commutation method for Jacobi operators. We start with a linear transformation which turns out to be unitary when restricted to proper subspaces of our Hilbert space. We use this transformation to construct an operator $H_{\gamma_1}$ from a given background operator $H$. This operator $H_{\gamma_1}$ will be the doubly commuted operator of $H$ as discussed in the Introduction. The results of Sections 4-6 appear to be without precedent.

Let $\mathfrak{H} = \ell^2((M_- - 1, M_+ + 1))$ be the underlying Hilbert space ($-\infty \le M_- < M_+ \le \infty$) and let $\psi(n)$ be a given real-valued sequence which is square summable near $M_-$. Choose a positive constant $\gamma > 0$ and define

$$c_\gamma(n) = 1 + \gamma \sum_{j=M_-}^{n} \psi(j)^2, \qquad n \ge M_-. \tag{4.1}$$

(We set in addition $c_\gamma(M_- - 1) = 1$ if $M_-$ is finite.) Denote the set of sequences in $\ell((M_- - 1, M_+ + 1))$ which are square summable near $M_-$ by $\mathfrak{H}_-$ and consider the following (linear) transformation

$$\begin{array}{rccl} U_\gamma: & \mathfrak{H}_- & \to & \mathfrak{H}_- \\ & f(n) & \mapsto & f_\gamma(n) = \sqrt{\frac{c_\gamma(n)}{c_\gamma(n-1)}} f(n) - \gamma\psi_\gamma(n) \sum\limits_{j=M_-}^{n} \psi(j) f(j). \end{array} \tag{4.2}$$

By inspection, the sequence $f_\gamma$ is also square summable near $M_-$ and the inverse transformation is given by

$$\begin{array}{rccl} U_\gamma^{-1}: & \mathfrak{H}_- & \to & \mathfrak{H}_- \\ & g(n) & \mapsto & \sqrt{\frac{d_\gamma(n)}{d_\gamma(n-1)}} g(n) + \gamma\psi(n) \sum\limits_{j=M_-}^{n} \psi_\gamma(j) g(j) \end{array}, \tag{4.3}$$

where

$$d_\gamma(n) = c_\gamma(n)^{-1} = 1 - \gamma \sum_{j=M_-}^{n} \psi_\gamma(j)^2, \qquad \psi_\gamma(n) = \frac{\psi(n)}{\sqrt{c_\gamma(n-1) c_\gamma(n)}}. \tag{4.4}$$

**Lemma 4.1.** *Define $\psi_\gamma$ as in (4.4). Then $\psi_\gamma \in \mathfrak{H}$ and*

$$\|\psi_\gamma\|^2 = \frac{1}{\gamma}\Big(1 - \lim_{n \to M_+} c_\gamma(n)^{-1}\Big). \tag{4.5}$$

*If $P, P_\gamma$ denote the orthogonal projections onto the one-dimensional subspaces of $\mathfrak{H}$ spanned by $\psi, \psi_\gamma$ (set $P = 0$ if $\psi \notin \mathfrak{H}$) the operator $U_\gamma$ is unitary from $(1-P)\mathfrak{H}$ onto $(1-P_\gamma)\mathfrak{H}$.*

*Proof.* For the claims concerning $\psi$ we use

$$\sum_{j=M_-}^{n} |\psi_\gamma(j)|^2 = \frac{1}{\gamma} \sum_{j=M_-}^{n} \Big(\frac{1}{c_\gamma(j-1)} - \frac{1}{c_\gamma(j)}\Big) = \frac{1}{\gamma}\Big(1 - \frac{1}{c_\gamma(n)}\Big). \tag{4.6}$$

Next we note that

$$c_\gamma(n) \sum_{j=M_-}^{n} \psi_\gamma(j) f_\gamma(j) = \sum_{j=M_-}^{n} \psi(j) f(j) \tag{4.7}$$

and a direct calculation shows

$$\sum_{j=M_-}^{n} |f_\gamma(j)|^2 = \sum_{j=M_-}^{n} |f(j)|^2 - \frac{\gamma}{c_\gamma(n)} |\sum_{j=M_-}^{n} f(j)\psi(j)|^2. \tag{4.8}$$

This clearly proves the lemma if $\psi \in \mathfrak{H}$. Otherwise, i.e., if $\psi \notin \mathfrak{H}$, consider $U_\gamma$, $U_\gamma^{-1}$ on the dense subspace $\ell_0((M_-, M_+))$ and take closures (cf., e.g., [54], Theorem 6.13). □

Using, e.g., the polarization identity, we further get

$$\sum_{j=M_-}^{n} \overline{g_\gamma(j)} f_\gamma(j) = \sum_{j=M_-}^{n} \overline{g(j)} f(j) - \frac{\gamma}{c_\gamma(n)} \sum_{j=M_-}^{n} \psi(j) f(j) \sum_{j=M_-}^{n} \psi(j) \overline{g(j)}. \tag{4.9}$$

Next we take two sequences $a, b$ satisfying

**Hypothesis (H.4.2).** Suppose

$$a, b \in \ell((M_- - 1, M_+ + 1)), \qquad a(n) \in \mathbb{R}\backslash\{0\},\ b(n) \in \mathbb{R} \tag{4.10}$$

and introduce the difference expression

$$(\tau f)(n) = a(n)f(n+1) + a(n-1)f(n-1) - b(n)f(n). \tag{4.11}$$

We want to consider a self-adjoint operator $H$ associated with $\tau$ and separated boundary conditions at $M_\pm$ and assume the existence of a sequence $\psi(\lambda_1, n)$ of the following kind.

**Hypothesis (H.4.3).** Suppose $\psi(\lambda)$ satisfies the following conditions.

(i). $\psi(\lambda, n)$ is a real-valued solution of $\tau\psi(\lambda) = \lambda\psi(\lambda)$.
(ii). $\psi(\lambda, n)$ is square summable near $M_-$ and fulfills the boundary condition (of $H$) at $M_-$ (if any, i.e., if $\tau$ is *l.c.* at $M_-$).
(iii). $\psi(\lambda, n)$ also fulfills the boundary condition (of $H$) at $M_+$ if $\tau$ is *l.c.* at $M_+$ ($\psi(\lambda, n)$ is then an eigenfunction of $H$).

Sufficient conditions for the above function to exist are

(a). $\lambda \in \sigma_p(H)$, or
(b). $\tau$ is *l.c.* at $M_-$ but not at $M_+$, or
(c). $\sigma(H) \neq \mathbb{R}$ (and $\lambda \in \mathbb{R}\backslash\sigma(H)$), or
(d). $\sigma(H_-) \neq \mathbb{R}$ (and $\lambda \in \mathbb{R}\backslash\sigma(H_-)$), where $H_-$ is a restriction of $H$ to $\ell^2((M_- - 1, \hat{M}+1))$ with $\hat{M} \in \mathbb{Z}$ and (for instance) a Dirichlet boundary condition at $\hat{M}+1$.

It follows that $H$ is explicitly given by

$$\begin{aligned} \mathfrak{D}(H) = \{f \in \mathfrak{H} |\ \tau f \in \mathfrak{H};\ & W_{M_- -1}(\psi(\lambda_1), f) = 0 \text{ if } \tau \text{ is } l.c. \text{ at } M_-, \\ & W_{M_+}(\psi(\lambda_1), f) = 0 \text{ if } \tau \text{ is } l.c. \text{ at } M_+\}. \end{aligned} \tag{4.12}$$

We now use Lemma 4.1 with $\psi(n) = \psi(\lambda_1, n)$, $\gamma = \gamma_1$, $U_\gamma = U_{\gamma_1}$ to prove

**Theorem 4.4.** *Suppose (H.4.2) and (H.4.3) and let $\tau_{\gamma_1}$ be the difference expression*

$$(\tau_{\gamma_1} f)(n) = a_{\gamma_1}(n)f(n+1) + a_{\gamma_1}(n-1)f(n-1) - b_{\gamma_1}(n)f(n), \tag{4.13}$$

*where*

$$a_{\gamma_1}(n) = a(n)\frac{\sqrt{c_{\gamma_1}(\lambda_1, n-1)c_{\gamma_1}(\lambda_1, n+1)}}{c_{\gamma_1}(\lambda_1, n)}, \tag{4.14}$$

$$\begin{aligned} b_{\gamma_1}(n) &= b(n) + \gamma_1\Big(\frac{a(n-1)\psi(\lambda_1, n-1)\psi(\lambda_1, n)}{c_{\gamma_1}(\lambda_1, n-1)} \\ &\quad - \frac{a(n)\psi(\lambda_1, n)\psi(\lambda_1, n+1)}{c_{\gamma_1}(\lambda_1, n)}\Big). \end{aligned} \tag{4.15}$$

*Then the operator $H_{\gamma_1}$ defined by*

$$\begin{aligned} H_{\gamma_1} f &= \tau_{\gamma_1} f, \\ \mathfrak{D}(H_{\gamma_1}) &= \{f \in \mathfrak{H} | \tau_{\gamma_1} f \in \mathfrak{H}; W_{\gamma_1, M_- -1}(\psi_{\gamma_1}(\lambda_1), f) = W_{\gamma_1, M_+}(\psi_{\gamma_1}(\lambda_1), f) = 0\}, \end{aligned} \tag{4.16}$$

*where $W_{\gamma_1,n}(u,v) = a_{\gamma_1}(n)(u(n)v(n+1) - u(n+1)v(n))$, is self-adjoint and has the eigenfunction*

$$\psi_{\gamma_1}(\lambda_1, n) = \frac{\psi(\lambda_1, n)}{\sqrt{c_{\gamma_1}(\lambda_1, n-1)c_{\gamma_1}(\lambda_1, n)}} \tag{4.17}$$

*associated with the eigenvalue $\lambda_1$. If $\psi(\lambda_1) \notin \mathfrak{H}$ (and hence $\tau$ is l.p. at $M_+$) we have*

$$(1 - P_{\gamma_1}(\lambda_1))H_{\gamma_1} = U_{\gamma_1} H U_{\gamma_1}^{-1}(1 - P_{\gamma_1}(\lambda_1)), \tag{4.18}$$

*where $U_{\gamma_1}$ is the unitary transformation of Lemma 4.1 and thus*

$$\begin{aligned} \sigma(H_{\gamma_1}) &= \sigma(H) \cup \{\lambda_1\}, & \sigma_{ac}(H_{\gamma_1}) &= \sigma_{ac}(H), \\ \sigma_p(H_{\gamma_1}) &= \sigma_p(H) \cup \{\lambda_1\}, & \sigma_{sc}(H_{\gamma_1}) &= \sigma_{sc}(H). \end{aligned} \tag{4.19}$$

*If $\psi(\lambda_1) \in \mathfrak{H}$ there is a unitary operator $\tilde{U}_{\gamma_1} = U_{\gamma_1} \oplus \sqrt{1 + \gamma_1\|\psi(\lambda_1)\|^2}\mathbf{1}$ on $(1 - P_{\gamma_1}(\lambda_1))\mathfrak{H} \oplus P_{\gamma_1}(\lambda_1)\mathfrak{H}$ such that*

$$H_{\gamma_1} = \tilde{U}_{\gamma_1} H \tilde{U}_{\gamma_1}^{-1} \tag{4.20}$$

*and thus*

$$\begin{array}{rclcrcl}\sigma(H_{\gamma_1}) & = & \sigma(H), & \quad & \sigma_{ac}(H_{\gamma_1}) & = & \sigma_{ac}(H),\\ \sigma_p(H_{\gamma_1}) & = & \sigma_p(H), & & \sigma_{sc}(H_{\gamma_1}) & = & \sigma_{sc}(H).\end{array} \tag{4.21}$$

*Proof.* It suffices to prove

$$(1-P_{\gamma_1}(\lambda_1))H_{\gamma_1} = U_{\gamma_1} H U_{\gamma_1}^{-1}(1-P_{\gamma_1}(\lambda_1)). \tag{4.22}$$

Let $f$ be a sequence which is square summable near $M_-$ such that $\tau f$ is also square summable near $M_-$ and assume that $f$ fulfills the boundary condition at $M_-$, if any. Then a straightforward calculation shows

$$\tau_{\gamma_1}(U_{\gamma_1} f) = U_{\gamma_1}(\tau f) \tag{4.23}$$

and we only have to check the boundary conditions at $M_\pm$. Equation (4.8) shows that $\tau_{\gamma_1}$ is *l.c.* at $M_-$ if and only if $\tau$ is and that $\tau_{\gamma_1}$ is *l.c.* at $M_+$ if $\tau$ is. The formula

$$W_{\gamma_1,n}(\psi_{\gamma_1}(\lambda_1), U_{\gamma_1} f) = \frac{W_n(\psi(\lambda_1), f)}{c_{\gamma_1}(\lambda_1, n)} \tag{4.24}$$

shows that

$$W_{\gamma_1,M_- -1}(\psi_{\gamma_1}(\lambda_1), U_{\gamma_1} f) = 0, \qquad f \in \mathfrak{D}(H). \tag{4.25}$$

We further claim that

$$W_{\gamma_1,M_+}(\psi_{\gamma_1}(\lambda_1), U_{\gamma_1} f) = 0, \qquad f \in \mathfrak{D}(H). \tag{4.26}$$

This is clear if $\psi(\lambda_1) \in \mathfrak{H}$. Otherwise, i.e., if $\psi(\lambda_1) \notin \mathfrak{H}$, we use

$$\frac{W_n(\psi(\lambda_1), f)}{c_{\gamma_1}(\lambda_1, n)} = \frac{\sum_{j=M_-}^n \psi(\lambda_1, j)(\lambda_1 - \tau) f(j)}{c_{\gamma_1}(\lambda_1, n)}. \tag{4.27}$$

The right hand side tends to zero for $f \in \mathfrak{D}(H)$ as can be seen from (4.8) and the fact that $U_{\gamma_1}$ is unitary. Combining (4.25) and (4.26) yields

$$(1-P_{\gamma_1}(\lambda_1))U_{\gamma_1}\mathfrak{D}(H) \subseteq (1-P_{\gamma_1}(\lambda_1))\mathfrak{D}(H_{\gamma_1}). \tag{4.28}$$

But $(1-P_{\gamma_1}(\lambda_1))U_{\gamma_1}\mathfrak{D}(H)$ cannot be properly contained in $(1-P_{\gamma_1}(\lambda_1))\mathfrak{D}(H_{\gamma_1})$ by the property of self-adjoint operators being maximally defined. ☐

*Remark* 4.5. (i). By choosing $\lambda_1 \in \sigma_{ac}(H) \cup \sigma_{sc}(H)$ (provided the continuous spectrum is not empty and a solution satisfying (H.4.3) exists) we can use the double commutation method to construct operators with eigenvalues embedded in the continuous spectrum.
(ii). If $M_+ = \infty$ and $H$ has an eigenfunction $\psi(\lambda_1)$ one can remove this eigenfunction from the spectrum upon choosing $\gamma_1 = -\|\psi(\lambda_1)\|^{-2}$. The corresponding function $\psi_{\gamma_1}(\lambda_1)$ is then no longer in $\mathfrak{H}$, implying that $\tau_{\gamma_1}$ is *l.p.* at $M_+$.
(iii). Especially, removing an eigenvalue from an operator which is *l.c.* at $\infty$ yields an operator which is *l.p.*. Thus $\tau_{\gamma_1}$ is not necessary *l.p.* if $\tau$ is. Moreover, this shows that one cannot insert additional eigenvalues into an operator which is *l.c.* at $M_+$ (remove this eigenvalue again to obtain a contradiction).
(iv). The limiting case $\gamma_1 = \infty$ can be handled analogously producing a unitarily equivalent operator if $\psi(\lambda_1) \notin \mathfrak{H}$ and removes the eigenvalue $\lambda_1$ otherwise.

The previous theorem tells us only how to transfer solutions of $\tau u = zu$ into solutions of $\tau_{\gamma_1} v = zv$ if $u$ is square summable near $M_-$. The following lemma treats the general case.

**Lemma 4.6.** *The sequence*

$$u_{\gamma_1}(z,n) = \frac{c_{\gamma_1}(\lambda_1,n)u(z,n) - \frac{\gamma_1}{z-\lambda_1}\psi(\lambda_1,n)W_n(\psi(\lambda_1),u(z))}{\sqrt{c_{\gamma_1}(\lambda_1,n-1)c_{\gamma_1}(\lambda_1,n)}}, \ z \in \mathbb{C}\backslash\{\lambda_1\} \tag{4.29}$$

*solves* $\tau_{\gamma_1} u = zu$ *if* $u(z)$ *solves* $\tau u = zu$. *If* $u(z)$ *is square summable near* $M_-$ *and fulfills the boundary condition at* $M_-$ *(if any) we have* $u_{\gamma_1}(z,n) = (U_{\gamma_1} u)(z,n)$ *justifying our notation. Furthermore, we note*

$$|u_{\gamma_1}(z,n)|^2 = |u(z,n)|^2 - \frac{\gamma_1}{|z-\lambda_1|^2}\Big(\frac{|W_n(\psi(\lambda_1),u(z))|^2}{c_{\gamma_1}(\lambda_1,n)} - \frac{|W_{n-1}(\psi(\lambda_1),u(z))|^2}{c_{\gamma_1}(\lambda_1,n-1)}\Big), \tag{4.30}$$

*and*

$$W_{\gamma_1,n}(\psi_{\gamma_1}(\lambda_1), u_{\gamma_1}(z)) = \frac{W_n(\psi(\lambda_1),u(z))}{c_{\gamma_1}(\lambda_1,n)}. \tag{4.31}$$

*Hence* $u_{\gamma_1}$ *is square summable near* $M_+$ *if* $u$ *is. If* $\hat{u}_\gamma(\hat{z})$ *is constructed analogously then*

$$W_{\gamma_1,n}(u_{\gamma_1}(z),\hat{u}_{\gamma_1}(\hat{z})) = W_n(u(z),\hat{u}(\hat{z})) + \frac{\gamma_1}{c_{\gamma_1}(\lambda_1,n)}\frac{z-\hat{z}}{(z-\lambda_1)(\hat{z}-\lambda_1)} \times W_n(\psi(\lambda_1),u(z))W_n(\psi(\lambda_1),\hat{u}(\hat{z})). \tag{4.32}$$

*Proof.* All facts are tedious but straightforward calculations. □

Next we want to give some conditions implying the *l.p.* case of $\tau_{\gamma_1}$ at $M_+$, assuming $M_+ = \infty$. Let $M_- < \hat{M} < \infty$ and let $H_+$ denote a self-adjoint operator associated with $\tau$ on $(\hat{M}-1,\infty)$ and the boundary condition induced by $\psi(\lambda_1)$ at $\hat{M}$ (cf. equation (4.12)).

**Hypothesis (H.4.7).** Suppose $H_+$ satisfies one of the following spectral conditions:
(i). $\sigma_{ess}(H_+) \neq \emptyset$.
(ii). $\sigma(H_+) = \sigma_{\rm d}(H_+) = \{\lambda_{+,j}\}_{j\in J_+}$ with $\sum_{j\in J_+}(1+\lambda_{+,j}^2)^{-1} = \infty$.

Clearly Hypothesis (H.4.7) is satisfied if $a, b$ are bounded near $\infty$ (which is equivalent to $H_+$ being bounded) since then $\tau$ is *l.p.* at $\infty$.

**Theorem 4.8.** *Assume (H.4.2), (H.4.3), and (H.4.7). Then* $\tau_{\gamma_1}$ *is l.p. at* $M_+ = \infty$.

*Proof.* Let $\gamma_{1,+} = c_{\gamma_1}(\lambda_1,\hat{M})^{-1}\gamma_1$ and consider the doubly commuted operator $H_{+,\gamma_{1,+}}$ of $H_+$. Then $\tau_{\gamma_1}|_{(\hat{M},\infty)} = \tau_{\gamma_{1,+}}$ and $H_{+,\gamma_{1,+}}$ also satisfies (H.4.7). Hence $\tau_{\gamma_1}$ is *l.p.* at $\infty$ as claimed. □

*Remark* 4.9. We can interchange the role of $M_-$ and $M_+$ in this section by substituting $M_- \leftrightarrow M_+$, $\sum_{j=M_-}^{n} \to \sum_{j=n+1}^{M_+}$ and $\gamma_1 \to -\gamma_1$.

Let $M_\pm = \pm\infty$ and $H$ be a given Jacobi operator satisfying (2.46). Our next aim is to show how the scattering data of the operators $H, H_{\gamma_1}$ are related, where $H_{\gamma_1}$ is defined as in Theorem 4.4.

**Lemma 4.10.** *Let* $H$ *be a given Jacobi operator satisfying (2.46). Then the doubly commuted operator* $H_{\gamma_1}$*, defined via* $\psi(\lambda_1,n) = f_-(k_1,n)$, $\lambda_1 = (k_1+k_1^{-1})/2$ *as in Theorem 4.4, has the transmission and reflection coefficients*

$$T_{\gamma_1}(k) = \mathrm{sgn}(k_1)\frac{k\,k_1-1}{k-k_1}T(k), \tag{4.33}$$

$$R_{-,\gamma_1}(k) = R_-(k), \qquad R_{+,\gamma_1}(k) = \left(\frac{k-k_1}{k\,k_1-1}\right)^2 R_+(k), \tag{4.34}$$

*where* $k$ *and* $z$ *are related via* $z = (k+k^{-1})/2$. *Furthermore, the norming constants* $\gamma_{-,j}$ *corresponding to* $\lambda_j \in \sigma_p(H)$, $j \in J$ *(cf.* (2.50)*) remain unchanged except for an additional eigenvalue* $\lambda_1$ *with norming constant* $\gamma_{-,1} = \gamma_1$ *if* $\psi(\lambda_1) \notin \mathfrak{H}$ *respectively with norming constant* $\tilde{\gamma}_{-,1} = \gamma_{-,1} + \gamma_1$ *if* $\psi(\lambda_1) \in \mathfrak{H}$ *and* $\gamma_{-,1}$ *denotes the original norming constant of* $\lambda_1 \in \sigma_p(H)$.

*Proof.* By Lemma 4.6 the Jost solutions $f_{\gamma_1,\pm}(k,n)$ are up to a constant given by

$$\frac{c_{\gamma_1}(\lambda_1,n-1)f_\pm(k,n)-\frac{\gamma_1}{z-\lambda_1}\psi(\lambda_1,n)W_{n-1}(\psi(\lambda_1),f_\pm(k))}{\sqrt{c_{\gamma_1}(\lambda_1,n-1)c_{\gamma_1}(\lambda_1,n)}}. \tag{4.35}$$

This constant is easily seen to be 1 for $f_{\gamma_1,-}(k,n)$. Thus we can compute $R_-(\lambda)$ using (4.32) (the second unknown constant cancels). The rest follows by a straightforward calculation. □

## 5. Double commutation and Weyl–Titchmarsh theory

In this section we want to reveal the connections between Weyl–Titchmarsh theory and the double commutation method. Without loss of generality we consider only the cases $\ell^2(\mathbb{N})$ and $\ell^2(\mathbb{Z})$. We start with the half-line $\mathbb{N}$ and freely use the notation employed in Appendices A–D.

Let $H_+$ be a self-adjoint operator associated with $\tau$ on $\mathbb{N}$ and a Dirichlet boundary condition at 0. Without loss of generality we assume $\psi(\lambda_1,1)=1$.

*Remark* 5.1. We have restricted ourselves to a Dirichlet boundary condition since the general boundary condition

$$\cos(\alpha)u(0)+\sin(\alpha)u(1)=0 \tag{5.1}$$

can be reduced to the case $\alpha=0$ by the transformation $b(1)\to b(1)+a(0)\tan(\alpha)$ for $\alpha\neq\pi/2$, whereas for $\alpha=\pi/2$ one can replace $\ell^2(\mathbb{N})$ by $\ell^2((1,\infty))$.

**Theorem 5.2.** *Assume (H.4.2), $\psi(\lambda_1,1)=1$ and let $m_+(z,0)$, $m_{+,\gamma_1}(z,0)$ denote the Weyl $m$-functions of $H_+$, $H_{+,\gamma_1}$. Then we have*

$$m_{+,\gamma_1}(z,0)=\frac{1}{1+\gamma_1}\Big(m_+(z,0)-\frac{\gamma_1}{z-\lambda_1}\Big). \tag{5.2}$$

*If $\mu_+$ and $\mu_{+,\gamma_1}$ denote the corresponding spectral functions of $H_+$ and $H_{+,\gamma_1}$ it follows that*

$$\mu_{+,\gamma_1}(\lambda)=\frac{1}{1+\gamma_1}\Big(\mu_+(\lambda)+\gamma_1\Theta(\lambda-\lambda_1)\Big), \tag{5.3}$$

*where $\Theta(.)$ denotes the (right continuous) step function*

$$\Theta(x)=\left\{\begin{array}{ll}1, & x\geq 0\\ 0, & x<0\end{array}\right. . \tag{5.4}$$

*Proof.* As in Appendix B we use the finite approximations $m_N(z,0)$ and $m_{N,\gamma_1}(z,0)$. If $\gamma_j(N)$, $\gamma_{j,\gamma_1}(N)$ are the corresponding norming constants we have

$$\gamma_{j,\gamma_1}(N)=\frac{1}{1+\gamma_1}\left\{\begin{array}{ll}\gamma_j(N)+\gamma_1, & \lambda_j=\lambda_1\\ \gamma_j(N), & \lambda_j\neq\lambda_1\end{array}\right. . \tag{5.5}$$

This follows since $\psi(z,0)=0$, $\psi(z,1)=1$ implies $\psi_{\gamma_1}(z,0)=0$, $\psi_{\gamma_1}(z,1)=(1+\gamma_1)^{-1/2}$. Hence we infer

$$m_{N,\gamma_1}(z,0)=\frac{1}{1+\gamma_1}\Big(m_N(z,0)-\frac{\gamma_1}{z-\lambda_1}\Big) \tag{5.6}$$

and the theorem follows upon taking the limit $N\to\infty$. □

*Remark* 5.3. If we transform the operator $H_+$ into it's diagonal form as in Appendix C the double commutation method gets particularly transparent: it corresponds to adding a step function to the spectral function. This approach can also be used to derive the unitary transformation stated in Section 2 in the following way. Take the spectral function $\mu_+$ of a given Jacobi operator, switch to $\mu_{+,\gamma_1}$, and compute the orthogonal polynomials with respect to this new measure (compare Appendix C and [1], Ch. 1). Now take a sequence $f(n)$ and its transform $F(z)$ and use (C.8) to obtain (4.2).

Next we turn to operators in $\ell^2(\mathbb{Z})$. Without loss of generality we assume

$$\psi(\lambda_1,0)=-\sin(\alpha),\quad \psi(\lambda_1,0)=\cos(\alpha),\quad \alpha\in[0,\pi). \tag{5.7}$$

**Theorem 5.4.** *Assume (H.4.2) and let* $\tilde{m}_\pm(z,\alpha)$, $\tilde{m}_{\pm,\gamma_1}(z,\alpha)$ *denote the Weyl* $\tilde{m}$*-functions of* $H$, $H_{\gamma_1}$ *as introduced in Appendix B. Then we have*

$$\tilde{m}_{\pm,\gamma_1}(z,\tilde{\alpha}) = \frac{c_{\gamma_1}(\lambda_1,0)}{c_{\gamma_1}(\lambda_1,-1)}\frac{1+\cot(\tilde{\alpha})^2}{1+\cot(\alpha)^2}\Big(\tilde{m}_\pm(z,\alpha) - \frac{\tilde{\gamma}_1}{z-\lambda_1} + \frac{\cot(\alpha)c_{\gamma_1}(\lambda_1,1)^{-1}}{a(0)(1+\cot(\tilde{\alpha})^2)}\Big), \tag{5.8}$$

*where*

$$\tilde{\gamma}_1 = \frac{\gamma_1}{c_{\gamma_1}(\lambda_1,0)}, \qquad \tan(\tilde{\alpha}) = \sqrt{\frac{c_{\gamma_1}(\lambda_1,1)}{c_{\gamma_1}(\lambda_1,-1)}}\tan(\alpha). \tag{5.9}$$

*Proof.* Consider the sequences

$$\phi_{\alpha,\gamma_1}(z,n), \quad \theta_{\alpha,\gamma_1}(z,n) - \Big(\frac{\tilde{\gamma}_1}{z-\lambda_1} - \frac{\cot(\alpha)c_{\gamma_1}(\lambda_1,1)^{-1}}{a(0)(1+\cot(\tilde{\alpha})^2)}\Big)\phi_{\alpha,\gamma_1}(z,n) \tag{5.10}$$

constructed from the fundamental system $\theta_\alpha(z,n)$, $\phi_\alpha(z,n)$ for $\tau$ (cf. (B.1)) as in Lemma 4.6. They form a fundamental system for $\tau_{\gamma_1}$ corresponding to the initial conditions associated with $\tilde{\alpha}$ up to constant multiples. Now use (4.31) to evaluate (B.3). □

The Weyl $M$-matrix and the corresponding spectral matrix can now be computed in a straightforward manner (cf. Appendix D).

## 6. Iteration of the double commutation method

Finally we demonstrate how to iterate the double commutation method. We choose a given background operator $H$ (with coefficients $a$, $b$ satisfying (H.4.2)) and further $\gamma_1 > 0, \lambda_1 \in \mathbb{R}$. Next choose $\psi(\lambda_1)$ as in Hypothesis (H.4.3) to define the transformation $U_{\gamma_1}$ and the operator $H_{\gamma_1}$. In the second step, we choose $\gamma_2 > 0, \lambda_2 \in \mathbb{R}$ and another function $\psi(\lambda_2)$ to define $\psi_{\gamma_1}(\lambda_2) = U_{\gamma_1}\psi(\lambda_2)$, a corresponding transformation $U_{\gamma_1,\gamma_2}$, and an operator $H_{\gamma_1,\gamma_2}$. Applying this procedure $N$-times results in

**Theorem 6.1.** *Assuming (H.4.2) let* $H$ *be a given background Jacobi operator in* $\mathfrak{H} = \ell^2((M_- - 1, M_+ + 1))$ *and let* $\gamma_j > 0$, $\lambda_j$, $1 \le j \le N$ *be such that there exist corresponding solutions* $\psi(\lambda_j,n)$ *of* $\tau\psi = \lambda_j\psi$ *satisfying Hypothesis (H.4.3). We set* $\psi_{\gamma_1,\dots,\gamma_k}(\lambda_j) = U_{\gamma_1,\dots,\gamma_k}\cdots U_{\gamma_1}\psi(\lambda_j)$ *and define the following matrices* $(1 \le \ell \le N)$

$$C^\ell(n) = \left\{\delta_r(s) + \sqrt{\gamma_r\gamma_s}\sum_{m=M_-}^{n}\psi(\lambda_r,m)\psi(\lambda_s,m)\right\}_{1\le r,s\le\ell}, \tag{6.1}$$

$$C^\ell_{i,j}(n) = \left\{\begin{array}{cc} C^{\ell-1}(n)_{r,s} & r,s\le\ell-1 \\ \sqrt{\gamma_s}\sum\limits_{m=M_-}^{n}\psi(\lambda_i,m)\psi(\lambda_s,m) & s\le\ell-1, r=\ell \\ \sqrt{\gamma_r}\sum\limits_{m=M_-}^{n}\psi(\lambda_r,m)\psi(\lambda_j,m) & r\le\ell-1, s=\ell \\ \sum\limits_{m=M_-}^{n}\psi(\lambda_i,m)\psi(\lambda_j,m) & r=s=\ell \end{array}\right\}_{1\le r,s\le\ell}, \tag{6.2}$$

$$\Psi^\ell(\lambda_j,n) = \left\{\begin{array}{cc} C^{\ell}(n)_{r,s} & r,s\le\ell \\ \sqrt{\gamma_s}\sum\limits_{m=M_-}^{n}\psi(\lambda_j,m)\psi(\lambda_s,m) & s\le\ell, r=\ell+1 \\ \sqrt{\gamma_r}\psi(\lambda_r,n) & r\le\ell, s=\ell+1 \\ \psi(\lambda_j,n) & r=s=\ell+1 \end{array}\right\}_{1\le r,s\le\ell+1}. \tag{6.3}$$

*Then we have (set* $C^0(n) = 1$*)*

$$c_{\gamma_\ell}(\lambda_\ell,n) = 1 + \gamma_\ell\sum_{m=M_-}^{n}\psi_{\gamma_1,\dots,\gamma_{\ell-1}}(\lambda_\ell,m)^2 = \frac{\det C^\ell(n)}{\det C^{\ell-1}(n)}, \tag{6.4}$$

*and hence*

$$\prod_{\ell=1}^{N} c_{\gamma_\ell}(\lambda_\ell, n) = \det C^N(n). \tag{6.5}$$

*Moreover,*

$$\sum_{m=M_-}^{n} \psi_{\gamma_1,\dots,\gamma_{\ell-1}}(\lambda_i, m)\psi_{\gamma_1,\dots,\gamma_{\ell-1}}(\lambda_j, m) = \frac{\det C^\ell_{i,j}(n)}{\det C^{\ell-1}(n)} \tag{6.6}$$

*and*

$$\psi_{\gamma_1,\dots,\gamma_\ell}(\lambda_j, n) = \frac{\det \Psi^\ell(\lambda_j, n)}{\sqrt{\det C^\ell(n-1)\det C^\ell(n)}}. \tag{6.7}$$

*In addition, we get*

$$a_{\gamma_1,\dots,\gamma_N}(n) = a(n)\frac{\sqrt{\det C^N(n-1)\det C^N(n+1)}}{\det C^N(n)}, \tag{6.8}$$

$$\begin{aligned} b_{\gamma_1,\dots,\gamma_N}(n) &= b(n) - \sum_{\ell=1}^{N}\gamma_\ell\Big(a(n)\frac{\det\Psi^\ell(\lambda_\ell,n)\det\Psi^\ell(\lambda_\ell,n+1)}{\det C^{\ell-1}(n)\det C^\ell(n)} \\ &\quad - a(n-1)\frac{\det\Psi^\ell(\lambda_\ell,n-1)\det\Psi^\ell(\lambda_\ell,n)}{\det C^{\ell-1}(n-1)\det C^\ell(n-1)}\Big) \\ &= -\lambda_N + a(n)\frac{\det C^N(n-1)}{\det C^N(n)}\frac{\det\Psi^N(\lambda_N,n+1)}{\det\Psi^N(\lambda_N,n)} \\ &\quad - a(n-1)\frac{\det C^N(n)}{\det C^N(n-1)}\frac{\det\Psi^N(\lambda_N,n-1)}{\det\Psi^N(\lambda_N,n)}, \end{aligned} \tag{6.9}$$

*the last equation only being valid if* $\det\Psi^N(\lambda_N, n) \neq 0$ *(e.g., if* $\lambda_N \le \inf\sigma(H)$*). The spectrum of* $H_{\gamma_1,\dots,\gamma_N}$ *is given by*

$$\begin{aligned} \sigma(H_{\gamma_1,\dots,\gamma_N}) &= \sigma(H)\cup\{\lambda_j\}_{j=1}^N, & \sigma_{ac}(H_{\gamma_1,\dots,\gamma_N}) &= \sigma_{ac}(H), \\ \sigma_p(H_{\gamma_1,\dots,\gamma_N}) &= \sigma_p(H)\cup\{\lambda_j\}_{j=1}^N, & \sigma_{sc}(H_{\gamma_1,\dots,\gamma_N}) &= \sigma_{sc}(H). \end{aligned} \tag{6.10}$$

*Moreover,*

$$\begin{aligned} &H_{\gamma_1,\dots,\gamma_N}(1 - \sum_{j=1}^N P_{\gamma_1,\dots,\gamma_N}(\lambda_j)) \\ &= (U_{\gamma_1,\dots,\gamma_N}\cdots U_{\gamma_1})H(U_{\gamma_1}^{-1}\cdots U_{\gamma_1,\dots,\gamma_N}^{-1})(1 - \sum_{j=1}^N P_{\gamma_1,\dots,\gamma_N}(\lambda_j)), \end{aligned} \tag{6.11}$$

*where* $P_{\gamma_1,\dots,\gamma_N}(\lambda_j)$ *denotes the projection onto the one-dimensional subspace of* $\mathfrak{H}$ *spanned by* $\psi_{\gamma_1,\dots,\gamma_N}(\lambda_j)$*.*

*Proof.* We start with (6.6). Using Sylvester's determinant identity (cf. [25], Sect. II.3) we obtain

$$\begin{aligned} &\det C^{\ell-1}(n)\det C^{\ell+1}_{i,j}(n) \\ &= \det C^\ell(n)\det C^\ell_{i,j}(n) - \gamma_\ell\det C^\ell_{\ell,j}(n)\det C^\ell_{i,\ell}(n), \end{aligned} \tag{6.12}$$

which proves (6.6) together with a look at (4.9) by induction on $N$. Next, (6.4) easily follows from (6.6). Similarly,

$$\begin{aligned} &\det C^\ell(n)\det\Psi^{\ell+1}(\lambda_j,n) \\ &= \det C^{\ell+1}(n)\det\Psi^\ell(\lambda_j,n) - \gamma_\ell\det\Psi^\ell(\lambda_\ell,n)\det C^\ell_{j,\ell}(n), \end{aligned} \tag{6.13}$$

and (4.3) prove (6.7). The rest follows in a straightforward manner. □

*Remark* 6.2. (i). If $f$ is square summable near $M_-$, $f_{\gamma_1,\dots,\gamma_j} = U_{\gamma_1,\dots,\gamma_j} \cdots U_{\gamma_1} f$ is given by substituting $\psi(\lambda_j) \to f$ in (6.7). Similarly we get the scalar product of $f_{\gamma_1,\dots,\gamma_i}$ and $g_{\gamma_1,\dots,\gamma_j}$ from (6.6) by substituting $f \to \psi(\lambda_i)$ and $g \to \psi(\lambda_j)$ in (6.2).
(ii). Equation (6.7) can be rephrased as

$$(\gamma_1\psi_{\gamma_1,\dots,\gamma_\ell}(\lambda_1,n),\dots,\gamma_\ell\psi_{\gamma_1,\dots,\gamma_\ell}(\lambda_\ell,n)) = \sqrt{\frac{\det C^\ell(n)}{\det C^\ell(n-1)}}(C^\ell(n))^{-1}(\gamma_1\psi(\lambda_1,n),\dots,\gamma_\ell\psi(\lambda_\ell,n)), \tag{6.14}$$

where $(C^\ell(n))^{-1}$ is the inverse matrix of $C^\ell(n)$.

Clearly Theorem 4.8 extends (by induction) to this more general situation.

**Theorem 6.3.** *Assume (H.4.2) and (H.4.7). Then $\tau_{\gamma_1,\dots,\gamma_N}$ is l.p. at $M_+$.*

Finally we also extend Lemma 4.10. For simplicity we assume $\psi(\lambda_j,n) \notin \mathfrak{H}$, $1 \le j \le N$.

**Lemma 6.4.** *Let $H$ be a given Jacobi operator satisfying (2.46). Then $H_{\gamma_1,\dots,\gamma_N}$, defined via $\psi(\lambda_\ell,n) = f_-(k_\ell,n)$, $\lambda_\ell = (k_\ell + k_\ell^{-1})/2 \in \mathbb{R}\backslash\sigma(H_{\gamma_1,\dots,\gamma_{\ell-1}})$, $1 \le \ell \le N$ has the transmission and reflection coefficients*

$$T_{\gamma_1,\dots,\gamma_N}(k) = \textstyle\prod_{\ell=1}^N \mathrm{sgn}(k_\ell)\frac{k\,k_\ell - 1}{k - k_\ell} T(k), \tag{6.15}$$

$$R_{-,\gamma_1,\dots,\gamma_N}(k) = R_-(k), \quad R_{+,\gamma_1,\dots,\gamma_N}(k) = \left(\prod_{\ell=1}^N \left(\frac{k - k_\ell}{k\,k_\ell - 1}\right)^2\right) R_+(k), \tag{6.16}$$

*where $z = (k + k^{-1})/2$. Furthermore, the norming constants $\gamma_{-,j}$ corresponding to $\lambda_j \in \sigma_p(H)$, $j \in J$ (cf.* (2.50)*) remain unchanged and the additional eigenvalues $\lambda_\ell$ have norming constants $\gamma_{-,\ell} = \gamma_\ell$.*

*Remark* 6.5. Of special importance is the case $a(n) = 1/2$, $b(n) = 0$. Here we have $f_\pm(k,n) = k^{\pm n}$, $T(k) = 1$, and $R_\pm(k) = 0$. It is well known from inverse scattering theory that $R_\pm(k)$, $|k| = 1$ together with the point spectrum and corresponding norming constants uniquely determine $a(n), b(n)$. Hence we infer from Lemma 3.3 that $H_{\gamma_1,\dots,\gamma_N}$ constructed from $\psi(\lambda_\ell,n) = f_-(k_\ell,n)$ as in Theorem 6.1 and $H_{\sigma_1,\dots,\sigma_N}$ constructed from $u^\ell_{\sigma_\ell} = \frac{1+\sigma_\ell}{2}k_\ell^n + (-1)^{\ell+1}\frac{1-\sigma_\ell}{2}k_\ell^{-n}$ as in Theorem 3.1 coincide if

$$\gamma_j = \left(\frac{1-\sigma_j}{1+\sigma_j}\right)^{-1} |k_j|^{-1-N} \frac{\prod_{\ell=1}^N |1 - k_j k_\ell|}{\prod_{\substack{\ell=1\\ \ell\neq j}}^N |k_j - k_\ell|}, \quad 1 \le j \le N. \tag{6.17}$$

For a direct proof compare [35].

## 7. Applications

First we state the discrete analogue of the FIT-formula derived in [22] for the isospectral torus of periodic Schrödinger operators. This yields an explicit realization of the isospectral torus of all algebro-geometric quasi-periodic finite-gap Jacobi operators.

Let $a(n), b(n)$ be given algebro-geometric quasi-periodic $g$-gap sequences characterized by the band-edges $E_0 < E_1 < \dots < E_{2g+1}$ and Dirichlet data $\{(\mu_j,\sigma_j)\}_{j=1}^g$ at the reference point $n = 0$ (cf. [7]), where $\mu_j \in [E_{2j-1}, E_{2j}]$ and $\sigma_j \in \{\pm\}$, $1 \le j \le g$. Then the spectrum of the associate Jacobi operator $H$ is of the type

$$\begin{aligned} \sigma(H) &= \sigma_{ac}(H) = \textstyle\bigcup_{n=1}^{g+1}[E_{2n-2}, E_{2n-1}], \\ \sigma_{sc}(H) &= \sigma_p(H) = \emptyset. \end{aligned} \tag{7.1}$$

and (cf. (2.29))

$$\sigma(H_\pm) = \sigma(H) \cup \{\mu_j | \sigma_j = \pm,\ 1 \le j \le g\}. \tag{7.2}$$

Then considerations as in Theorem 3.1 readily yield that all other isospectral algebro-geometric $g$-gap sequences can be realized in the following way

$$\begin{aligned} a_{(\tilde\mu_1,\tilde\sigma_1),\dots,(\tilde\mu_g,\tilde\sigma_g)}(n) &= -\sqrt{a(n-g)a(n-g+2)}\,\times \\ &\quad \sqrt{\frac{C_{n-g}(\psi_{\sigma_1}(\mu_1),\psi_{-\tilde\sigma_1}(\tilde\mu_1),\dots,\psi_{\sigma_g}(\mu_g),\psi_{-\tilde\sigma_g}(\tilde\mu_g))}{C_{n-g+1}(\psi_{\sigma_1}(\mu_1),\psi_{-\tilde\sigma_1}(\tilde\mu_1),\dots,\psi_{\sigma_g}(\mu_g),\psi_{-\tilde\sigma_g}(\tilde\mu_g))}}\,\times \\ &\quad \sqrt{\frac{C_{n-g+2}(\psi_{\sigma_1}(\mu_1),\psi_{-\tilde\sigma_1}(\tilde\mu_1),\dots,\psi_{\sigma_g}(\mu_g),\psi_{-\tilde\sigma_g}(\tilde\mu_g))}{C_{n-g+1}(\psi_{\sigma_1}(\mu_1),\psi_{-\tilde\sigma_1}(\tilde\mu_1),\dots,\psi_{\sigma_g}(\mu_g),\psi_{-\tilde\sigma_g}(\tilde\mu_g))}}, \end{aligned} \tag{7.3}$$

$$\begin{aligned} b_{(\tilde\mu_1,\tilde\sigma_1),\dots,(\tilde\mu_g,\tilde\sigma_g)}(n) &= a(n-g)\frac{C_{n-g+2}(\psi_{\sigma_1}(\mu_1),\psi_{-\tilde\sigma_1}(\tilde\mu_1),\dots,\psi_{\sigma_g}(\mu_g))}{C_{n-g+1}(\psi_{\sigma_1}(\mu_1),\psi_{-\tilde\sigma_1}(\tilde\mu_1),\dots,\psi_{\sigma_g}(\mu_g))}\,\times \\ &\quad \frac{C_{n-g}(\psi_{\sigma_1}(\mu_1),\psi_{-\tilde\sigma_1}(\tilde\mu_1),\dots,\psi_{\sigma_g}(\mu_g),\psi_{-\tilde\sigma_g}(\tilde\mu_g))}{C_{n-g+1}(\psi_{\sigma_1}(\mu_1),\psi_{-\tilde\sigma_1}(\tilde\mu_1),\dots,\psi_{\sigma_g}(\mu_g),\psi_{-\tilde\sigma_g}(\tilde\mu_g))} \\ &\quad + a(n+1)\frac{C_{n-g}(\psi_{\sigma_1}(\mu_1),\psi_{-\tilde\sigma_1}(\tilde\mu_1),\dots,\psi_{\sigma_g}(\mu_g))}{C_{n-g+1}(\psi_{\sigma_1}(\mu_1),\psi_{-\tilde\sigma_1}(\tilde\mu_1),\dots,\psi_{\sigma_g}(\mu_g))}\,\times \\ &\quad \frac{C_{n-g+1}(\psi_{\sigma_1}(\mu_1),\psi_{-\tilde\sigma_1}(\tilde\mu_1),\dots,\psi_{\sigma_g}(\mu_g),\psi_{-\tilde\sigma_g}(\tilde\mu_g))}{C_{n-g}(\psi_{\sigma_1}(\mu_1),\psi_{-\tilde\sigma_1}(\tilde\mu_1),\dots,\psi_{\sigma_g}(\mu_g),\psi_{-\tilde\sigma_g}(\tilde\mu_g))} - \tilde\mu_g, \end{aligned} \tag{7.4}$$

where $\psi_\pm(z,n)$ are the branches of the Baker-Akhiezer function associated with $a,b$ (i.e., the solutions of $\tau\psi = z\psi$ which are square summable near $\pm\infty$) and the new sequences are associated with the new Dirichlet data $\{(\tilde\mu_j,\tilde\sigma_j)\}_{j=1}^g$ at the same reference point $n=0$. Even though $\psi_\pm(z,n)$ is not necessarily positive as required in our Theorem 3.1, the above sequences can be shown to be well-defined by using the explicit theta-function representations for $\psi_\pm(z,n)$ (cf., e.g., [7]) as long as $\tilde\mu_j \in [E_{2j-1},E_{2j}]$ and $\tilde\sigma_j \in \{\pm\}$, $1\le j\le g$. In fact, consider the hyperelliptic Riemann surface $K_g$ associated with the function

$$R_{2g+2}(z)^{1/2} = \prod_{j=0}^{2g+1}(z-E_j)^{1/2} \tag{7.5}$$

and branch points $E_0 < E_1 < \cdots < E_{2g+1}$. A point $P \in K_g$ will be denoted by $P = (z, \pm R_{2g+2}(z)^{1/2})$ and we add two points $\infty_\pm \in K_g$ such that $K_g$ is compact. Introduce

$$\underline{z}(P,n) = \underline{\hat A}_{P_0}(P) - \sum_{j=1}^g \underline{\hat A}_{P_0}(\hat\mu_j) + 2n\underline{\hat A}_{P_0}(\infty_+) - \underline{\hat\Xi}_{P_0}, \tag{7.6}$$

where $\underline{\hat A}_{P_0}$ is Abel's map with base point $P_0=(E_0,0)$ and $\underline{\hat\Xi}_{P_0}$ is the vector of Riemann constants (cf. [7] for more details). Then

$$a(n) = \tilde a[\theta(\underline{z}(\infty_+,n-1))\theta(\underline{z}(\infty_+,n+1))/\theta(\underline{z}(\infty_+,n))^2]^{1/2}, \tag{7.7}$$

$$\begin{aligned} b(n) &= -E_0 + \tilde a\frac{\theta(\underline{z}(\infty_+,n-1))\theta(\underline{z}(P_0,n+1))}{\theta(\underline{z}(\infty_+,n))\theta(\underline{z}(P_0,n))} \\ &\quad + \tilde a\frac{\theta(\underline{z}(\infty_+,n))\theta(\underline{z}(P_0,n-1))}{\theta(\underline{z}(\infty_+,n-1))\theta(\underline{z}(P_0,n))}, \end{aligned} \tag{7.8}$$

where $\theta$ is Riemann's theta function associated with $K_g$ and $\tilde a$ is a constant depending only on $K_g$ (i.e.,on $\{E_j\}_{j=0}^{2g+1}$). Performing one single commutation at a point $Q=(z,\sigma R_{2g+2}(z)^{1/2}) \in K_g$ (i.e., choosing $\psi_\sigma(z,n)$ to perform the commutation) it is shown in [7], Chapter 9 that the new sequences are again given by (7.7), (7.8) if $\underline{z}(P,n)$ is replaced by

$$\underline{\tilde z}(P,n) = \underline{z}(P,n) + \underline{\hat A}_{P_0}(Q) + \underline{\hat A}_{P_0}(\infty_+). \tag{7.9}$$

As a consequence we note that for the standard procedure as in Theorem 2.6 (i.e., with $Q = (\lambda_1, \sigma_1 R_{2g+2}(\lambda_1)^{1/2})$, $\sigma_1 \in \{\pm 1\}$) the corresponding commuted operator $H_{\sigma_1}$ is again quasi-periodic and isospectral to $H$.

Hence, choosing $Q = \hat{\mu}_j$ we obtain

$$\underline{\tilde{z}}(P,n) = \underline{z}(P,n) + \underline{\hat{A}}_{P_0}(\hat{\mu}_j) + \underline{\hat{A}}_{P_0}(\infty_+) \tag{7.10}$$

and the Dirichlet eigenvalue at $\hat{\mu}_j$ is formally replaced by one at $\infty_-$ (since $\underline{\hat{A}}_{P_0}(\infty_-) = -\underline{\hat{A}}_{P_0}(\infty_+)$). The corresponding sequences are neither real-valued nor well-defined. To repair this we perform a second single commutation choosing $Q = (\tilde{\mu}_j, -\tilde{\sigma}_j R_{2g+2}(\tilde{\mu}_j)^{1/2})$. The resulting sequences $a_{(\tilde{\mu}_j,\tilde{\sigma}_j)}$, $b_{(\tilde{\mu}_j,\tilde{\sigma}_j)}$ are associated with

$$\underline{z}_{(\tilde{\mu}_j,\tilde{\sigma}_j)}(P,n) = \underline{z}(P,n+1) + \underline{\hat{A}}_{P_0}(\hat{\mu}_j) - \underline{\hat{A}}_{P_0}((\tilde{\mu}_j, \tilde{\sigma}_j R_{2g+2}(\tilde{\mu}_j)^{1/2})) \tag{7.11}$$

and are again real-valued. Moreover, we have replaced the Dirichlet eigenvalue $(\mu_j,\sigma_j)$ by $(\tilde{\mu}_j,\tilde{\sigma}_j)$ and we have shifted the reference point for the Dirichlet boundary condition by one (since $\underline{z}(P,n+1)$ and not $\underline{z}(P,n)$ occurs in (7.11)) whereas everything else remains unchanged. From Section 3 we know that $a_{(\tilde{\mu}_j,\tilde{\sigma}_j)}$, $b_{(\tilde{\mu}_j,\tilde{\sigma}_j)}$ are equivalently given by

$$a_{(\tilde{\mu}_j,\tilde{\sigma}_j)}(n+1) = -\sqrt{a(n)a(n+2)}\sqrt{\frac{C_n(\psi_{\sigma_j}(\mu_j), \psi_{-\tilde{\sigma}_j}(\tilde{\mu}_j))C_{n+2}(\psi_{\sigma_j}(\mu_j), \psi_{-\tilde{\sigma}_j}(\tilde{\mu}_j))}{C_{n+1}(\psi_{\sigma_j}(\mu_j), \psi_{-\tilde{\sigma}_j}(\tilde{\mu}_j))^2}}, \tag{7.12}$$

$$\begin{aligned} b_{(\tilde{\mu}_j,\tilde{\sigma}_j)}(n+1) &= a(n)\frac{\psi_{\sigma_j}(\mu_j,n+2)C_n(\psi_{\sigma_j}(\mu_j), \psi_{-\tilde{\sigma}_j}(\tilde{\mu}_j))}{\psi_{\sigma_j}(\mu_j,n+1)C_{n+1}(\psi_{\sigma_j}(\mu_j), \psi_{-\tilde{\sigma}_j}(\tilde{\mu}_j))} + \\ & \quad a(n+1)\frac{\psi_{\sigma_j}(\mu_j,n)C_{n+1}(\psi_{\sigma_j}(\mu_j), \psi_{-\tilde{\sigma}_j}(\tilde{\mu}_j))}{\psi_{\sigma_j}(\mu_j,n+1)C_n(\psi_{\sigma_j}(\mu_j), \psi_{-\tilde{\sigma}_j}(\tilde{\mu}_j))} - \tilde{\mu}_j, \end{aligned} \tag{7.13}$$

where the $n+1$ on the left-hand-side takes the aforementioned shift of reference point into account. Thus, applying this procedure $g$ times we can replace all Dirichlet eigenvalues proving (7.3), (7.4).

The reader might be puzzled by the fact that the Dirichlet eigenvalue $\hat{\mu}_j$ is shifted to $\infty_-$ (as opposed to $\infty_+$) which seemingly distinguishes $\infty_-$ from $\infty_+$. However, this apparent asymmetry between $\infty_+$ and $\infty_-$ is related to our way of factorizing $H$. If we would instead split up $H$ as

$$H = \tilde{A}_{\sigma_j}^* \tilde{A}_{\sigma_j} + \mu_j, \tag{7.14}$$

where

$$(\tilde{A}_{\sigma_j})f(n) = -\sqrt{-\frac{a(n-1)\psi_{\sigma_j}(\mu_j,n)}{\psi_{\sigma_j}(\mu_j,n-1)}}f(n-1) + \sqrt{-\frac{a(n-1)\psi_{\sigma_j}(\mu_j,n-1)}{\psi_{\sigma_j}(\mu_j,n)}}f(n), \tag{7.15}$$

with $\tilde{A}_{\sigma_j}^*$ being the adjoint of $\tilde{A}_{\sigma_j}$, the role of $\infty_+$ and $\infty_-$ would be interchanged.

We stress again that (7.3), (7.4) represent an explicit realization of the isospectral torus of all algebro-geometric quasi-periodic $g$-gap Jacobi operators with spectrum (7.1).

Next we turn to bounded solutions $(a(n,t), b(n,t))$ of the Toda equations and construct $N$-soliton solutions on these (arbitrary) background solutions using the single commutation method.

The corresponding Jacobi operators $H(t)$ satisfy $\inf(\sigma(H(t))) = \inf(\sigma(H(0))) > -\infty$ for all $t \in \mathbb{R}$. Furthermore, this implies the existence of principal solutions $u_\pm(\lambda,n,t)$ which satisfy

$$H(t)u_\pm(\lambda,n,t) = \lambda u_\pm(\lambda,n,t), \tag{7.16}$$

$$\frac{d}{dt}u_\pm(\lambda,n,t) = P(t)u_\pm(\lambda,n,t), \quad (n,t) \in \mathbb{Z}\times\mathbb{R}, \tag{7.17}$$

where the difference expression $P(t)$ associated with $(a(t), b(t))$ is defined by

$$(P(t)f)(n) = a(n,t)f(n+1) - a(n-1,t)f(n-1). \tag{7.18}$$

(7.16) and (7.17) then imply the Toda lattice equations,

$$\left.\begin{aligned} \frac{d}{dt}a(n,t) &= a(n,t)\Big(b(n,t) - b(n+1,t)\Big) \\ \frac{d}{dt}b(n,t) &= 2\Big(a(n,t-1)^2 - a(n,t)^2\Big) \end{aligned}\right., \quad (n,t) \in \mathbb{Z}\times\mathbb{R} \tag{7.19}$$

which are well-known to be equivalent to the Lax equation

$$\frac{d}{dt}H(t) - [P(t), H(t)] = 0, \quad t \in \mathbb{R} \tag{7.20}$$

(where $[.,.]$ denotes the commutator).

Next, let $H(t)$ be as above and choose

$$\lambda_N < \cdots < \lambda_1 < \inf(\sigma(H(0))), \quad \sigma_j \in [-1,1], \quad 1 \le j \le N \in \mathbb{N}. \tag{7.21}$$

Then Theorem 3.1 implies

$$\begin{aligned} a_{\sigma_1,\dots,\sigma_N}(n,t) &= -\sqrt{a(n,t)a(n+N,t)} \times \\ &\quad \frac{\sqrt{C_n(u^1_{\sigma_1},\dots,u^N_{\sigma_N})C_{n+2}(u^1_{\sigma_1},\dots,u^N_{\sigma_N})}}{C_{n+1}(u^1_{\sigma_1},\dots,u^N_{\sigma_N})}, \end{aligned} \tag{7.22}$$

$$\begin{aligned} b_{\sigma_1,\dots,\sigma_N}(n,t) &= -\lambda_N \\ &\quad + a(n,t)\frac{C_{n+2}(u^1_{\sigma_1},\dots,u^{N-1}_{\sigma_{N-1}})C_n(u^1_{\sigma_1},\dots,u^N_{\sigma_N})}{C_{n+1}(u^1_{\sigma_1},\dots,u^{N-1}_{\sigma_{N-1}})C_{n+1}(u^1_{\sigma_1},\dots,u^N_{\sigma_N})} \\ &\quad + a(n+N-1,t)\frac{C_n(u^1_{\sigma_1},\dots,u^{N-1}_{\sigma_{N-1}})C_{n+1}(u^1_{\sigma_1},\dots,u^N_{\sigma_N})}{C_{n+1}(u^1_{\sigma_1},\dots,u^{N-1}_{\sigma_{N-1}})C_n(u^1_{\sigma_1},\dots,u^N_{\sigma_N})}, \end{aligned} \tag{7.23}$$

where

$$u^\ell_{\sigma_\ell}(n,t) = \frac{1+\sigma_\ell}{2}u_+(\lambda_\ell,n,t) + (-1)^{\ell+1}\frac{1-\sigma_\ell}{2}u_-(\lambda_\ell,n,t). \tag{7.24}$$

Moreover, for $\lambda < \lambda_N$,

$$u_{\sigma_1,\dots,\sigma_N,\pm}(\lambda,n,t) = \frac{\pm\sqrt{\prod_{j=0}^{N-1}(-a(n+j,t))}C_n(u^1_{\sigma_1},\dots,u^\ell_{\sigma_N},u_\pm(\lambda))}{\sqrt{C_n(u^1_{\sigma_1},\dots,u^N_{\sigma_N})C_{n+1}(u^1_{\sigma_1},\dots,u^N_{\sigma_N})}} \tag{7.25}$$

are the principal solutions of $\tau_{\sigma_1,\dots,\sigma_N}(t)u = \lambda u$ satisfying

$$\frac{d}{dt}u_{\sigma_1,\dots,\sigma_N,\pm}(\lambda,n,t) = P_{\sigma_1,\dots,\sigma_N}(t)u_{\sigma_1,\dots,\sigma_N,\pm}(\lambda,n,t), \tag{7.26}$$

where $P_{\sigma_1,\dots,\sigma_N}(t)$ is defined as in (7.18) with $a$ replaced by $a_{\sigma_1,\dots,\sigma_N}$. We also have (cf. (3.11), (3.12))

$$\rho_{o,\sigma_1,\dots,\sigma_N}(n,t) = -\sqrt{-a(n,t)\frac{C_{n+2}(u^1_{\sigma_1},\dots,u^{N-1}_{\sigma_{N-1}})C_n(u^1_{\sigma_1},\dots,u^N_{\sigma_N})}{C_{n+1}(u^1_{\sigma_1},\dots,u^{N-1}_{\sigma_{N-1}})C_{n+1}(u^1_{\sigma_1},\dots,u^N_{\sigma_N})}}, \tag{7.27}$$

$$\rho_{e,\sigma_1,\dots,\sigma_N}(n,t) = \sqrt{-a(n+N-1,t)\frac{C_n(u^1_{\sigma_1},\dots,u^{N-1}_{\sigma_{N-1}})C_{n+1}(u^1_{\sigma_1},\dots,u^N_{\sigma_N})}{C_{n+1}(u^1_{\sigma_1},\dots,u^{N-1}_{\sigma_{N-1}})C_n(u^1_{\sigma_1},\dots,u^N_{\sigma_N})}}. \tag{7.28}$$

Finally, the sequences $a_{\sigma_1,\dots,\sigma_N}(n,t)$, $b_{\sigma_1,\dots,\sigma_N}(n,t)$ fulfill the Toda lattice equations (7.19) and the sequence

$$\rho_{\sigma_1,\dots,\sigma_N}(n,t) = \left\{ \begin{array}{ll} \rho_{e,\sigma_1,\dots,\sigma_N}(m,t), & n = 2m \\ \rho_{o,\sigma_1,\dots,\sigma_N}(m,t), & n = 2m+1 \end{array} \right., \tag{7.29}$$

fulfills the Kac–van Moerbeke lattice equation

$$\frac{d}{dt}\rho(n,t) = \rho(n,t)\Big(\rho(n+1,t)^2 - \rho(n-1,t)^2\Big). \tag{7.30}$$

At the end we derive the $N$-soliton solutions relative to an arbitrary Toda background solution $(a(t), b(t))$ using the double commutation method.

Denote by $\psi(\lambda,n,t)$ the solutions of $\tau(t)\psi = \lambda\psi$ which are square summable near $-\infty$ and satisfy

$$\frac{d}{dt}\psi(\lambda,n,t) = P(t)\psi(\lambda,n,t). \tag{7.31}$$

As in Theorem 6.1 we define the following matrices

$$C^N(n,t) = \left\{ \delta_r(s) + \sqrt{\gamma_r \gamma_s} \sum_{m=M_-}^{n} \psi(\lambda_r, m, t)\psi(\lambda_s, m, t) \right\}_{1 \le r,s \le N}, \tag{7.32}$$

$$\Psi^N(\lambda_j, n, t) = \left\{ \begin{array}{cc} C^N(n,t)_{r,s} & {\scriptstyle r,s\le N} \\ \sqrt{\gamma_s} \sum\limits_{m=M_-}^{n} \psi(\lambda_j, m, t)\psi(\lambda_s, m, t) & {\scriptstyle s\le \ell, r=N+1} \\ \sqrt{\gamma_r}\psi(\lambda_r, n, t) & {\scriptstyle r\le \ell, s=N+1} \\ \psi(\lambda_j, n, t) & {\scriptstyle r=s=N+1} \end{array} \right\}_{1 \le r,s \le N+1}. \tag{7.33}$$

Then the sequences

$$a_{\gamma_1,\dots,\gamma_N}(n,t) = a(n,t) \frac{\sqrt{\det C^N(n-1,t) \det C^N(n+1,t)}}{\det C^N(n,t)}, \tag{7.34}$$

$$b_{\gamma_1,\dots,\gamma_N}(n,t) = b(n,t) - \frac{1}{2} \frac{d}{dt} \ln \frac{\det C^N(n,t)}{\det C^N(n-1,t)}. \tag{7.35}$$

satisfy the Toda lattice equations (7.19). Moreover,

$$\psi_{\gamma_1,\dots,\gamma_N}(\lambda_j, n, t) = \frac{\det \Psi^N(\lambda_j, n, t)}{\sqrt{\det C^N(n-1,t) \det C^N(n,t)}} \tag{7.36}$$

satisfies

$$\frac{d}{dt} \psi_{\gamma_1,\dots,\gamma_N}(\lambda_j, n, t) = P_{\gamma_1,\dots,\gamma_N}(t) \psi_{\gamma_1,\dots,\gamma_N}(\lambda_j, n, t), \tag{7.37}$$

where again $P_{\gamma_1,\dots,\gamma_N}(t)$ is defined as in (7.18) with $a$ replaced by $a_{\gamma_1,\dots,\gamma_N}$.

## 8. Appendices

Appendix A lists some formulas for Jacobi operators which are used in Sections 2 and 3. Appendices B–D contain some facts about Weyl–Titchmarsh theory for Jacobi operators which are needed in Section 3. Finally Appendix D states a *l.p.* criterion which seems to be novel and of independent interest.

Appendices B–D generalize some well-known facts about Sturm–Liouville operators (to be found, e.g., in [11],[28],[49],[54]) to Jacobi operators. The following material is essentially taken from [1],[3],[5],[8].

## Appendix A. General Background

Assume (H.4.2) and define the Jacobi difference expression

$$(\tau f)(n) = a(n) f(n+1) + a(n-1) f(n-1) - b(n) f(n). \tag{A.1}$$

A simple calculation yields Green's formula for $f, g \in \ell(\mathbb{Z})$

$$\sum_{j=m}^{n} \Big( f(\tau g) - g \tau f \Big)(j) = W_n(f,g) - W_{m-1}(f,g), \tag{A.2}$$

where we have introduced the modified Wronskian

$$W_n(f,g) = a(n) \Big( f(n) g(n+1) - f(n+1) g(n) \Big), \ n \in \mathbb{Z}. \tag{A.3}$$

The main object of our interest will be the equation

$$\tau u = z\, u, \qquad u \in \ell(\mathbb{Z}), \ z \in \mathbb{C}. \tag{A.4}$$

A glance at (A.2) shows that the modified Wronskian of two solutions is constant and nonzero if and only if they are linearly independent. If we choose $f = u(z)$, $g = \overline{u(z)}$ in (A.2), where $u(z)$ is a solution of (A.4) with $z \in \mathbb{C}\backslash\mathbb{R}$, we obtain

$$[u(z)]_n = [u(z)]_{m-1} - \sum_{j=m}^{n} |u(z,j)|^2, \tag{A.5}$$

where $[.]_n$ denotes the Weyl bracket

$$[u(z)]_n = \frac{W_n(u(z), \overline{u(z)})}{2\,\mathrm{i}\,\mathrm{Im}(z)} = a(n)\frac{\mathrm{Im}(u(z,n)\overline{u(z,n+1)})}{\mathrm{Im}(z)}, \quad n \in \mathbb{Z}. \tag{A.6}$$

Taking limits in (A.2) shows that $W_{\pm\infty}(f,g) = \lim_{n\to\pm\infty} W_n(f,g)$ exists if $f, g, \tau f$, and $\tau g$ are square summable near $\pm\infty$.

## Appendix B. Weyl $m$-functions

Let $\theta_\alpha(z,.), \phi_\alpha(z,.)$ be the fundamental system of (A.4) corresponding to the initial conditions

$$\begin{aligned} \phi_\alpha(z,0) &= -\sin(\alpha), & \phi_\alpha(z,1) &= \cos(\alpha), \\ \theta_\alpha(z,0) &= \frac{\cos(\alpha)}{a(0)}, & \theta_\alpha(z,1) &= \frac{\sin(\alpha)}{a(0)} \end{aligned} \tag{B.1}$$

such that

$$W(\theta_\alpha(z), \phi_\alpha(z)) = 1. \tag{B.2}$$

Next pick $\lambda_1 \in \mathbb{R}$ and define the following rational function with respect to $z$,

$$m_N(z,\alpha) = \frac{W_N(\phi_\alpha(\lambda_1), \theta_\alpha(z))}{W_N(\phi_\alpha(\lambda_1), \phi_\alpha(z))}, \qquad N \in \mathbb{Z}\backslash\{0\}, \tag{B.3}$$

which has poles at the zeros $\lambda_j(N) \in \mathbb{R}$, $\lambda_1(N) \equiv \lambda_1$ of $W_N(\phi_\alpha(\lambda_1), \phi_\alpha(.)) = 0$. The fact that one can rewrite $m_N(z,\alpha)$ with $\lambda_1$ replaced by $\lambda_j(N)$ together with

$$\lim_{z\to\lambda_j(N)} W_N(\phi_\alpha(\lambda_j(N)), \theta_\alpha(z)) \;=\; -1, \tag{B.4}$$

$$\lim_{z\to\lambda_j(N)} \frac{W_N(\phi_\alpha(\lambda_j(N)), \phi_\alpha(z))}{z - \lambda_j(N)} \;=\; W_N(\phi_\alpha(\lambda_j(N)), \frac{d}{dz}\phi_\alpha(\lambda_j(N))) \tag{B.5}$$

imply that all poles of $m_N(z,\alpha)$ are simple. Using (A.2) to evaluate (B.5) one infers that $\mp 1$ times the residue at $\lambda_j(N)$ is given by

$$\gamma_j(\alpha,N) = \Big( \sum_{n=\substack{1 \\ N+1}}^{\substack{N \\ 0}} \phi_\alpha(\lambda_j(N),n)^2 \Big)^{-1}, \quad N \gtrless 0. \tag{B.6}$$

The $\gamma_j(\alpha,N)$ are called norming constants. Hence one gets

$$m_N(z,\alpha) = \sum_j \frac{\mp\gamma_j(\alpha,N)}{z - \lambda_j(N)} + \begin{cases} \frac{\pm\tan(\alpha)^{\pm 1}}{a(0)}, \ \alpha \in \substack{[0,\pi) \\ (0,\pi]} \\ \frac{\pm z - b(\substack{1 \\ 0})}{a(0)^2}, \ \alpha = \substack{\pi \\ 0} \end{cases}, \quad N \gtrless 0. \tag{B.7}$$

(We note that $\lambda_j(N)$ depend on $\alpha$ for $j > 1$.) Furthermore, the function

$$u_N(z,n) = \theta_\alpha(z,n) - m_N(z,\alpha)\phi_\alpha(z,n) \tag{B.8}$$

satisfies

$$\sum_{n=\substack{1 \\ N+1}}^{\substack{N \\ 0}} |u_N(z,n)|^2 = \pm\frac{\mathrm{Im}(m_N(z,\alpha))}{\mathrm{Im}(z)}, \quad N \gtrless 0, \tag{B.9}$$

i.e., $\pm m_N(z,\alpha)$ are Herglotz functions for $N \gtrless 0$.

Next we want to investigate the limits $N \to \pm\infty$. Fix $z \in \mathbb{C}\backslash\mathbb{R}$. Then, as in the Sturm-Liouville case, the function $m_N(z,\alpha)$ (for different values of $\lambda_1 \in \mathbb{R}$) lies on a circle given by

$$\{m \in \mathbb{C} | [\theta_\alpha(z) - m\phi_\alpha(z)]_N = 0\}. \tag{B.10}$$

Since $[.]_N$ is decreasing in $N$ for $N > 0$, the circle corresponding to $N+1$ lies inside the circle corresponding to $N$. Similarly for $N < 0$. Hence these circles either tend to a limit point or a limit circle, depending on whether

$$\sum^{\pm\infty} |\phi_\alpha(z,n)|^2 = \infty, \quad \text{or} \quad \sum^{\pm\infty} |\phi_\alpha(z,n)|^2 < \infty. \tag{B.11}$$

Accordingly, one says that $\tau$ is limit point (*l.p.*) respectively limit circle (*l.c.*) at $\pm\infty$. One can show that this definition is independent of $z \in \mathbb{C}\backslash\mathbb{R}$. Thus the pointwise convergence of $m_N(z,\alpha)$ is clear in the *l.p.* case. In the *l.c.* case both Wronskians in (B.3) converge and we may set

$$\tilde{m}_\pm(z,\alpha) = \lim_{N\to\pm\infty} m_N(z,\alpha). \tag{B.12}$$

*Remark* B.1. (i). $\tilde{m}_\pm(z,0)$ are not the usual Weyl $m$-functions defined in the literature. For a connection with the standard Weyl $m$-functions $m_\pm(z)$ see (C.20), (C.21). We have chosen to introduce $\tilde{m}_\pm(z,\alpha)$ in order to simplify our notation in various places.
(ii). This explicit construction of converging sequences, even in the *l.c.* case, also works for Sturm-Liouville operators and seems to be novel to the best of our knowledge. Previously one usually proved the existence of such sequences using Helly's selection theorem (cf., e.g., [11]).

Moreover, the above sequences are locally bounded in $z$ (fix an $N$ 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 ([50], p. 168) they converge uniformly on every compact set in $\mathbb{C}_\pm = \{z \in \mathbb{C} | \pm\,\mathrm{Im}(z) > 0\}$, implying that $\pm\tilde{m}_\pm(z,\alpha)$ are again Herglotz functions.

Upon setting

$$u_\pm(z,n) = \theta_\alpha(z,n) - \tilde{m}_\pm(z,\alpha)\phi_\alpha(z,n) \tag{B.13}$$

we get a function which is square summable near $\pm\infty$

$$\sum_{n=\substack{1\\-\infty}}^{\substack{\infty\\0}} |u_\pm(z,n)|^2 = \pm\frac{\mathrm{Im}(\tilde{m}_\pm(z,\alpha))}{\mathrm{Im}(z)}. \tag{B.14}$$

In addition,

$$W_{\pm\infty}(\phi_\alpha(\lambda_1), u_\pm(z)) = 0, \tag{B.15}$$

if $\tau$ is *l.c.* at $\pm\infty$. We remark that (independently of the *l.c.* and *l.p.* case at $\pm\infty$)

$$\tilde{m}_\pm(z) = \tilde{m}_\pm(z,0) = \frac{-u_\pm(z,1)}{a(0)u_\pm(z,0)} \tag{B.16}$$

and that $\tilde{m}_\pm(z,\alpha)$ can be expressed in terms of $\tilde{m}_\pm(z,\beta)$ (use that $u_\pm$ is unique up to a constant) by

$$\tilde{m}_\pm(z,\alpha) = \frac{1}{a(0)} \frac{a(0)\cos(\beta-\alpha)\tilde{m}_\pm(z,\beta) - \sin(\beta-\alpha)}{a(0)\sin(\beta-\alpha)\tilde{m}_\pm(z,\beta) + \cos(\beta-\alpha)}. \tag{B.17}$$

## Appendix C. Weyl–Titchmarsh Theory on $\mathbb{N}$

Let $H_+$ be a given self-adjoint operator associated with $\tau$ on $\mathbb{N}$ and a Dirichlet boundary condition at $n = 0$. Abbreviate $\phi(z,n) = \phi_0(z,n)$ and let $u_+(z,n)$, $z \in \mathbb{C}\backslash\sigma(H_+)$ be a solution of (A.4) which is square summable near $\infty$ and fulfills the boundary condition at $\infty$ (if any). The resolvent of $H_+$ then reads

$$((H_+ - z)^{-1} f)(n) = \sum_{m\in\mathbb{N}} G_+(z,m,n) f(m), \quad z \in \mathbb{C}\backslash\sigma(H_+), \tag{C.1}$$

where

$$G_+(z,m,n) = \frac{1}{W(\phi(z),u_+(z))} \left\{ \begin{array}{ll} \phi(z,n)u_+(z,m), & m \geq n \\ \phi(z,m)u_+(z,n), & m \leq n \end{array} \right. . \tag{C.2}$$

Since $\phi(z,n)$ is a polynomial in $z$ we infer by induction

$$\phi(H_+,n)\delta_1 = \delta_n, \qquad \delta_n(k) = \left\{ \begin{array}{ll} 1, & k=n \\ 0, & k \neq n \end{array} \right. , \tag{C.3}$$

implying that $\delta_1$ is a cyclic vector for $H_+$. If $E_+(.)$ denotes the family of spectral projections corresponding to $H_+$ we introduce the measure

$$d\rho_+(.) = d\langle \delta_1, E_+(.)\delta_1\rangle. \tag{C.4}$$

Equation (C.3) now shows that the polynomials $\phi(z,n)$, $n \in \mathbb{N}$ are orthogonal with respect to this measure, i.e.,

$$\langle \phi(j),\phi(k)\rangle = \int_{-\infty}^{\infty} \phi(\lambda,j)\phi(\lambda,k)\, d\rho_+(\lambda) = \delta_j(k), \tag{C.5}$$

implying

$$a(n) = \langle \phi(n+1), \lambda\phi(n)\rangle, \quad b(n) = -\langle \phi(n), \lambda\phi(n)\rangle, \;\; n \in \mathbb{N}. \tag{C.6}$$

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

$$(Uf)(\lambda) \;=\; \sum_{n=1}^{\infty} f(n)\phi(\lambda,n), \tag{C.7}$$

$$(U^{-1}F)(n) \;=\; \int_{\mathbb{R}} \phi(\lambda,n)F(\lambda)d\rho_+(\lambda). \tag{C.8}$$

A simple calculation for $F(\lambda) = (Uf)(\lambda)$ shows that

$$\sum_{n=1}^{\infty} |f(n)|^2 = \int_{\mathbb{R}} |F(\lambda)|^2 d\rho_+(\lambda). \tag{C.9}$$

Thus $U$ extends to a unitary transformation

$$\tilde{U} : \ell^2(\mathbb{N}) \to L^2(\mathbb{R}, d\rho_+) \tag{C.10}$$

(since the set of polynomials is dense in $L^2(\mathbb{R}, d\rho_+)$, [5], Theorem VII.1.7) which maps the operator $H_+$ to the multiplication operator by $\lambda$,

$$\tilde{U} H_+ \tilde{U}^{-1} = \tilde{H}, \tag{C.11}$$

where

$$\tilde{H}F(\lambda) = \lambda F(\lambda), \quad \mathfrak{D}(\tilde{H}) = \{F \in L^2(\mathbb{R}, d\rho_+) | \lambda F(\lambda) \in L^2(\mathbb{R}, d\rho_+)\}. \tag{C.12}$$

This is easily verified for $f \in \ell_0(\mathbb{N})$. If $\tau$ is *l.p.* at $\infty$ note that $\ell_0(\mathbb{N})$ is a core for $H_+$ and if $\tau$ is *l.c.* at $\infty$ note that $d\rho_+$ is a pure point measure and that eigenfunctions are mapped onto eigenfunctions (all finite linear combinations of eigenfunctions form again a core).

This implies that the spectrum of $H_+$ can be characterized as follows. Let the Lebesgue decomposition of $d\rho_+$ be given by

$$d\rho_+ = d\rho_{+,p} + d\rho_{+,ac} + d\rho_{+,sc}, \tag{C.13}$$

then we have ($\rho_+(\lambda) = \int_{(-\infty,\lambda]} d\rho_+$)

$$\sigma(H_+) \;=\; \{\lambda \in \mathbb{R} | \lambda \text{ is a growth point of } \rho_+\}, \tag{C.14}$$

$$\sigma_p(H_+) \;=\; \{\lambda \in \mathbb{R} | \lambda \text{ is a growth point of } \rho_{+,p}\}, \tag{C.15}$$

$$\sigma_{ac}(H_+) \;=\; \{\lambda \in \mathbb{R} | \lambda \text{ is a growth point of } \rho_{+,ac}\}, \tag{C.16}$$

$$\sigma_{sc}(H_+) \;=\; \{\lambda \in \mathbb{R} | \lambda \text{ is a growth point of } \rho_{+,sc}\}. \tag{C.17}$$

The Stieltjes transform of the spectral function $\rho_+$ is called the Weyl $m$-function

$$m_+(z) = \int_{\mathbb{R}} \frac{d\rho_+(\lambda)}{\lambda - z}, \qquad z \in \mathbb{C}\backslash\mathbb{R}. \tag{C.18}$$

Conversely, the spectral function $\rho_+$ can be recovered from $m_+(z)$ by the Stieltjes inversion formula

$$\rho_+(\lambda) = \frac{1}{\pi} \lim_{\delta\downarrow 0} \lim_{\varepsilon\downarrow 0} \int_{-\infty}^{\lambda+\delta} \mathrm{Im}(m_+(\nu + \mathrm{i}\,\varepsilon)) d\nu. \tag{C.19}$$

We have normalized $\rho_+$ such that it is right continuous and satisfies $\lim_{\lambda\to-\infty} \rho_+(\lambda) = 0$. One infers

$$m_+(z) = G_+(z,1,1) = \frac{-u_+(1)}{a(0)u_+(0)} = \tilde{m}_+(z), \tag{C.20}$$

and we remark that the local compact convergence of $m_N(z,0)$ to $\tilde{m}_+(z) = m_+(z)$ implies the convergence of the associated spectral functions at every point of continuity ([2], p. 332). The second Weyl $m$-function is usually defined as

$$m_-(z) = G_-(z,-1,-1) = \frac{-u_-(-1)}{a(-1)u_-(0)} = -\frac{z + b(0) + a(0)^2\tilde{m}_-(z)}{a(-1)^2}. \tag{C.21}$$

$m_\pm(z)$, like $\pm\tilde{m}_\pm(z)$, are Herglotz functions.

## Appendix D. Weyl–Titchmarsh Theory on $\mathbb{Z}$

In Appendix C we have dealt with the half-line $\mathbb{N}$. In this appendix we extend these results to all of $\mathbb{Z}$.

Let $H$ be a given self-adjoint operator associated with $\tau$. Let $u_\pm(z,n)$ be a solution of (A.4) which is square summable near $\pm\infty$ (provided such a solution exists) and fulfills the boundary condition at $\pm\infty$ if any. The resolvent of $H$ then reads

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

where

$$G(z,m,n) = \frac{1}{W(u_-(z),u_+(z))} \left\{ \begin{array}{ll} u_-(z,n)u_+(z,m), & m \geq n \\ u_-(z,m)u_+(z,n), & m \leq n \end{array} \right. . \tag{D.2}$$

Consider the vector-valued polynomials

$$\underline{\phi}(z,n) = \Big(\phi_1(z,n), \phi_2(z,n)\Big), \tag{D.3}$$

where $\phi_{1,2}(z,n)$ are solutions of (A.4) satisfying the initial conditions

$$\begin{array}{ll} \phi_1(z,0) = 0, & \phi_1(z,1) = 1, \\ \phi_2(z,0) = 1, & \phi_2(z,1) = 0. \end{array} \tag{D.4}$$

The analog of (C.3) reads

$$\phi_1(H,n)\delta_1 + \phi_2(H,n)\delta_0 = \delta_n. \tag{D.5}$$

This is obvious for $n = 0, 1$ and the rest follows from induction upon applying $H$ to (D.5). If $E(.)$ denotes the spectral resolution of the identity corresponding to $H$ we introduce the measures

$$d\rho_{j,k}(.) = d\langle \delta_j, E(.)\delta_k \rangle, \tag{D.6}$$

and the (hermitian) matrix-valued measure

$$d\rho = \left( \begin{array}{cc} d\rho_{1,1} & d\rho_{1,2} \\ d\rho_{2,1} & d\rho_{2,2} \end{array} \right). \tag{D.7}$$

By (D.5) the vector-valued polynomials are orthogonal with respect to $d\rho$

$$\begin{aligned} \langle \underline{\phi}(m), \underline{\phi}(n)\rangle &= \sum_{j,k=1}^{2} \int_{\mathbb{R}} \phi_j(\lambda, m)\ \phi_k(\lambda, n) d\rho_{j,k}(\lambda) \\ &\equiv \int_{\mathbb{R}} \underline{\phi}(\lambda, m) d\rho(\lambda)\ \underline{\phi}(\lambda, n) = \delta_n(m). \end{aligned} \tag{D.8}$$

The analogous formulas to (C.6) then read

$$a(n) = \langle \underline{\phi}(n+1), \lambda\underline{\phi}(n)\rangle, \quad b(n) = \langle \underline{\phi}(n), \lambda\underline{\phi}(n)\rangle, \ \ n \in \mathbb{Z}. \tag{D.9}$$

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

$$(Uf)(\lambda) = \sum_{n\in\mathbb{Z}} f(n)\underline{\phi}(\lambda, n), \tag{D.10}$$

$$(U^{-1}\underline{F})(n) = \int_{\mathbb{R}} \underline{\phi}(\lambda, n) d\rho(\lambda)\underline{F}(\lambda). \tag{D.11}$$

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

$$\sum_{n\in\mathbb{Z}} |f(n)|^2 = \int_{\mathbb{R}} \overline{\underline{F}(\lambda)} d\rho(z)\underline{F}(\lambda). \tag{D.12}$$

Thus $U$ extends to a unitary transformation

$$\tilde{U} : \ell^2(\mathbb{Z}) \to L^2(\mathbb{R}, d\rho) \tag{D.13}$$

which maps the operator $H$ to the multiplication operator by $\lambda$,

$$\tilde{U} H \tilde{U}^{-1} = \tilde{H}, \tag{D.14}$$

where

$$\tilde{H}\underline{F}(\lambda) = z\underline{F}(\lambda), \quad \mathfrak{D}(\tilde{H}) = \{\underline{F} \in L^2(\mathbb{R}, d\rho) | \lambda\underline{F}(\lambda) \in L^2(\mathbb{R}, d\rho)\}, \tag{D.15}$$

as in Appendix B.

In order to characterize the spectrum of $H$ one only needs to consider the trace $d\rho^t$ of $d\rho$

$$d\rho^t = d\rho_{1,1} + d\rho_{2,2}. \tag{D.16}$$

Let the Lebesgue decomposition of $d\rho^t$ be given by

$$d\rho^t = d\rho^t_p + d\rho^t_{ac} + d\rho^t_{sc}, \tag{D.17}$$

then we have ($\rho^t(\lambda) = \int_{(-\infty,\lambda]} d\rho^t$, etc.)

$$\sigma(H) = \{\lambda \in \mathbb{R} | \lambda \text{ is a growth point of } \rho^t\}, \tag{D.18}$$

$$\sigma_p(H) = \{\lambda \in \mathbb{R} | \lambda \text{ is a growth point of } \rho^t_p\}, \tag{D.19}$$

$$\sigma_{ac}(H) = \{\lambda \in \mathbb{R} | \lambda \text{ is a growth point of } \rho^t_{ac}\}, \tag{D.20}$$

$$\sigma_{sc}(H) = \{\lambda \in \mathbb{R} | \lambda \text{ is a growth point of } \rho^t_{sc}\}. \tag{D.21}$$

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

$$M(z) = \int_{-\infty}^{\infty} \frac{d\rho(\lambda)}{\lambda - z}, \qquad z \in \mathbb{C}\backslash\mathbb{R}. \tag{D.22}$$

Explicit evaluation yields

$$\begin{aligned} M(z) &= \begin{pmatrix} G(z,0,0) & G(z,1,0) \\ G(z,0,1) & G(z,1,1) \end{pmatrix} \\ &= \frac{a(0)^{-2}}{\tilde{m}_-(z) - \tilde{m}_+(z)} \begin{pmatrix} 1 & -a(0)\tilde{m}_+(z) \\ -a(0)\tilde{m}_+(z) & a(0)^2\tilde{m}_+(z)\tilde{m}_-(z) \end{pmatrix}. \end{aligned} \tag{D.23}$$

Finally, assuming $\rho$ to be right continuous and normalizing $\rho(-\infty)=0$ one obtains

$$\rho_{j,k}(\lambda)=\frac{1}{\pi}\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\int_{-\infty}^{\lambda+\delta}\mathrm{Im}(M_{j,k}(\nu+\mathrm{i}\,\varepsilon))d\nu,\quad 1\le j,k\le 2. \tag{D.24}$$

## Appendix E. A limit point criterion

**Lemma E.1.** *Let $w$, $a$, $b$ be real–valued sequences, $w>0$, $a<0$. Define*

$$(\tau u)(n)=\frac{1}{w(n)}\Big(a(n)u(n+1)+a(n-1)u(n-1)-b(n)u(n)\Big) \tag{E.1}$$

*and suppose that $\tau$ is bounded from below. Then $\tau$ is in the l.p. case at $\infty$ if $\sum^{\infty}|w(n)/a(n)|^{1/2}=\infty$.*

*Proof.* Since $\tau$ is bounded from below, there exists a principal solution $u_+>0$ of $\tau u=\lambda u$ near $\infty$ for $\lambda\in\mathbb{R}$ sufficiently small. (See, e.g. [33], [44] for the definition and basic properties of (non)principal solutions associated with $\tau$.) Then $\hat{u}_+$ defined by

$$\hat{u}_+(n)=u_+(n)\sum^{n}\frac{1}{a(m)u_+(m)u_+(m+1)} \tag{E.2}$$

is nonprincipal near $\infty$, i.e.,

$$\sum^{\infty}\frac{1}{a(m)\hat{u}_+(m)\hat{u}_+(m+1)}<\infty. \tag{E.3}$$

Now suppose that $\tau$ is l.c. at $\infty$ which implies

$$\sum^{\infty}w(m)\big|\hat{u}_+(m)\big|^2<\infty. \tag{E.4}$$

Then Cauchy's inequality yields the contradiction

$$\begin{aligned}\infty=\sum^{\infty}|w(n)/a(n)|^{1/2} &=\\ \sum^{\infty}|(w(m)\hat{u}_+(m)\hat{u}_+(m+1))/(a(m)\hat{u}_+(m)\hat{u}_+(m+1))|^{1/2} &\le\\ \left|\sum^{\infty}w(m)|\hat{u}_+(m)|^2\right|^{1/2}\left|\sum^{\infty}|a(m)\hat{u}_+(m)\hat{u}_+(m+1)|^{-1}\right|^{1/2} &< \infty.\end{aligned} \tag{E.5}$$

□

For further *l.p.* criteria we refer the reader, e.g., to [1], [36].

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Department of Mathematics, University of Missouri, Columbia, MO 65211, USA
*E-mail address*: fritz@math.missouri.edu

Department of Mathematics, University of Missouri, Columbia, MO 65211, USA and Department of Theoretical Physics, Technical University of Graz, A-8010 Graz, Austria
*Current address*: Institut für Mathematik, Strudlhofgasse 4, 1090 Wien, Austria
*E-mail address*: Gerald.Teschl@univie.ac.at
*URL*: http://www.mat.univie.ac.at/~gerald/