TOPICS IN SPECTRAL AND INVERSE SPECTRAL THEORY

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The undersigned, appointed by the Dean of the Graduate School, have examined the dissertation entitled.

TOPICS IN SPECTRAL AND INVERSE SPECTRAL THEORY

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A candidate for the degree of Doctor of Philosophy

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ABSTRACT

This dissertation is concerned with two major classes of operators and provides various spectral and inverse spectral results for them.

In the first part of this work a special class of one-dimensional discrete unitary operators is under investigation. The underlying Weyl–Titchmarsh theory and a Borg-type inverse spectral result are established for this class of operators.

The second part of this work is devoted to some spectral theoretical questions for one- and multi-dimensional Schrödinger operators. In particular, the Weyl–Titchmarsh theory for one-dimensional self-adjoint Schrödinger operators with strongly singular potentials is established. In addition, a general perturbation theory for non-self-adjoint operators is developed and subsequently applied to a large class of non-self-adjoint multi-dimensional Schrödinger operators.

Introduction

In this dissertation we investigate various spectral and inverse spectral questions related to the following classes of operators: a special class of unitary operators associated with orthogonal polynomials on the unit circle, a class of one-dimensional self-adjoint Schrödinger operators with strongly singular potentials, and a class of factorable non-self-adjoint perturbations which includes multi-dimensional Schrödinger operators with complex-valued potentials.

The material in this work is split into four chapters, each containing a thorough investigation of a separate topic.

Chapter 1 is devoted to the study of Weyl–Titchmarsh theory relevant to a special class of unitary semi- and doubly infinite five-diagonal matrices (CMV), which, from the spectral theoretic point of view, are the most natural unitary analogs of semi- and doubly infinite self-adjoint Jacobi matrices. Chapter 1 contains numerous results on full- and half-lattice CMV operators which include relations between such objects as orthogonal polynomials on the unit circle, finite measures on the unit circle, spectral functions, spectral measures, resolvents, and Green's functions of CMV operators, generalized eigenfunctions, transfer matrices, associated Weyl–Titchmarsh

m-functions, Weyl disks, Verblunsky coefficients, etc.

In Chapter 2, we study an inverse spectral problem associated with CMV operators and proved a general Borg-type result for full-lattice unitary CMV operators with reflectionless coefficients (a natural extension of periodic coefficients). This result allows one to reconstruct a CMV operator from the end points of its spectrum in the case of a one-arc spectrum and the reflectionless assumption on the coefficients. In Chapter 2, we also derive exponential Herglotz representations of Caratheodory functions and an infinite sequence of trace formulas, which become corner stones in the proof of our Borg-type theorem. In addition, we prove a unitary invariance lemma for a certain class of transformations which shows that our result is sharp in the sense that one cannot obtain any additional information on the coefficients under the given assumptions.

Chapter 3 is dedicated to the study of spectral theory of one-dimensional Schrödinger operators with strongly singular potentials. In this chapter we examine two kinds of spectral theoretic situations: First, we recall the case of self-adjoint half-line Schrödinger operators on $[a,\infty)$, $a \in \mathbb{R}$, with a regular finite end point a and the case of Schrödinger operators on the real line with locally integrable potentials, which naturally lead to Herglotz functions and 2×2 matrix-valued Herglotz functions representing the associated Weyl–Titchmarsh coefficients. Second, we contrast this with the case of self-adjoint half-line Schrödinger operators on (a,∞) with a potential strongly singular at the end point a. We focus on situations where the potential is "so singular" that the associated maximally defined Schrödinger operator is self-adjoint (equivalently, the associated minimally defined Schrödinger operator is essentially self-adjoint), and hence no boundary condition is required at the finite end point a. We show that the Weyl–Titchmarsh coefficient in this strongly singular context still determines the associated spectral function, but ceases to posses the Herglotz property. However, we show that Herglotz function techniques still continue to play a decisive role in the spectral theory for strongly singular Schrödinger operators.

In Chapter 4, we investigate various spectral theoretic aspects of perturbed non-self-adjoint operators. Specifically, we consider a class of factorizable non-self-adjoint perturbations of a given unperturbed non-self-adjoint operator and provide an indepth study of a variant of the Birman–Schwinger principle as well as local and global Weinstein–Aronszajn formulas (following results of Howland [96]). In addition, we provide two concrete applications of the abstract perturbation results. First, we obtain a certain generalization of the celebrated Jost and Pais formula (see [104], [74], [142], [165, Proposition 5.7]) for Schrödinger operators with complex-valued potentials in dimensions two and three. Our formula allows a reduction of appropriate ratios of Fredholm determinants associated with operators in $L^2(\Omega; d^n x)$ to a Fredholm determinant associated with an operator in $L^2(\partial\Omega; d^{n-1}\sigma)$. Second, we provide a new proof of the formula connecting the scattering operator $S(\lambda)$ in $L^2(S^{n-1}; d^{n-1}\sigma)$, related to the pair of Schrödinger operators $H_0 = \Delta$ and $H = H_0 + V$ in $L^2(\mathbb{R}^n; d^n x)$, $n = 2, 3$, with a ratio of modified perturbation determinants.

Finally, Appendix A summarizes basic facts on Caratheodory and Schur functions relevant to Chapters 1 and 2, Appendix B provides basic facts on Herglotz functions used in Chapter 3, and Appendix C gives some properties of the Dirichlet and Neumann Laplacians considered in Chapter 4.

The material of each of these four chapters (together with the corresponding appendices) has been accepted for publication as follows: Chapter 1 is based on [79], Chapter 2 is based on [80], Chapter 3 is based on [81], and Chapter 4 is based on [72].

Chapter 1

Weyl–Titchmarsh Theory for CMV Operators Associated with Orthogonal Polynomials on the Unit Circle

1.1 Introduction

The aim of this chapter is to develop Weyl–Titchmarsh theory for a special class of unitary doubly infinite five-diagonal matrices. The corresponding unitary semi-infinite five-diagonal matrices were recently introduced by Cantero, Moral, and Velázquez (CMV) [28] in 2003. In [171, Sects. 4.5, 10.5], Simon introduced the corresponding notion of unitary doubly infinite five-diagonal matrices and coined the term "extended" CMV matrices. To simplify notations we will often just speak of CMV operators whether or not they are half-lattice or full-lattice operators indexed by $\mathbb{N}$ or $\mathbb{Z}$, respectively.

CMV operators on $\mathbb{Z}$ are intimately related to a completely integrable version of the defocusing nonlinear Schrödinger equation (continuous in time but discrete in space), a special case of the Ablowitz–Ladik system. Relevant references in this context are, for instance, [1], [2], [60], [68], [132], [138], [139], and the literature cited therein. A recent application to a Borg-type theorem (an inverse spectral result), which motivated us to develop Weyl–Titchmarsh theory, is discussed in Chapter 2. For more details we refer to Chapter 2 and, in particular, to Theorem 2.1.1.

We denote by $\mathbb{D}$ the open unit disk in $\mathbb{C}$ and let α be a sequence of complex numbers in $\mathbb{D}$, $\alpha = \{\alpha_k\}_{k\in\mathbb{Z}} \subset \mathbb{D}$. The unitary CMV operator U on $\ell^2(\mathbb{Z})$ then can be written as a special five-diagonal doubly infinite matrix in the standard basis of $\ell^2(\mathbb{Z})$ according to [171, Sects. 4.5, 10.5]) as

$$U = \begin{pmatrix} \ddots & \ddots & \ddots & \ddots & \ddots & & & & \\ & 0 & -\alpha_0\rho_{-1} & -\overline{\alpha_{-1}}\alpha_0 & -\alpha_1\rho_0 & \rho_0\rho_1 & & \text{\huge 0} & \\ & & \rho_{-1}\rho_0 & \overline{\alpha_{-1}}\rho_0 & -\overline{\alpha_0}\alpha_1 & \overline{\alpha_0}\rho_1 & 0 & & \\ & & & 0 & -\alpha_2\rho_1 & -\overline{\alpha_1}\alpha_2 & -\alpha_3\rho_2 & \rho_2\rho_3 & \\ & \text{\huge 0} & & & \rho_1\rho_2 & \overline{\alpha_1}\rho_2 & -\overline{\alpha_2}\alpha_3 & \overline{\alpha_2}\rho_3 & 0 \\ & & & & & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}. \tag{1.1.1}$$

Here the sequence of positive real numbers $\{\rho_k\}_{k\in\mathbb{Z}}$ is defined by

$$\rho_k = \sqrt{1 - |\alpha_k|^2}, \quad k \in \mathbb{Z}, \tag{1.1.2}$$

and terms of the form $-\overline{\alpha_k}\alpha_{k+1}$, $k \in \mathbb{Z}$, represent the diagonal entries in the infinite matrix (1.1.1), specifically, $-\overline{\alpha_k}\alpha_{k+1}$ is the (k,k) diagonal entry. For the corresponding half-lattice CMV operators $U_{+,k_0}^{(s)}$, $s \in [0, 2\pi)$ in $\ell^2([k_0,\infty)\cap\mathbb{Z})$ we refer to (1.2.29).

The relevance of this unitary operator U on $\ell^2(\mathbb{Z})$, more precisely, the relevance of the corresponding half-lattice CMV operator $U_{+,0}$ in $\ell^2(\mathbb{N}_0)$ (cf. (1.2.31)) is derived from its intimate relationship with the trigonometric moment problem and hence with finite measures on the unit circle $\partial\mathbb{D}$. (Here $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$.) Let $\{\alpha_k\}_{k\in\mathbb{N}} \subset \mathbb{D}$ and define the transfer matrix

$$S(\zeta,k)=\begin{pmatrix}\zeta & \alpha_k\\ \overline{\alpha_k}\zeta & 1\end{pmatrix},\quad \zeta\in\partial\mathbb{D},\ k\in\mathbb{N}, \tag{1.1.3}$$

with spectral parameter $\zeta\in\partial\mathbb{D}$. Consider the system of difference equations

$$\begin{pmatrix}\varphi_+(\zeta,k)\\ \varphi_+^*(\zeta,k)\end{pmatrix}=S(\zeta,k)\begin{pmatrix}\varphi_+(\zeta,k-1)\\ \varphi_+^*(\zeta,k-1)\end{pmatrix},\quad \zeta\in\partial\mathbb{D},\ k\in\mathbb{N} \tag{1.1.4}$$

with initial condition

$$\begin{pmatrix}\varphi_+(\zeta,0)\\ \varphi_+^*(\zeta,0)\end{pmatrix}=\begin{pmatrix}1\\ 1\end{pmatrix},\quad \zeta\in\partial\mathbb{D}. \tag{1.1.5}$$

Then $\varphi_+(\,\cdot\,,k)$ are monic polynomials of degree k and

$$\varphi_+^*(\zeta,k)=\zeta^k\overline{\varphi_+(1/\overline{\zeta},k)},\quad \zeta\in\partial\mathbb{D},\ k\in\mathbb{N}_0, \tag{1.1.6}$$

the reversed *-polynomial of $\varphi_+(\cdot,k)$, is at most of degree k. These polynomials were first introduced by Szegő in the 1920's in his work on the asymptotic distribution of eigenvalues of sections of Toeplitz forms [177], [178] (see also [92, Chs. 1–4], [179, Ch. XI]). Szegő's point of departure was the trigonometric moment problem and hence the theory of orthogonal polynomials on the unit circle: Given a probability measure $d\sigma_+$ supported on an infinite set on the unit circle, find monic polynomials of degree k in $\zeta=e^{i\theta}$, $\theta\in[0,2\pi]$, such that

$$\int_0^{2\pi} d\sigma_+(e^{i\theta})\,\overline{\varphi_+(e^{i\theta},k)}\varphi_+(e^{i\theta},k')=\gamma_k^{-2}\delta_{k,k'},\quad k,k'\in\mathbb{N}_0, \tag{1.1.7}$$

where (cf. (1.1.2))

$$\gamma_k^2=\begin{cases}1, & k=0,\\ \prod_{j=1}^k\rho_j^{-2}, & k\in\mathbb{N}.\end{cases} \tag{1.1.8}$$

One then also infers

$$\int_0^{2\pi} d\sigma_+(e^{i\theta})\,\overline{\varphi_+^*(e^{i\theta},k)}\varphi_+^*(e^{i\theta},k') = \gamma_{k''}^{-2}, \quad k'' = \max\{k,k'\},\ k,k' \in \mathbb{N}_0 \tag{1.1.9}$$

and obtains that $\varphi_+(\cdot,k)$ is orthogonal to $\{\zeta^j\}_{j=0,\dots,k-1}$ in $L^2(\partial\mathbb{D};d\sigma_+)$ and $\varphi_+^*(\cdot,k)$ is orthogonal to $\{\zeta^j\}_{j=1,\dots,k}$ in $L^2(\partial\mathbb{D};d\sigma_+)$. Additional comments in this context will be provided in Remark 1.2.9. For a detailed account of the relationship of $U_{+,0}$ with orthogonal polynomials on the unit circle we refer to the monumental two-volume treatise by Simon [171] (see also [170] and [172] for a description of some of the principal results in [171]) and the exhaustive bibliography therein. For classical results on orthogonal polynomials on the unit circle we refer, for instance, to [4], [64]–[66], [92], [118], [177]–[179], [187]–[189]. More recent references relevant to the spectral theoretic content of this chapter are [61]–[63], [90], [126], [147], [169].

We note that $S(\zeta,k)$ in (1.1.3) is not the transfer matrix that leads to the half-lattice CMV operator $U_{+,0}$ in $\ell^2(\mathbb{N}_0)$ (cf. (1.2.29)). After a suitable change of basis introduced by Cantero, Moral, and Velázquez [28], the transfer matrix $S(\zeta,k)$ turns into $T(\zeta,k)$ as defined in (1.2.18).

In Section 1.2 we provide an extensive treatment of Weyl–Titchmarsh theory for half-lattice CMV operators U_{+,k_0} on $\ell([k_0,\infty)\cap\mathbb{Z})$ and discuss various systems of orthonormal Laurent polynomials on the unit circle, the half-lattice spectral function of U_{+,k_0}, variants of half-lattice Weyl–Titchmarsh functions, and the Green's function of U_{+,k_0}. In particular, we discuss the spectral representation of U_{+,k_0}. While many of these results can be found in Simon's two-volume treatise [171], we survey some of this material here from an operator theoretic point of view, starting directly from the

CMV operator. Section 1.3 then contains our new results on Weyl–Titchmarsh theory for full-lattice CMV operators U on $\ell^2(\mathbb{Z})$. Again we discuss systems of orthonormal Laurent polynomials on the unit circle, the 2×2 matrix-valued spectral and Weyl–Titchmarsh functions of U, its Green's matrix, and the spectral representation of U.

1.2 Weyl–Titchmarsh Theory for CMV Operators on Half-Lattices

In this section we describe the Weyl–Titchmarsh theory for CMV operators on half-lattices.

In the following, let $\ell^2(\mathbb{Z})$ be the usual Hilbert space of all square summable complex-valued sequences with scalar product $(\cdot,\cdot)$ linear in the second argument. The *standard basis* in $\ell^2(\mathbb{Z})$ is denoted by

$$\{\delta_k\}_{k\in\mathbb{Z}}, \quad \delta_k = (\dots,0,\dots,0,\underbrace{1}_{k},0,\dots,0,\dots)^\top,\ k \in \mathbb{Z}. \tag{1.2.1}$$

$\ell_0^\infty(\mathbb{Z})$ denotes the set of sequences of compact support (i.e., $f = \{f(k)\}_{k\in\mathbb{Z}} \in \ell_0^\infty(\mathbb{Z})$ if there exist $M(f), N(f) \in \mathbb{Z}$ such that $f(k) = 0$ for $k < M(f)$ and $k > N(f)$). We use the analogous notation for compactly supported sequences on half-lattices $[k_0, \pm\infty) \cap \mathbb{Z}$, $k_0 \in \mathbb{Z}$, and then write $\ell_0^\infty([k_0, \pm\infty) \cap \mathbb{Z})$, etc. For $J \subseteq \mathbb{R}$ an interval, we will identify $\ell^2(J \cap \mathbb{Z}) \oplus \ell^2(J \cap \mathbb{Z})$ and $\ell^2(J \cap \mathbb{Z}) \otimes \mathbb{C}^2$ and then use the simplified notation $\ell^2(J \cap \mathbb{Z})^2$. For simplicity, the identity operator on $\ell^2(J \cap \mathbb{Z})$ is abbreviated by I without separately indicating its dependence on J.

Moreover, we denote by $\mathbb{D} = \{z \in \mathbb{C} \,|\, |z| < 1\}$ the open unit disk in the complex plane $\mathbb{C}$, by $\partial\mathbb{D} = \{\zeta \in \mathbb{C} \,|\, |\zeta| = 1\}$ its counterclockwise oriented boundary, and we freely use the notation employed in Appendix A. By a *Laurent polynomial* we denote a finite linear combination of terms z^k, $k \in \mathbb{Z}$, with complex-valued coefficients.

Throughout this chapter we make the following basic assumption:

Hypothesis 1.2.1. Let α be a sequence of complex numbers such that

$$\alpha = \{\alpha_k\}_{k\in\mathbb{Z}} \subset \mathbb{D}. \tag{1.2.2}$$

Given a sequence α satisfying (1.2.2), we define the sequence of positive real numbers $\{\rho_k\}_{k\in\mathbb{Z}}$ and two sequences of complex numbers with positive real parts $\{a_k\}_{k\in\mathbb{Z}}$ and $\{b_k\}_{k\in\mathbb{Z}}$ by

$$\rho_k = \sqrt{1 - |\alpha_k|^2}, \quad k \in \mathbb{Z}, \tag{1.2.3}$$

$$a_k = 1 + \alpha_k, \quad k \in \mathbb{Z}, \tag{1.2.4}$$

$$b_k = 1 - \alpha_k, \quad k \in \mathbb{Z}. \tag{1.2.5}$$

Following Simon [171], we call α_k the Verblunsky coefficients in honor of Verblunsky's pioneering work in the theory of orthogonal polynomials on the unit circle [188], [189].

Next, we also introduce a sequence of 2×2 unitary matrices θ_k by

$$\theta_k = \begin{pmatrix} -\alpha_k & \rho_k \\ \rho_k & \overline{\alpha_k} \end{pmatrix}, \quad k \in \mathbb{Z}, \tag{1.2.6}$$

and two unitary operators V and W on $\ell^2(\mathbb{Z})$ by their matrix representations in the standard basis of $\ell^2(\mathbb{Z})$ as follows,

$$V = \begin{pmatrix} \ddots & & & \text{\Large 0} \\ & \theta_{2k-2} & & \\ & & \theta_{2k} & \\ \text{\Large 0} & & & \ddots \end{pmatrix}, \quad W = \begin{pmatrix} \ddots & & & \text{\Large 0} \\ & \theta_{2k-1} & & \\ & & \theta_{2k+1} & \\ \text{\Large 0} & & & \ddots \end{pmatrix}, \tag{1.2.7}$$

where

$$\begin{pmatrix} V_{2k-1,2k-1} & V_{2k-1,2k} \\ V_{2k,2k-1} & V_{2k,2k} \end{pmatrix} = \theta_{2k}, \quad \begin{pmatrix} W_{2k,2k} & W_{2k,2k+1} \\ W_{2k+1,2k} & W_{2k+1,2k+1} \end{pmatrix} = \theta_{2k+1}, \quad k \in \mathbb{Z}. \tag{1.2.8}$$

Moreover, we introduce the unitary operator U on $\ell^2(\mathbb{Z})$ by

$$U = VW, \tag{1.2.9}$$

or in matrix form, in the standard basis of $\ell^2(\mathbb{Z})$, by

$$U = \begin{pmatrix} \ddots & \ddots & \ddots & \ddots & \ddots & & & & \Large 0 \\ & 0 & -\alpha_0\rho_{-1} & -\overline{\alpha_{-1}}\alpha_0 & -\alpha_1\rho_0 & \rho_0\rho_1 & & & \\ & & \rho_{-1}\rho_0 & \overline{\alpha_{-1}}\rho_0 & -\overline{\alpha_0}\alpha_1 & \overline{\alpha_0}\rho_1 & 0 & & \\ & & & 0 & -\alpha_2\rho_1 & -\overline{\alpha_1}\alpha_2 & -\alpha_3\rho_2 & \rho_2\rho_3 & \\ & \Large 0 & & & \rho_1\rho_2 & \overline{\alpha_1}\rho_2 & -\overline{\alpha_2}\alpha_3 & \overline{\alpha_2}\rho_3 & 0 \\ & & & & & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}. \tag{1.2.10}$$

Here terms of the form $-\overline{\alpha_k}\alpha_{k+1}$, $k \in \mathbb{Z}$, represent the diagonal entries in the infinite matrix (1.2.10), specifically, $-\overline{\alpha_k}\alpha_{k+1}$ is the (k,k) diagonal entry. We will call the operator U on $\ell^2(\mathbb{Z})$ the CMV operator since (1.2.6)–(1.2.10) in the context of the semi-infinite (i.e., half-lattice) case were first obtained by Cantero, Moral, and Velázquez in [28].

Finally, let $\mathbb{U}$ denote the unitary operator on $\ell^2(\mathbb{Z})^2$ defined by

$$\mathbb{U} = \begin{pmatrix} U & 0 \\ 0 & U^\top \end{pmatrix} = \begin{pmatrix} VW & 0 \\ 0 & WV \end{pmatrix} = \begin{pmatrix} 0 & V \\ W & 0 \end{pmatrix}^2. \tag{1.2.11}$$

One observes remnants of a certain "supersymmetric" structure in $\left(\begin{smallmatrix} 0 & V \\ W & 0 \end{smallmatrix}\right)$ which is also reflected in the following result.

Lemma 1.2.2. *Let $z \in \mathbb{C}\backslash\{0\}$ and $\{u(z,k)\}_{k\in\mathbb{Z}}, \{v(z,k)\}_{k\in\mathbb{Z}}$ be sequences of complex functions. Then the following items (i)–(vi) are equivalent:*

$$(i) \quad Uu(z,\cdot) = zu(z,\cdot), \quad (Wu)(z,\cdot) = zv(z,\cdot). \tag{1.2.12}$$

$$(ii) \quad U^\top v(z,\cdot) = zv(z,\cdot), \quad (Vv)(z,\cdot) = u(z,\cdot). \tag{1.2.13}$$

$$(iii) \quad (Wu)(z,\cdot) = zv(z,\cdot), \quad (Vv)(z,\cdot) = u(z,\cdot). \tag{1.2.14}$$

$$(iv) \quad \mathbb{U}\begin{pmatrix} u(z,\cdot) \\ v(z,\cdot) \end{pmatrix} = z\begin{pmatrix} u(z,\cdot) \\ v(z,\cdot) \end{pmatrix}, \quad (Wu)(z,\cdot) = zv(z,\cdot). \tag{1.2.15}$$

$$(v) \quad \mathbb{U}\begin{pmatrix} u(z,\cdot) \\ v(z,\cdot) \end{pmatrix} = z\begin{pmatrix} u(z,\cdot) \\ v(z,\cdot) \end{pmatrix}. \quad (Vv)(z,\cdot) = u(z,\cdot). \tag{1.2.16}$$

$$(vi) \quad \begin{pmatrix} u(z,k) \\ v(z,k) \end{pmatrix} = T(z,k)\begin{pmatrix} u(z,k-1) \\ v(z,k-1) \end{pmatrix}, \quad k \in \mathbb{Z}, \tag{1.2.17}$$

where the transfer matrices $T(z,k)$, $z \in \mathbb{C}\backslash\{0\}$, $k \in \mathbb{Z}$, are given by

$$T(z,k) = \begin{cases} \frac{1}{\rho_k}\begin{pmatrix} \alpha_k & z \\ 1/z & \overline{\alpha_k} \end{pmatrix}, & k \text{ odd,} \\ \frac{1}{\rho_k}\begin{pmatrix} \overline{\alpha_k} & 1 \\ 1 & \alpha_k \end{pmatrix}, & k \text{ even.} \end{cases} \tag{1.2.18}$$

Proof. The equivalence of (1.2.12) and (1.2.14) follows from (1.2.9) after one defines $v(z,\cdot) = \frac{1}{z}(Wu)(z,\cdot)$. Since $\theta_k^\top = \theta_k$, one has $V^\top = V$, $W^\top = W$ and hence, $U^\top = (VW)^\top = WV$. Thus, defining $u(z,\cdot) = (Vv)(z,\cdot)$, one gets the equivalence of (1.2.13) and (1.2.14). The equivalence of (1.2.14), (1.2.15), and (1.2.16) follows immediately from (1.2.11).

Next, we will prove that (1.2.14) is equivalent to (1.2.17). Assuming k to be odd one obtains the equivalence of the following items (i)–(v):

$$(i) \quad \begin{pmatrix} u(z,k) \\ v(z,k) \end{pmatrix} = T(z,k)\begin{pmatrix} u(z,k-1) \\ v(z,k-1) \end{pmatrix}. \tag{1.2.19}$$

$$(ii) \quad \rho_k\begin{pmatrix} u(z,k) \\ v(z,k) \end{pmatrix} = \begin{pmatrix} \alpha_k & z \\ 1/z & \overline{\alpha_k} \end{pmatrix}\begin{pmatrix} u(z,k-1) \\ v(z,k-1) \end{pmatrix}. \tag{1.2.20}$$

$$(iii) \quad \begin{cases} zv(z,k-1) = -\alpha_k u(z,k-1) + \rho_k u(z,k), \\ z\rho_k v(z,k) = u(z,k-1) + \overline{\alpha_k} z v(z,k-1). \end{cases} \tag{1.2.21}$$

$$(iv) \quad \begin{cases} zv(z,k-1) = -\alpha_k u(z,k-1) + \rho_k u(z,k), \\ zv(z,k) = \rho_k u(z,k-1) + \overline{\alpha_k} u(z,k). \end{cases} \tag{1.2.22}$$

$$(v) \quad z\begin{pmatrix} v(z,k-1) \\ v(z,k) \end{pmatrix} = \theta_k \begin{pmatrix} u(z,k-1) \\ u(z,k) \end{pmatrix}. \tag{1.2.23}$$

If k is even, one similarly proves that the following items (vi)–$(viii)$ are equivalent:

$$(vi) \quad \begin{pmatrix} u(z,k) \\ v(z,k) \end{pmatrix} = T(z,k) \begin{pmatrix} u(z,k-1) \\ v(z,k-1) \end{pmatrix}. \tag{1.2.24}$$

$$(vii) \quad \rho_k \begin{pmatrix} v(z,k) \\ u(z,k) \end{pmatrix} = \begin{pmatrix} \alpha_k & 1 \\ 1 & \overline{\alpha_k} \end{pmatrix} \begin{pmatrix} v(z,k-1) \\ u(z,k-1) \end{pmatrix}. \tag{1.2.25}$$

$$(viii) \quad \begin{pmatrix} u(z,k-1) \\ u(z,k) \end{pmatrix} = \theta_k \begin{pmatrix} v(z,k-1) \\ v(z,k) \end{pmatrix}. \tag{1.2.26}$$

Thus, taking into account (1.2.7), one concludes that

$$\begin{cases} Wu(z,\cdot) = zv(z,\cdot), \\ Vv(z,\cdot) = u(z,\cdot) \end{cases} \tag{1.2.27}$$

is equivalent to

$$\begin{pmatrix} u(z,k) \\ v(z,k) \end{pmatrix} = T(z,k) \begin{pmatrix} u(z,k-1) \\ v(z,k-1) \end{pmatrix}, \quad k \in \mathbb{Z}. \tag{1.2.28}$$

□

We note that in studying solutions of $Uu(z,\cdot) = zu(z,\cdot)$ as in Lemma 1.2.2 (i), the purpose of the additional relation $(Wu)(z,\cdot) = zv(z,\cdot)$ in (1.2.12) is to introduce a new variable v that improves our understanding of the structure of such solutions u. An analogous comment applies to solutions of $U^\top v(z,\cdot) = zv(z,\cdot)$ and the relation $(Vv)(z,\cdot) = u(z,\cdot)$ in Lemma 1.2.2 (ii).

If one sets $\alpha_{k_0} = e^{is}$, $s \in [0, 2\pi)$, for some reference point $k_0 \in \mathbb{Z}$, then the operator U splits into a direct sum of two half-lattice operators $U_{-,k_0-1}^{(s)}$ and $U_{+,k_0}^{(s)}$ acting on $\ell^2((-\infty, k_0-1] \cap \mathbb{Z})$ and on $\ell^2([k_0, \infty) \cap \mathbb{Z})$, respectively. Explicitly, one obtains

$$\begin{aligned} &U = U_{-,k_0-1}^{(s)} \oplus U_{+,k_0}^{(s)} \ \text{ in } \ \ell^2((-\infty, k_0-1] \cap \mathbb{Z}) \oplus \ell^2([k_0, \infty) \cap \mathbb{Z}) \\ &\text{if } \ \alpha_{k_0} = e^{is}, \ s \in [0, 2\pi). \end{aligned} \tag{1.2.29}$$

(Strictly speaking, setting $\alpha_{k_0} = e^{is}$, $s \in [0, 2\pi)$, for some reference point $k_0 \in \mathbb{Z}$ contradicts our basic Hypothesis 1.2.1. However, as long as the exception to Hypothesis 1.2.1 refers to only one or two sites (cf. also (1.2.181)), we will safely ignore this inconsistency in favor of the notational simplicity it provides by avoiding the introduction of a properly modified hypothesis on $\{\alpha_k\}_{k\in\mathbb{Z}}$.) Similarly, one obtains $W_{-,k_0-1}^{(s)}$, $V_{-,k_0-1}^{(s)}$ and $W_{+,k_0}^{(s)}$, $V_{+,k_0}^{(s)}$ such that

$$U_{\pm,k_0}^{(s)} = V_{\pm,k_0}^{(s)} W_{\pm,k_0}^{(s)}. \tag{1.2.30}$$

For simplicity we will abbreviate

$$U_{\pm,k_0} = U_{\pm,k_0}^{(s=0)} = V_{\pm,k_0}^{(s=0)} W_{\pm,k_0}^{(s=0)} = V_{\pm,k_0} W_{\pm,k_0}. \tag{1.2.31}$$

In addition, we introduce on $\ell^2([k_0, \pm\infty) \cap \mathbb{Z})^2$ the half-lattice operators $\mathbb{U}_{\pm,k_0}^{(s)}$ by

$$\mathbb{U}_{\pm,k_0}^{(s)} = \begin{pmatrix} U_{\pm,k_0}^{(s)} & 0 \\ 0 & (U_{\pm,k_0}^{(s)})^\top \end{pmatrix} = \begin{pmatrix} V_{\pm,k_0}^{(s)} W_{\pm,k_0}^{(s)} & 0 \\ 0 & W_{\pm,k_0}^{(s)} V_{\pm,k_0}^{(s)} \end{pmatrix}. \tag{1.2.32}$$

By $\mathbb{U}_{\pm,k_0}$ we denote the half-lattice operators defined for $s = 0$,

$$\mathbb{U}_{\pm,k_0} = \mathbb{U}_{\pm,k_0}^{(s=0)} = \begin{pmatrix} U_{\pm,k_0} & 0 \\ 0 & (U_{\pm,k_0})^\top \end{pmatrix} = \begin{pmatrix} V_{\pm,k_0} W_{\pm,k_0} & 0 \\ 0 & W_{\pm,k_0} V_{\pm,k_0} \end{pmatrix}. \tag{1.2.33}$$

Lemma 1.2.3. *Let $z \in \mathbb{C}\backslash\{0\}$, $k_0 \in \mathbb{Z}$, and $\{\widehat{p}_+(z,k,k_0)\}_{k\geq k_0}$, $\{\widehat{r}_+(z,k,k_0)\}_{k\geq k_0}$ be sequences of complex functions. Then, the following items (i)–(vi) are equivalent:*

$$(i) \quad U_{+,k_0}\widehat{p}_+(z,\cdot,k_0) = z\widehat{p}_+(z,\cdot,k_0), \quad W_{+,k_0}\widehat{p}_+(z,\cdot,k_0) = z\widehat{r}_+(z,\cdot,k_0). \tag{1.2.34}$$

$$(ii) \quad (U_{+,k_0})^\top\widehat{r}_+(z,\cdot,k_0) = z\widehat{r}_+(z,\cdot,k_0), \quad V_{+,k_0}\widehat{r}_+(z,\cdot,k_0) = \widehat{p}_+(z,\cdot,k_0). \tag{1.2.35}$$

$$(iii) \quad W_{+,k_0}\widehat{p}_+(z,\cdot,k_0) = z\widehat{r}_+(z,\cdot,k_0), \quad V_{+,k_0}\widehat{r}_+(z,\cdot,k_0) = \widehat{p}_+(z,\cdot,k_0). \tag{1.2.36}$$

$$(iv) \quad \mathbb{U}_{+,k_0}\begin{pmatrix}\widehat{p}_+(z,\cdot,k_0)\\ \widehat{r}_+(z,\cdot,k_0)\end{pmatrix} = z\begin{pmatrix}\widehat{p}_+(z,\cdot,k_0)\\ \widehat{r}_+(z,\cdot,k_0)\end{pmatrix}, \quad W_{+,k_0}\widehat{p}_+(z,\cdot,k_0) = z\widehat{r}_+(z,\cdot,k_0). \tag{1.2.37}$$

$$(v) \quad \mathbb{U}_{+,k_0}\begin{pmatrix}\widehat{p}_+(z,\cdot,k_0)\\ \widehat{r}_+(z,\cdot,k_0)\end{pmatrix} = z\begin{pmatrix}\widehat{p}_+(z,\cdot,k_0)\\ \widehat{r}_+(z,\cdot,k_0)\end{pmatrix}, \quad V_{+,k_0}\widehat{r}_+(z,\cdot,k_0) = \widehat{p}_+(z,\cdot,k_0). \tag{1.2.38}$$

$$(vi) \quad \begin{pmatrix}\widehat{p}_+(z,k,k_0)\\ \widehat{r}_+(z,k,k_0)\end{pmatrix} = T(z,k)\begin{pmatrix}\widehat{p}_+(z,k-1,k_0)\\ \widehat{r}_+(z,k-1,k_0)\end{pmatrix}, \quad k > k_0, \tag{1.2.39}$$

$$\text{assuming } \widehat{p}_+(z,k_0,k_0) = \begin{cases} z\widehat{r}_+(z,k_0,k_0), & k_0 \text{ odd},\\ \widehat{r}_+(z,k_0,k_0), & k_0 \text{ even}.\end{cases} \tag{1.2.40}$$

Next, consider sequences $\{\widehat{p}_-(z,k,k_0)\}_{k\leq k_0}$, $\{\widehat{r}_-(z,k,k_0)\}_{k\leq k_0}$. Then, the following items (vii)–(xii) are equivalent:

$$(vii) \quad U_{-,k_0}\widehat{p}_-(z,\cdot,k_0) = z\widehat{p}_-(z,\cdot,k_0), \quad W_{-,k_0}\widehat{p}_-(z,\cdot,k_0) = z\widehat{r}_-(z,\cdot,k_0). \tag{1.2.41}$$

$$(viii) \quad (U_{-,k_0})^\top\widehat{r}_-(z,\cdot,k_0) = z\widehat{r}_-(z,\cdot,k_0), \quad V_{-,k_0}\widehat{r}_-(z,\cdot,k_0) = \widehat{p}_-(z,\cdot,k_0). \tag{1.2.42}$$

$$(ix) \quad W_{-,k_0}\widehat{p}_-(z,\cdot,k_0) = z\widehat{r}_-(z,\cdot,k_0), \quad V_{-,k_0}\widehat{r}_-(z,\cdot,k_0) = \widehat{p}_-(z,\cdot,k_0). \tag{1.2.43}$$

$$(x) \quad \mathbb{U}_{-,k_0}\begin{pmatrix}\widehat{p}_-(z,\cdot,k_0)\\ \widehat{r}_-(z,\cdot,k_0)\end{pmatrix} = z\begin{pmatrix}\widehat{p}_-(z,\cdot,k_0)\\ \widehat{r}_-(z,\cdot,k_0)\end{pmatrix}, \quad W_{-,k_0}\widehat{p}_-(z,\cdot,k_0) = z\widehat{r}_-(z,\cdot,k_0). \tag{1.2.44}$$

$$(xi) \quad \mathbb{U}_{-,k_0}\begin{pmatrix}\widehat{p}_-(z,\cdot,k_0)\\ \widehat{r}_-(z,\cdot,k_0)\end{pmatrix} = z\begin{pmatrix}\widehat{p}_-(z,\cdot,k_0)\\ \widehat{r}_-(z,\cdot,k_0)\end{pmatrix}, \quad V_{-,k_0}\widehat{r}_-(z,\cdot,k_0) = \widehat{p}_-(z,\cdot,k_0). \tag{1.2.45}$$

$$(xii) \quad \begin{pmatrix}\widehat{p}_-(z,k-1),k_0\\ \widehat{r}_-(z,k-1,k_0)\end{pmatrix} = T(z,k)^{-1}\begin{pmatrix}\widehat{p}_-(z,k,k_0)\\ \widehat{r}_-(z,k,k_0)\end{pmatrix}, \quad k \leq k_0, \tag{1.2.46}$$

$$\textit{assuming } \widehat{p}_-(z,k_0,k_0) = \begin{cases} -\widehat{r}_-(z,k_0,k_0), & k_0 \textit{ odd,} \\ -z\widehat{r}_-(z,k_0,k_0), & k_0 \textit{ even.} \end{cases} \tag{1.2.47}$$

Proof. Repeating the first part of the proof of Lemma 1.2.2 one obtains the equivalence of (1.2.34), (1.2.35), (1.2.36), (1.2.37), and (1.2.38). Moreover, repeating the second part of the proof of Lemma 1.2.2 one obtains that

$$(W_{+,k_0}\widehat{p}_+(z,\cdot,k_0))(k) = z\widehat{r}_+(z,k,k_0), \tag{1.2.48}$$

$$(V_{+,k_0}\widehat{r}_+(z,\cdot,k_0))(k) = \widehat{p}_+(z,k,k_0), \quad k > k_0 \tag{1.2.49}$$

is equivalent to

$$\begin{pmatrix} \widehat{p}_+(z,k,k_0) \\ \widehat{r}_+(z,k,k_0) \end{pmatrix} = T(z,k) \begin{pmatrix} \widehat{p}_+(z,k-1,k_0) \\ \widehat{r}_+(z,k-1,k_0) \end{pmatrix}, \quad k > k_0. \tag{1.2.50}$$

If k_0 is odd, then the operators V_{+,k_0} and W_{+,k_0} have the following structure,

$$V_{+,k_0} = \begin{pmatrix} \theta_{k_0+1} & & 0 \\ & \theta_{k_0+3} & \\ 0 & & \ddots \end{pmatrix}, \quad W_{+,k_0} = \begin{pmatrix} 1 & & 0 \\ & \theta_{k_0+2} & \\ 0 & & \ddots \end{pmatrix}, \tag{1.2.51}$$

and hence,

$$W_{+,k_0}\widehat{p}_+(z,\cdot,k_0))(k_0) = z\widehat{r}_+(z,k_0,k_0) \tag{1.2.52}$$

is equivalent to

$$\widehat{p}_+(z,k_0,k_0) = z\widehat{r}_+(z,k_0,k_0). \tag{1.2.53}$$

Thus, one infers that (1.2.36) is equivalent to (1.2.39), (1.2.40) for k_0 odd. If k_0 is even, then the operators V_{+,k_0} and W_{+,k_0} have the following structure,

$$V_{+,k_0} = \begin{pmatrix} 1 & & 0 \\ & \theta_{k_0+2} & \\ 0 & & \ddots \end{pmatrix}, \quad W_{+,k_0} = \begin{pmatrix} \theta_{k_0+1} & & 0 \\ & \theta_{k_0+3} & \\ 0 & & \ddots \end{pmatrix}, \tag{1.2.54}$$

and hence,

$$(V_{+,k_0}\widehat{r}_+(z,\cdot,k_0))(k_0) = \widehat{p}_+(z,k_0,k_0) \tag{1.2.55}$$

is equivalent to

$$\widehat{p}_+(z,k_0,k_0) = \widehat{r}_+(z,k_0,k_0). \tag{1.2.56}$$

Thus, one infers that (1.2.36) is equivalent to (1.2.39), (1.2.40) for k_0 even.

The results for $\widehat{p}_-(z,\cdot,k_0)$ and $\widehat{r}_-(z,\cdot,k_0)$ are proved analogously. $\square$

Analogous comments to those made right after the proof of Lemma 1.2.2 apply in the present context of Lemma 1.2.3.

Definition 1.2.4. We denote by $\left(\begin{smallmatrix} p_+(z,k,k_0) \\ r_+(z,k,k_0) \end{smallmatrix}\right)_{k\geq k_0}$ and $\left(\begin{smallmatrix} q_+(z,k,k_0) \\ s_+(z,k,k_0) \end{smallmatrix}\right)_{k\geq k_0}$, $z \in \mathbb{C}\backslash\{0\}$, two linearly independent solutions of (1.2.39) with the following initial conditions:

$$\begin{pmatrix} p_+(z,k_0,k_0) \\ r_+(z,k_0,k_0) \end{pmatrix} = \begin{cases} \left(\begin{smallmatrix} z \\ 1 \end{smallmatrix}\right), & k_0 \text{ odd}, \\ \left(\begin{smallmatrix} 1 \\ 1 \end{smallmatrix}\right), & k_0 \text{ even}, \end{cases} \quad \begin{pmatrix} q_+(z,k_0,k_0) \\ s_+(z,k_0,k_0) \end{pmatrix} = \begin{cases} \left(\begin{smallmatrix} z \\ -1 \end{smallmatrix}\right), & k_0 \text{ odd}, \\ \left(\begin{smallmatrix} -1 \\ 1 \end{smallmatrix}\right), & k_0 \text{ even}. \end{cases} \tag{1.2.57}$$

Similarly, we denote by $\left(\begin{smallmatrix} p_-(z,k,k_0) \\ r_-(z,k,k_0) \end{smallmatrix}\right)_{k\leq k_0}$ and $\left(\begin{smallmatrix} q_-(z,k,k_0) \\ s_-(z,k,k_0) \end{smallmatrix}\right)_{k\leq k_0}$, $z \in \mathbb{C}\backslash\{0\}$, two linearly independent solutions of (1.2.46) with the following initial conditions:

$$\begin{pmatrix} p_-(z,k_0,k_0) \\ r_-(z,k_0,k_0) \end{pmatrix} = \begin{cases} \left(\begin{smallmatrix} 1 \\ -1 \end{smallmatrix}\right), & k_0 \text{ odd}, \\ \left(\begin{smallmatrix} -z \\ 1 \end{smallmatrix}\right), & k_0 \text{ even}, \end{cases} \quad \begin{pmatrix} q_-(z,k_0,k_0) \\ s_-(z,k_0,k_0) \end{pmatrix} = \begin{cases} \left(\begin{smallmatrix} 1 \\ 1 \end{smallmatrix}\right), & k_0 \text{ odd}, \\ \left(\begin{smallmatrix} z \\ 1 \end{smallmatrix}\right), & k_0 \text{ even}. \end{cases} \tag{1.2.58}$$

Using (1.2.17) one extends $\left(\begin{smallmatrix} p_+(z,k,k_0) \\ r_+(z,k,k_0) \end{smallmatrix}\right)_{k\geq k_0}$, $\left(\begin{smallmatrix} q_+(z,k,k_0) \\ s_+(z,k,k_0) \end{smallmatrix}\right)_{k\geq k_0}$, $z \in \mathbb{C}\backslash\{0\}$, to $k < k_0$. In the same manner, one extends $\left(\begin{smallmatrix} p_-(z,k,k_0) \\ r_-(z,k,k_0) \end{smallmatrix}\right)_{k\leq k_0}$ and $\left(\begin{smallmatrix} q_-(z,k,k_0) \\ s_-(z,k,k_0) \end{smallmatrix}\right)_{k\leq k_0}$, $z \in \mathbb{C}\backslash\{0\}$, to $k > k_0$. These extensions will be denoted by $\left(\begin{smallmatrix} p_\pm(z,k,k_0) \\ r_\pm(z,k,k_0) \end{smallmatrix}\right)_{k\in\mathbb{Z}}$ and $\left(\begin{smallmatrix} q_\pm(z,k,k_0) \\ s_\pm(z,k,k_0) \end{smallmatrix}\right)_{k\in\mathbb{Z}}$. Moreover, it follows from (1.2.17) that $p_\pm(z,k,k_0)$, $q_\pm(z,k,k_0)$, $r_\pm(z,k,k_0)$, and $s_\pm(z,k,k_0)$, $k, k_0 \in \mathbb{Z}$, are Laurent polynomials in z.

In particular, one computes

k	$k_0 - 1$	k_0 odd	$k_0 + 1$
$\begin{pmatrix} p_+(z,k,k_0) \\ r_+(z,k,k_0) \end{pmatrix}$	$\dfrac{1}{\rho_{k_0}} \begin{pmatrix} z(1-\overline{\alpha_{k_0}}) \\ 1-\alpha_{k_0} \end{pmatrix}$	$\begin{pmatrix} z \\ 1 \end{pmatrix}$	$\dfrac{1}{\rho_{k_0+1}} \begin{pmatrix} 1+\overline{\alpha_{k_0+1}}z \\ z+\alpha_{k_0+1} \end{pmatrix}$
$\begin{pmatrix} q_+(z,k,k_0) \\ s_+(z,k,k_0) \end{pmatrix}$	$\dfrac{1}{\rho_{k_0}} \begin{pmatrix} z(-1-\overline{\alpha_{k_0}}) \\ 1+\alpha_{k_0} \end{pmatrix}$	$\begin{pmatrix} z \\ -1 \end{pmatrix}$	$\dfrac{1}{\rho_{k_0+1}} \begin{pmatrix} -1+\overline{\alpha_{k_0+1}}z \\ z-\alpha_{k_0+1} \end{pmatrix}$
$\begin{pmatrix} p_-(z,k,k_0) \\ r_-(z,k,k_0) \end{pmatrix}$	$\dfrac{1}{\rho_{k_0}} \begin{pmatrix} -z-\overline{\alpha_{k_0}} \\ 1/z+\alpha_{k_0} \end{pmatrix}$	$\begin{pmatrix} 1 \\ -1 \end{pmatrix}$	$\dfrac{1}{\rho_{k_0+1}} \begin{pmatrix} -1+\overline{\alpha_{k_0+1}} \\ 1-\alpha_{k_0+1} \end{pmatrix}$
$\begin{pmatrix} q_-(z,k,k_0) \\ s_-(z,k,k_0) \end{pmatrix}$	$\dfrac{1}{\rho_{k_0}} \begin{pmatrix} z-\overline{\alpha_{k_0}} \\ 1/z-\alpha_{k_0} \end{pmatrix}$	$\begin{pmatrix} 1 \\ 1 \end{pmatrix}$	$\dfrac{1}{\rho_{k_0+1}} \begin{pmatrix} 1+\overline{\alpha_{k_0+1}} \\ 1+\alpha_{k_0+1} \end{pmatrix}$
k	$k_0 - 1$	k_0 even	$k_0 + 1$
$\begin{pmatrix} p_+(z,k,k_0) \\ r_+(z,k,k_0) \end{pmatrix}$	$\dfrac{1}{\rho_{k_0}} \begin{pmatrix} 1-\alpha_{k_0} \\ 1-\overline{\alpha_{k_0}} \end{pmatrix}$	$\begin{pmatrix} 1 \\ 1 \end{pmatrix}$	$\dfrac{1}{\rho_{k_0+1}} \begin{pmatrix} z+\alpha_{k_0+1} \\ 1/z+\overline{\alpha_{k_0+1}} \end{pmatrix}$
$\begin{pmatrix} q_+(z,k,k_0) \\ s_+(z,k,k_0) \end{pmatrix}$	$\dfrac{1}{\rho_{k_0}} \begin{pmatrix} 1+\alpha_{k_0} \\ -1-\overline{\alpha_{k_0}} \end{pmatrix}$	$\begin{pmatrix} -1 \\ 1 \end{pmatrix}$	$\dfrac{1}{\rho_{k_0+1}} \begin{pmatrix} z-\alpha_{k_0+1} \\ -1/z+\overline{\alpha_{k_0+1}} \end{pmatrix}$
$\begin{pmatrix} p_-(z,k,k_0) \\ r_-(z,k,k_0) \end{pmatrix}$	$\dfrac{1}{\rho_{k_0}} \begin{pmatrix} 1+\alpha_{k_0}z \\ -z-\overline{\alpha_{k_0}} \end{pmatrix}$	$\begin{pmatrix} -z \\ 1 \end{pmatrix}$	$\dfrac{1}{\rho_{k_0+1}} \begin{pmatrix} z(1-\alpha_{k_0+1}) \\ -1+\overline{\alpha_{k_0+1}} \end{pmatrix}$
$\begin{pmatrix} q_-(z,k,k_0) \\ s_-(z,k,k_0) \end{pmatrix}$	$\dfrac{1}{\rho_{k_0}} \begin{pmatrix} 1-\alpha_{k_0}z \\ z-\overline{\alpha_{k_0}} \end{pmatrix}$	$\begin{pmatrix} z \\ 1 \end{pmatrix}$	$\dfrac{1}{\rho_{k_0+1}} \begin{pmatrix} z(1+\alpha_{k_0+1}) \\ 1+\overline{\alpha_{k_0+1}} \end{pmatrix}$

Remark 1.2.5. We note that Lemmas 1.2.2 and 1.2.3 are crucial for many of the proofs to follow. For instance, we note that the equivalence of items (i) and (vi) in Lemma 1.2.2 proves that for each $z \in \mathbb{C}\backslash\{0\}$, the solutions $\{u(z,k)\}_{k\in\mathbb{Z}}$ of $Uu(z,\cdot) = zu(z,\cdot)$ form a two-dimensional space, which implies that such solutions are linear combinations of $\{p_\pm(z,k,k_0)\}_{k\in\mathbb{Z}}$ and $\{q_\pm(z,k,k_0)\}_{k\in\mathbb{Z}}$ (with z-dependent coefficients). This equivalence also proves that any solution of $Uu(z,\cdot) = zu(z,\cdot)$ is determined by its values at a site k_0 of u and the auxiliary variable v. Moreover, taking into account item (vi) of Lemma 1.2.2, this also implies that such a solution is determined by its values at two consecutive sites $k_0 - 1$ and k_0. Similar comments

apply to the solutions of $U^\top v(z,\cdot) = zv(z,\cdot)$. In the context of Lemma 1.2.3, we remark that its importance lies in the fact that it shows that in the case of half-lattice CMV operators, the analogous equations have a one-dimensional space of solutions for each $z \in \mathbb{C}\backslash\{0\}$, due to the restriction on k_0 that appears in items (vi) and (xii) of Lemma 1.2.3. As a consequence, the corresponding solutions are determined by their value at a single site k_0.

Next, for all $z \in \mathbb{C}\backslash\{0\}$, $k, k_0 \in \mathbb{Z}$, we introduce the following modified Laurent polynomials $\widetilde{p}_\pm(z,k,k_0)$ and $\widetilde{q}_\pm(z,k,k_0)$, as follows,

$$\widetilde{p}_+(z,k,k_0) = \begin{cases} p_+(z,k,k_0)/z, & k_0 \text{ odd}, \\ p_+(z,k,k_0), & k_0 \text{ even}, \end{cases} \tag{1.2.59}$$

$$\widetilde{q}_+(z,k,k_0) = \begin{cases} q_+(z,k,k_0)/z, & k_0 \text{ odd}, \\ q_+(z,k,k_0), & k_0 \text{ even}, \end{cases} \tag{1.2.60}$$

$$\widetilde{p}_-(z,k,k_0) = \begin{cases} p_-(z,k,k_0), & k_0 \text{ odd}, \\ p_-(z,k,k_0)/z, & k_0 \text{ even}, \end{cases} \tag{1.2.61}$$

$$\widetilde{q}_-(z,k,k_0) = \begin{cases} q_-(z,k,k_0), & k_0 \text{ odd}, \\ q_-(z,k,k_0)/z, & k_0 \text{ even}. \end{cases} \tag{1.2.62}$$

Remark 1.2.6. By Lemma 1.2.3, $\left(\begin{smallmatrix} p_\pm(z,k,k_0) \\ r_\pm(z,k,k_0) \end{smallmatrix}\right)_{k \gtrless k_0}$, $z \in \mathbb{C}\backslash\{0\}$, $k_0 \in \mathbb{Z}$, are generalized eigenvectors of the operators $\mathbb{U}_{\pm,k_0}$. Moreover, by Lemma 1.2.2, $\left(\begin{smallmatrix} p_\pm(z,k,k_0) \\ r_\pm(z,k,k_0) \end{smallmatrix}\right)_{k \in \mathbb{Z}}$ and $\left(\begin{smallmatrix} q_\pm(z,k,k_0) \\ s_\pm(z,k,k_0) \end{smallmatrix}\right)_{k \in \mathbb{Z}}$, $z \in \mathbb{C}\backslash\{0\}$, $k_0 \in \mathbb{Z}$, are generalized eigenvectors of $\mathbb{U}$.

Lemma 1.2.7. *The Laurent polynomials $\widetilde{p}_\pm(z,k,k_0)$, $r_\pm(z,k,k_0)$, $\widetilde{q}_\pm(z,k,k_0)$, and $s_\pm(z,k,k_0)$ satisfy the following relations for all $z \in \mathbb{C}\backslash\{0\}$ and $k, k_0 \in \mathbb{Z}$,*

$$r_+(z,k,k_0) = \overline{\widetilde{p}_+(1/\overline{z},k,k_0)}, \tag{1.2.63}$$

$$s_+(z,k,k_0) = -\overline{\widetilde{q}_+(1/\overline{z},k,k_0)}, \tag{1.2.64}$$

$$r_-(z,k,k_0) = -\overline{\widetilde{p}_-(1/\overline{z},k,k_0)}, \tag{1.2.65}$$

$$s_-(z,k,k_0) = \overline{\widetilde{q}_-(1/\overline{z},k,k_0)}. \tag{1.2.66}$$

Proof. Let $\{u(z,k)\}_{k\in\mathbb{Z}}$, $\{v(z,k)\}_{k\in\mathbb{Z}}$ be two sequences of complex functions, then the following items (i)–(iii) are seen to be equivalent:

$$(i) \quad Wu(z,\cdot) = zv(z,\cdot), \quad Vv(z,\cdot) = u(z,\cdot). \tag{1.2.67}$$

$$(ii) \quad \frac{1}{z}u(z,\cdot) = W^*v(z,\cdot), \quad v(z,\cdot) = V^*u(z,\cdot). \tag{1.2.68}$$

$$(iii) \quad \frac{1}{\overline{z}}\overline{u(z,\cdot)} = W\overline{v(z,\cdot)}, \quad \overline{v(z,\cdot)} = V\overline{u(z,\cdot)}, \tag{1.2.69}$$

where equations (1.2.67)–(1.2.69) are meant in the algebraic sense and hence V, V^*, W, and W^* are considered as difference expressions rather than difference operators. Thus, the assertion of the Lemma follows from Lemma 1.2.3, Definition 1.2.4, and equalities (1.2.59)–(1.2.62). □

Lemma 1.2.8. *Let $k_0 \in \mathbb{Z}$. Then the sets of Laurent polynomials $\{p_+(\cdot,k,k_0)\}_{k\geq k_0}$ (resp., $\{p_-(\cdot,k,k_0)\}_{k\leq k_0}$) and $\{r_+(\cdot,k,k_0)\}_{k\geq k_0}$ (resp., $\{r_-(\cdot,k,k_0)\}_{k\leq k_0}$) form orthonormal bases in $L^2(\partial\mathbb{D}; d\mu_+(\cdot,k_0))$ (resp., $L^2(\partial\mathbb{D}; d\mu_-(\cdot,k_0))$), where*

$$d\mu_\pm(\zeta,k_0) = d(\delta_{k_0}, E_{U_{\pm,k_0}}(\zeta)\delta_{k_0})_{\ell^2([k_0,\pm\infty)\cap\mathbb{Z})}, \quad \zeta\in\partial\mathbb{D}, \tag{1.2.70}$$

and $dE_{U_{\pm,k_0}}(\cdot)$ denote the operator-valued spectral measures of the operators $U_{\pm,k_0}$,

$$U_{\pm,k_0} = \oint_{\partial\mathbb{D}} dE_{U_{\pm,k_0}}(\zeta)\,\zeta. \tag{1.2.71}$$

Proof. It follows from the definition of the transfer matrix $T(z,k)$ in (1.2.18) and the recursion relations (1.2.39) and (1.2.46) that

$$\begin{aligned} &\overline{\operatorname{span}\{p_\pm(\cdot,k,k_0)\}_{k\gtreqless k_0}} = \overline{\operatorname{span}\{r_\pm(\cdot,k,k_0)\}_{k\gtreqless k_0}} \\ &\quad = \overline{\operatorname{span}\{\zeta^k\}_{k\in\mathbb{Z}}} = L^2(\partial\mathbb{D}; d\mu), \end{aligned} \tag{1.2.72}$$

where $d\mu$ is any finite (nonnegative) Borel measure on $\partial\mathbb{D}$. Thus, one concludes that the systems of Laurent polynomials $\{p_\pm(\cdot,k,k_0)\}_{k \gtrless k_0}$ and $\{r_\pm(\cdot,k,k_0)\}_{k \gtrless k_0}$ are complete in $L^2(\partial\mathbb{D}; d\mu_\pm(\cdot,k_0))$.

Next, consider the following equations

$$(U_{+,k_0})^\top \delta_k = \sum_{j=k-2}^{k+2} (U_{+,k_0})^\top(j,k)\delta_j = \sum_{j=k-2}^{k+2} (U_{+,k_0})(k,j)\delta_j, \tag{1.2.73}$$

$$(U_{+,k_0})\delta_k = \sum_{j=k-2}^{k+2} (U_{+,k_0})(j,k)\delta_j = \sum_{j=k-2}^{k+2} (U_{+,k_0})^\top(k,j)\delta_j, \tag{1.2.74}$$

and

$$z\widehat{p}_+(z,k,k_0) = (U_{+,k_0}\widehat{p}_+(z,\cdot,k_0))(k) = \sum_{j=k-2}^{k+2} (U_{+,k_0})(k,j)\widehat{p}_+(z,j,k_0), \tag{1.2.75}$$

$$z\widehat{r}_+(z,k,k_0) = ((U_{+,k_0})^\top \widehat{r}_+(z,\cdot,k_0))(k) = \sum_{j=k-2}^{k+2} (U_{+,k_0})^\top(k,j)\widehat{r}_+(z,j,k_0). \tag{1.2.76}$$

By Lemma 1.2.3 the latter ones have unique solutions $\widetilde{p}_+(z,k,k_0)$ and $r_+(z,k,k_0)$ satisfying $\widetilde{p}_+(z,k_0,k_0) = r_+(z,k_0,k_0) = 1$. Moreover, due to the algebraic nature of the proof of Lemma 1.2.3, (1.2.75) and (1.2.76) remain valid if $z \in \mathbb{C}\backslash\{0\}$ is replaced by a unitary operator on a Hilbert space and the left- and right-hand sides are applied to the vector δ_{k_0}. Thus, $\{\widetilde{p}_+((U_{+,k_0})^\top,k,k_0)\delta_{k_0}\}_{k\geq k_0}$ and $\{r_+(U_{+,k_0},k,k_0)\delta_{k_0}\}_{k\geq k_0}$ are the unique solutions of

$$(U_{+,k_0})^\top \widehat{p}_+((U_{+,k_0})^\top,k,k_0)\delta_{k_0} = \sum_{j=k-2}^{k+2} (U_{+,k_0})(k,j)\widehat{p}_+((U_{+,k_0})^\top,j,k_0)\delta_{k_0}, \tag{1.2.77}$$

$$U_{+,k_0}\widehat{r}_+(U_{+,k_0},k,k_0)\delta_{k_0} = \sum_{j=k-2}^{k+2} (U_{+,k_0})^\top(k,j)\widehat{r}_+(U_{+,k_0},j,k_0)\delta_{k_0} \tag{1.2.78}$$

with value δ_{k_0} at $k=k_0$, respectively. In particular, comparing (1.2.73), (1.2.74) with

(1.2.77), (1.2.78), one concludes that for $k \geq k_0$,

$$\delta_k = \widetilde{p}_+((U_{+,k_0})^\top, k, k_0)\delta_{k_0}, \tag{1.2.79}$$

$$\delta_k = r_+(U_{+,k_0}, k, k_0)\delta_{k_0}. \tag{1.2.80}$$

Using the spectral representation for the operators U_{+,k_0} and $(U_{+,k_0})^\top$ one obtains (all scalar products $(\cdot,\cdot)$ in the remainder of this proof are with respect to the Hilbert space $\ell^2([k_0,\pm\infty)\cap\mathbb{Z})$ and for simplicity we omit the corresponding subscript in $(\cdot,\cdot)$),

$$(\delta_k, \delta_\ell) = \oint_{\partial\mathbb{D}} d(\delta_{k_0}, E_{(U_{+,k_0})^\top}(\zeta)\delta_{k_0})\, \overline{p_+(\zeta,k,k_0)} p_+(\zeta,\ell,k_0), \tag{1.2.81}$$

$$(\delta_k, \delta_\ell) = \oint_{\partial\mathbb{D}} d(\delta_{k_0}, E_{U_{+,k_0}}(\zeta)\delta_{k_0})\, \overline{r_+(\zeta,k,k_0)} r_+(\zeta,\ell,k_0), \quad k,\ell \in \mathbb{Z}. \tag{1.2.82}$$

Finally, one notes that

$$d\mu_+(\zeta,k_0) = d(\delta_{k_0}, E_{U_{+,k_0}}(\zeta)\delta_{k_0}) = d(\delta_{k_0}, E_{(U_{+,k_0})^\top}(\zeta)\delta_{k_0}) \tag{1.2.83}$$

since

$$\begin{aligned} &\oint_{\partial\mathbb{D}} d\mu_+(\zeta,k_0)\,\zeta^k = \Big(\delta_{k_0}, U_{+,k_0}^k \delta_{k_0}\Big) = \Big(\delta_{k_0}, \big(U_{+,k_0}^k\big)^\top \delta_{k_0}\Big) \\ &\quad = \Big(\delta_{k_0}, \big(U_{+,k_0}^\top\big)^k \delta_{k_0}\Big) = \oint_{\partial\mathbb{D}} d(\delta_{k_0}, E_{(U_{+,k_0})^\top}(\zeta)\delta_{k_0})\,\zeta^k, \quad k \in \mathbb{Z}. \end{aligned} \tag{1.2.84}$$

Thus, the Laurent polynomials $\{p_+(\cdot,k,k_0)\}_{k\geq k_0}$ and $\{r_+(\cdot,k,k_0)\}_{k\geq k_0}$ are orthonormal in $L^2(\partial\mathbb{D}; d\mu_+(\cdot,k_0))$.

The results for $\{p_-(\cdot,k,k_0)\}_{k\leq k_0}$ and $\{r_-(\cdot,k,k_0)\}_{k\leq k_0}$ are proved similarly. $\square$

We note that the measures $d\mu_\pm(\cdot,k_0)$, $k_0 \in \mathbb{Z}$, are not only nonnegative but also supported on an infinite set.

Remark 1.2.9. In connection with our introductory remarks in (1.1.3)–(1.1.9) we note that $d\sigma_+ = d\mu_+(\cdot, 0)$ and

$$\begin{aligned} p_+(\zeta,k,0) &= \begin{cases} \gamma_k \zeta^{-(k-1)/2}\varphi_+(\zeta,k), & k \text{ odd},\\ \gamma_k \zeta^{-k/2}\varphi_+^*(\zeta,k), & k \text{ even}, \end{cases} \\ r_+(\zeta,k,0) &= \begin{cases} \gamma_k \zeta^{-(k+1)/2}\varphi_+^*(\zeta,k), & k \text{ odd},\\ \gamma_k \zeta^{-k/2}\varphi_+(\zeta,k), & k \text{ even}; \end{cases} \quad \zeta \in \partial\mathbb{D}. \end{aligned} \tag{1.2.85}$$

Let $\phi \in C(\partial\mathbb{D})$ and define the operator of multiplication by ϕ, $M_{\pm,k_0}(\phi)$, acting on $L^2(\partial\mathbb{D}; d\mu_\pm(\cdot,k_0))$ by

$$(M_{\pm,k_0}(\phi)f)(\zeta) = \phi(\zeta)f(\zeta), \quad f \in L^2(\partial\mathbb{D}; d\mu_\pm(\cdot,k_0)). \tag{1.2.86}$$

In the special case $\phi = id$ (where $id(\zeta) = \zeta$, $\zeta \in \partial\mathbb{D}$), the corresponding multiplication operator is denoted by $M_{\pm,k_0}(id)$. The spectrum of $M_{\pm,k_0}(\phi)$ is given by

$$\sigma(M_{\pm,k_0}(\phi)) = \operatorname{ess.ran}_{d\mu_\pm(\cdot,k_0)}(\phi), \tag{1.2.87}$$

where the essential range of ϕ with respect to a measure $d\mu$ on $\partial\mathbb{D}$ is defined by

$$\operatorname{ess.ran}_{d\mu}(\phi) = \{z \in \mathbb{C} \,|\, \text{for all } \varepsilon > 0, \mu(\{\zeta \in \partial\mathbb{D} \,|\, |\phi(\zeta) - z| < \varepsilon\}) > 0\}. \tag{1.2.88}$$

Corollary 1.2.10. *Let $k_0 \in \mathbb{Z}$ and $\phi \in C(\partial\mathbb{D})$. Then the operators $\phi(U_{\pm,k_0})$ and $\phi(U^\top_{\pm,k_0})$ are unitarily equivalent to the operators $M_{\pm,k_0}(\phi)$ of multiplication by ϕ defined on $L^2(\partial\mathbb{D}; d\mu_\pm(\cdot,k_0))$. In particular,*

$$\sigma(\phi(U_{\pm,k_0})) = \sigma(\phi(U^\top_{\pm,k_0})) = \operatorname{ess.ran}_{d\mu_\pm(\cdot,k_0)}(\phi), \tag{1.2.89}$$

$$\sigma(U_{\pm,k_0}) = \sigma(U^\top_{\pm,k_0}) = \operatorname{supp}(d\mu_\pm(\cdot,k_0)) \tag{1.2.90}$$

and the spectrum of $U_{\pm,k_0}$ is simple.

Proof. Consider the following linear maps $\dot{\mathcal{U}}_\pm$ from $\ell_0^\infty([k_0,\pm\infty)\cap\mathbb{Z})$ into the set of Laurent polynomials on $\partial\mathbb{D}$ defined by

$$(\dot{\mathcal{U}}_\pm f)(\zeta) = \sum_{k=k_0}^{\pm\infty} r_\pm(\zeta,k,k_0)f(k), \quad f\in\ell_0^\infty([k_0,\pm\infty)\cap\mathbb{Z}). \tag{1.2.91}$$

A simple calculation for $F(\zeta)=(\dot{\mathcal{U}}_\pm f)(\zeta)$, $f\in\ell_0^\infty([k_0,\pm\infty)\cap\mathbb{Z})$, shows that

$$\sum_{k=k_0}^{\pm\infty}|f(k)|^2 = \oint_{\partial\mathbb{D}} d\mu_\pm(\zeta,k_0)\,|F(\zeta)|^2. \tag{1.2.92}$$

Since $\ell_0^\infty([k_0,\pm\infty)\cap\mathbb{Z})$ is dense in $\ell^2([k_0,\pm\infty)\cap\mathbb{Z})$, $\dot{\mathcal{U}}_\pm$ extend to bounded linear operators $\mathcal{U}_\pm\colon \ell^2([k_0,\pm\infty)\cap\mathbb{Z})\to L^2(\partial\mathbb{D};d\mu_\pm(\cdot,k_0))$. Since by (1.2.72), the sets of Laurent polynomials are dense in $L^2(\partial\mathbb{D};d\mu_\pm(\cdot,k_0))$, the maps $\mathcal{U}_\pm$ are onto and one infers

$$(\mathcal{U}_\pm^{-1}F)(k) = \oint_{\partial\mathbb{D}} d\mu_\pm(\zeta,k_0)\,\overline{r_\pm(\zeta,k,k_0)}F(\zeta), \quad F\in L^2(\partial\mathbb{D};d\mu_\pm(\cdot,k_0)). \tag{1.2.93}$$

In particular, $\mathcal{U}_\pm$ are unitary. Moreover, we claim that $\mathcal{U}_\pm$ map the operators $\phi(U_{\pm,k_0})$ on $\ell^2([k_0,\pm\infty)\cap\mathbb{Z})$ to the operators $M_{\pm,k_0}(\phi)$ of multiplication by ϕ acting on $L^2(\partial\mathbb{D};d\mu_\pm(\cdot,k_0))$,

$$\mathcal{U}_\pm\phi(U_{\pm,k_0})\mathcal{U}_\pm^{-1} = M_{\pm,k_0}(\phi). \tag{1.2.94}$$

Indeed,

$$\begin{aligned}
&(\mathcal{U}_\pm\phi(U_{\pm,k_0})\mathcal{U}_\pm^{-1}F(\cdot))(\zeta) = (\mathcal{U}_\pm\phi(U_{\pm,k_0})f(\cdot))(\zeta)\\
&\quad= \sum_{k=k_0}^{\pm\infty}(\phi(U_{\pm,k_0})f(\cdot))(k)r_\pm(\zeta,k,k_0) = \sum_{k=k_0}^{\pm\infty}(\phi(U_{\pm,k_0}^\top)r_\pm(\zeta,\cdot,k_0))(k)f(k)\\
&\quad= \sum_{k=k_0}^{\pm\infty}\phi(\zeta)r_\pm(\zeta,k,k_0)f(k) = \phi(\zeta)F(\zeta)
\end{aligned}$$

$$= (M_{\pm,k_0}(\phi)F)(\zeta), \quad F \in L^2(\partial\mathbb{D}; d\mu_\pm(\cdot,k_0)). \tag{1.2.95}$$

The result for $\phi(U^\top_{\pm,k_0})$ is proved analogously. $\square$

Corollary 1.2.11. *Let $k_0 \in \mathbb{Z}$.*

The Laurent polynomials $\{p_+(\cdot,k,k_0)\}_{k\geq k_0}$ can be constructed by Gram–Schmidt orthogonalizing

$$\begin{cases} \zeta,\, 1,\, \zeta^2,\, \zeta^{-1},\, \zeta^3,\, \zeta^{-2}, \dots, & k_0 \text{ odd,} \\ 1,\, \zeta,\, \zeta^{-1},\, \zeta^2,\, \zeta^{-2}, \zeta^3, \dots, & k_0 \text{ even} \end{cases} \tag{1.2.96}$$

in $L^2(\partial\mathbb{D}; d\mu_+(\cdot,k_0))$.

The Laurent polynomials $\{r_+(\cdot,k,k_0)\}_{k\geq k_0}$ can be constructed by Gram–Schmidt orthogonalizing

$$\begin{cases} 1,\, \zeta,\, \zeta^{-1},\, \zeta^2,\, \zeta^{-2}, \zeta^3, \dots, & k_0 \text{ odd,} \\ 1,\, \zeta^{-1},\, \zeta,\, \zeta^{-2},\, \zeta^2, \zeta^{-3}, \dots, & k_0 \text{ even} \end{cases} \tag{1.2.97}$$

in $L^2(\partial\mathbb{D}; d\mu_+(\cdot,k_0))$.

The Laurent polynomials $\{p_-(\cdot,k,k_0)\}_{k\leq k_0}$ can be constructed by Gram–Schmidt orthogonalizing

$$\begin{cases} 1,\, -\zeta,\, \zeta^{-1},\, -\zeta^2,\, \zeta^{-2}, -\zeta^3, \dots, & k_0 \text{ odd,} \\ -\zeta,\, 1,\, -\zeta^2,\, \zeta^{-1},\, -\zeta^3,\, \zeta^{-2}, \dots, & k_0 \text{ even} \end{cases} \tag{1.2.98}$$

in $L^2(\partial\mathbb{D}; d\mu_-(\cdot,k_0))$.

The Laurent polynomials $\{r_-(\cdot,k,k_0)\}_{k\leq k_0}$ can be constructed by Gram–Schmidt orthogonalizing

$$\begin{cases} -1,\, \zeta^{-1},\, -\zeta,\, \zeta^{-2},\, -\zeta^2, \zeta^{-3}, \dots, & k_0 \text{ odd,} \\ 1,\, -\zeta,\, \zeta^{-1},\, -\zeta^2,\, \zeta^{-2}, -\zeta^3, \dots, & k_0 \text{ even} \end{cases} \tag{1.2.99}$$

in $L^2(\partial\mathbb{D}; d\mu_-(\cdot,k_0))$.

Proof. The statements follow from Definition 1.2.4 and Lemma 1.2.8. $\square$

The following result clarifies which measures arise as spectral measures of half-lattice CMV operators and it yields the reconstruction of Verblunsky coefficients from the spectral measures and the corresponding orthogonal polynomials.

Theorem 1.2.12. *Let $k_0 \in \mathbb{Z}$ and $d\mu_\pm(\cdot, k_0)$ be nonnegative finite measures on $\partial\mathbb{D}$ which are supported on infinite sets and normalized by*

$$\oint_{\partial\mathbb{D}} d\mu_\pm(\zeta, k_0) = 1. \tag{1.2.100}$$

Then $d\mu_\pm(\cdot, k_0)$ are necessarily the spectral measures for some half-lattice CMV operators $U_{\pm,k_0}$ with coefficients $\{\alpha_k\}_{k\geq k_0+1}$, respectively $\{\alpha_k\}_{k\leq k_0}$, defined as follows,

$$\alpha_k = -\begin{cases} \big(p_+(\cdot, k-1, k_0), M_{\pm,k_0}(id) r_+(\cdot, k-1, k_0)\big)_{L^2(\partial\mathbb{D}; d\mu_+(\cdot, k_0))}, & k \text{ odd}, \\ \big(r_+(\cdot, k-1, k_0), p_+(\cdot, k-1, k_0)\big)_{L^2(\partial\mathbb{D}; d\mu_+(\cdot, k_0))}, & k \text{ even} \end{cases} \tag{1.2.101}$$

for all $k \geq k_0 + 1$ and

$$\alpha_k = -\begin{cases} \big(p_-(\cdot, k-1, k_0), M_{\pm,k_0}(id) r_-(\cdot, k-1, k_0)\big)_{L^2(\partial\mathbb{D}; d\mu_-(\cdot, k_0))}, & k \text{ odd}, \\ \big(r_-(\cdot, k-1, k_0), p_-(\cdot, k-1, k_0)\big)_{L^2(\partial\mathbb{D}; d\mu_-(\cdot, k_0))}, & k \text{ even} \end{cases} \tag{1.2.102}$$

for all $k \leq k_0$. Here the Laurent polynomials $\{p_+(\cdot, k, k_0), r_+(\cdot, k, k_0)\}_{k\geq k_0}$ and $\{p_-(\cdot, k, k_0), r_-(\cdot, k, k_0)\}_{k\leq k_0}$ denote the orthonormal polynomials constructed in Corollary 1.2.11.

Proof. Using Corollary 1.2.11 one constructs the orthonormal Laurent polynomials $\{p_+(\zeta, k, k_0), r_+(\zeta, k, k_0)\}_{k\geq k_0}$, $\zeta \in \partial\mathbb{D}$. Because of their orthogonality properties one concludes

$$r_+(\zeta, k, k_0) = \begin{cases} \zeta\overline{p_+(\zeta, k, k_0)}, & k_0 \text{ odd}, \\ \overline{p_+(\zeta, k, k_0)}, & k_0 \text{ even}, \end{cases} \quad \zeta \in \partial\mathbb{D},\ k \geq k_0. \tag{1.2.103}$$

Next we will establish the recursion relation (1.2.39). Consider the following Laurent polynomial $p(\zeta)$, $\zeta \in \partial\mathbb{D}$, for some fixed $k > k_0$,

$$p(\zeta) = \begin{cases} \rho_k p_+(\zeta, k, k_0) - \zeta r_+(\zeta, k-1, k_0), & k \text{ odd}, \\ \rho_k p_+(\zeta, k, k_0) - r_+(\zeta, k-1, k_0), & k \text{ even}, \end{cases} \quad \zeta \in \partial\mathbb{D}, \tag{1.2.104}$$

where $\rho_k \in (0, \infty)$ is chosen such that the leading term of $p_+(\cdot, k, k_0)$ cancels the leading term of $r_+(\cdot, k-1, k_0)$. Using Corollary 1.2.11 one checks that the Laurent polynomial $p(\cdot)$ is proportional to $p_+(\cdot, k-1, k_0)$. Hence, one arrives at the following recursion relation,

$$\rho_k p_+(\zeta, k, k_0) = \begin{cases} \alpha_k p_+(\zeta, k-1, k_0) + \zeta r_+(\zeta, k-1, k_0), & k \text{ odd}, \\ \overline{\alpha_k} p_+(\zeta, k-1, k_0) + r_+(\zeta, k-1, k_0), & k \text{ even}, \end{cases} \quad \zeta \in \partial\mathbb{D}, \tag{1.2.105}$$

where $\alpha_k \in \mathbb{C}$ is the proportionality constant. Taking the scalar product of both sides with $p_+(\zeta, k-1, k_0)$ yields the expressions for α_k, $k \geq k_0 + 1$, in (1.2.101). Moreover, applying (1.2.103) one obtains

$$\rho_k r_+(\zeta, k, k_0) = \begin{cases} \overline{\alpha_k} r_+(\zeta, k-1, k_0) + \frac{1}{\zeta} p_+(\zeta, k-1, k_0), & k \text{ odd}, \\ \alpha_k r_+(\zeta, k-1, k_0) + p_+(\zeta, k-1, k_0), & k \text{ even}, \end{cases} \quad \zeta \in \partial\mathbb{D}, \tag{1.2.106}$$

and hence (1.2.39). Since $\rho_k > 0$, $k \in \mathbb{Z}$, it remains to show that $\rho_k^2 = 1 - |\alpha_k|^2$ and hence that $|\alpha_k| < 1$. This follows from the orthonormality of Laurent polynomials $\{p_+(\cdot, k, k_0)\}_{k \geq k_0}$ in $L^2(\partial\mathbb{D}; d\mu_+(\cdot, k_0))$,

$$\begin{aligned} |\alpha_k|^2 &= \|\alpha_k p_+(\cdot, k-1, k_0)\|^2_{L^2(\partial\mathbb{D}; d\mu_+(\cdot, k_0))} \\ &= \|\rho_k p_+(\cdot, k, k_0) - id(\cdot) r_+(\cdot, k-1, k_0)\|^2_{L^2(\partial\mathbb{D}; d\mu_+(\cdot, k_0))} \\ &= \rho_k^2 + 1 - 2\mathrm{Re}\Big(\big(\rho_k p_+(\cdot, k, k_0), id(\cdot) r_+(\cdot, k-1, k_0)\big)_{L^2(\partial\mathbb{D}; d\mu_+(\cdot, k_0))} \Big) \end{aligned}$$

$$
\begin{aligned}
&= \rho_k^2 + 1 \\
&\quad - 2\mathrm{Re}\Big(\big(\rho_k p_+(\cdot,k,k_0), [\rho_k p_+(\cdot,k,k_0) - \alpha_k p_+(\cdot,k-1,k_0)]\big)_{L^2(\partial\mathbb{D};d\mu_+(\cdot,k_0))}\Big) \\
&= 1 - \rho_k^2, \quad k \text{ odd}.
\end{aligned} \tag{1.2.107}
$$

Similarly one treats the case k even. Finally, using Lemma 1.2.3 one concludes that $\binom{p_+(z,k,k_0)}{r_+(z,k,k_0)}_{k\geq k_0}$, $z \in \mathbb{C}\backslash\{0\}$, $k_0 \in \mathbb{Z}$, is a generalized eigenvector of the operator $\mathbb{U}_{+,k_0}$ defined in (1.2.33) associated with the coefficients α_k, ρ_k introduced above. Thus, the measure $d\mu_+(\cdot,k_0)$ is the spectral measure of the operator U_{+,k_0} in (1.2.31).

Similarly one proves the result for $d\mu_-(\cdot,k_0)$ and (1.2.102) for $k \leq k_0$. $\square$

Lemma 1.2.13. *Let $z \in \mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\})$ and $k_0 \in \mathbb{Z}$. Then the sets of two-dimensional Laurent polynomials* $\binom{\widetilde{p}_\pm(z,k,k_0)}{r_\pm(z,k,k_0)}_{k\gtreqless k_0}$ *and* $\binom{\widetilde{q}_\pm(z,k,k_0)}{s_\pm(z,k,k_0)}_{k\gtreqless k_0}$ *are related by,*

$$
\begin{pmatrix} \widetilde{q}_\pm(z,k,k_0) \\ s_\pm(z,k,k_0) \end{pmatrix} = \pm \oint_{\partial\mathbb{D}} d\mu_\pm(\zeta,k_0)\, \frac{\zeta+z}{\zeta-z} \left(\begin{pmatrix} \widetilde{p}_\pm(\zeta,k,k_0) \\ r_\pm(\zeta,k,k_0) \end{pmatrix} - \begin{pmatrix} \widetilde{p}_\pm(z,k,k_0) \\ r_\pm(z,k,k_0) \end{pmatrix} \right), \quad k \gtreqless k_0. \tag{1.2.108}
$$

Proof. First, we prove (1.2.108) for k_0 even, which by (1.2.59)–(1.2.62) is equivalent to

$$
\begin{pmatrix} q_+(z,k,k_0) \\ s_+(z,k,k_0) \end{pmatrix} = \oint_{\partial\mathbb{D}} \frac{\zeta+z}{\zeta-z} \left(\begin{pmatrix} p_+(\zeta,k,k_0) \\ r_+(\zeta,k,k_0) \end{pmatrix} - \begin{pmatrix} p_+(z,k,k_0) \\ r_+(z,k,k_0) \end{pmatrix} \right) d\mu_+(\zeta,k_0), \quad z \in \mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\}),\ k > k_0,\ k_0 \text{ even}. \tag{1.2.109}
$$

Let $k_0 \in \mathbb{Z}$ be even. It suffices to show that the right-hand side of (1.2.109), temporarily denoted by the symbol $RHS(z,k,k_0)$, satisfies

$$
T(z,k+1)^{-1} RHS(z,k+1,k_0) = RHS(z,k,k_0), \quad k > k_0, \tag{1.2.110}
$$

$$T(z,k_0+1)^{-1}RHS(z,k_0+1,k_0) = \begin{pmatrix} q_+(z,k_0,k_0) \\ s_+(z,k_0,k_0) \end{pmatrix} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}. \tag{1.2.111}$$

One verifies these statements using the following equality,

$$\begin{aligned} &T(z,k+1)^{-1}RHS(z,k+1,k_0) = RHS(z,k,k_0) \\ &\quad + \oint_{\partial\mathbb{D}} \frac{\zeta+z}{\zeta-z} \left(T(z,k+1)^{-1} - T(\zeta,k+1)^{-1}\right) \begin{pmatrix} p_+(\zeta,k+1,k_0) \\ r_+(\zeta,k+1,k_0) \end{pmatrix} d\mu_+(\zeta,k_0), \\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad k \in \mathbb{Z}. \end{aligned} \tag{1.2.112}$$

For $k > k_0$, the last term on the right-hand side of (1.2.112) is equal to zero since for k odd, $T(z,k+1)$ does not depend on z, and for k even, by Corollary 1.2.11, $p_+(\zeta,k+1,k_0)$ and $r_+(\zeta,k+1,k_0)$ are orthogonal in $L^2(\partial\mathbb{D};d\mu_+(\cdot,k_0))$ to $\operatorname{span}\{1,\zeta\}$ and $\operatorname{span}\{1,\zeta^{-1}\}$, respectively. Indeed,

$$\begin{aligned} &\oint_{\partial\mathbb{D}} \frac{\zeta+z}{\zeta-z}\Big(T(z,k+1)^{-1} - T(\zeta,k+1)^{-1}\Big)\begin{pmatrix} p_+(\zeta,k+1,k_0) \\ r_+(\zeta,k+1,k_0) \end{pmatrix} d\mu_+(\zeta,k_0) \\ &\quad = \oint_{\partial\mathbb{D}} \frac{\zeta+z}{\zeta-z}\,\frac{1}{\rho_{k+1}} \begin{pmatrix} 0 & z-\zeta \\ (1/z)-(1/\zeta) & 0 \end{pmatrix} \begin{pmatrix} p_+(\zeta,k+1,k_0) \\ r_+(\zeta,k+1,k_0) \end{pmatrix} d\mu_+(\zeta,k_0) \\ &\quad = \frac{1}{\rho_{k+1}} \oint_{\partial\mathbb{D}} \begin{pmatrix} 0 & -(\zeta+z) \\ (1/\zeta)+(1/z) & 0 \end{pmatrix} \begin{pmatrix} p_+(\zeta,k+1,k_0) \\ r_+(\zeta,k+1,k_0) \end{pmatrix} d\mu_+(\zeta,k_0) \\ &\quad = \frac{1}{\rho_{k+1}} \oint_{\partial\mathbb{D}} \begin{pmatrix} -\overline{((1/\zeta)+\overline{z})}r_+(\zeta,k,k_0) \\ \overline{(\zeta+(1/\overline{z}))}p_+(\zeta,k,k_0) \end{pmatrix} d\mu_+(\zeta,k_0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \end{aligned} \tag{1.2.113}$$

This proves (1.2.110).

For $k = k_0$ one obtains $RHS(z,k_0,k_0) = 0$ since $p_+(\zeta,k_0,k_0) = r_+(\zeta,k_0,k_0) = 1$. By Corollary 1.2.11, $p_+(\zeta,k_0+1,k_0)$ and $r_+(\zeta,k_0+1,k_0)$ are orthogonal to constants in $L^2(\partial\mathbb{D};d\mu_+(\cdot,k_0))$ and by the recursion relation (1.2.17),

$$\begin{aligned} p_+(\zeta,k_0+1,k_0) &= (\zeta+\alpha_{k_0+1})/\rho_{k_0+1}, \\ r_+(\zeta,k_0+1,k_0) &= ((1/\zeta)+\overline{\alpha_{k_0+1}})/\rho_{k_0+1}. \end{aligned} \tag{1.2.114}$$

Thus,

$$
\begin{aligned}
&\oint_{\partial\mathbb{D}} \frac{\zeta+z}{\zeta-z}\Big(T(z,k_0+1)^{-1}-T(\zeta,k_0+1)^{-1}\Big)\begin{pmatrix} p_+(\zeta,k_0+1,k_0) \\ r_+(\zeta,k_0+1,k_0)\end{pmatrix} d\mu_+(\zeta,k_0) \\
&\quad = \oint_{\partial\mathbb{D}} \frac{1}{\rho_{k_0+1}}\begin{pmatrix} -\overline{((1/\zeta)+\overline{z})}, r_+(\zeta,k_0+1,k_0) \\ \overline{(\zeta+(1/\overline{z}))}, p_+(\zeta,k_0+1,k_0)\end{pmatrix} d\mu_+(\zeta,k_0) \\
&\quad = \begin{pmatrix} -\,\|r_+(\zeta,k_0+1,k_0)\|^2_{L^2(\partial\mathbb{D};d\mu_+(\cdot,k_0))} \\ \|p_+(\zeta,k_0+1,k_0)\|^2_{L^2(\partial\mathbb{D};d\mu_+(\cdot,k_0))}\end{pmatrix} = \begin{pmatrix} -1 \\ 1\end{pmatrix}.
\end{aligned} \tag{1.2.115}
$$

This proves (1.2.111).

Next, we prove that

$$
\begin{pmatrix} s_+(z,k,k_0) \\ \widetilde{q}_+(z,k,k_0)\end{pmatrix} = \oint_{\partial\mathbb{D}} \frac{\zeta+z}{\zeta-z}\left(\begin{pmatrix} r_+(\zeta,k,k_0) \\ \widetilde{p}_+(\zeta,k,k_0)\end{pmatrix} - \begin{pmatrix} r_+(z,k,k_0) \\ \widetilde{p}_+(z,k,k_0)\end{pmatrix}\right) d\mu_+(\zeta,k_0),
$$
$$
z\in\mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\}),\ k>k_0,\ k_0 \text{ odd}. \tag{1.2.116}
$$

Let $k_0\in\mathbb{Z}$ be odd. We note that

$$
\begin{pmatrix} u(z,k) \\ v(z,k)\end{pmatrix} = T(z,k)\begin{pmatrix} u(z,k-1) \\ v(z,k-1)\end{pmatrix}
$$

is equivalent to

$$
\begin{pmatrix} v(z,k) \\ \widetilde{u}(z,k)\end{pmatrix} = \widetilde{T}(z,k)\begin{pmatrix} v(z,k-1) \\ \widetilde{u}(z,k-1)\end{pmatrix}, \tag{1.2.117}
$$

where

$$
\widetilde{u}(z,k) = u(z,k)/z, \quad \widetilde{T}(z,k) = \begin{pmatrix} 0 & 1 \\ 1/z & 0\end{pmatrix} T(z,k) \begin{pmatrix} 0 & z \\ 1 & 0\end{pmatrix}. \tag{1.2.118}
$$

Thus, it suffices to show that the right-hand side of (1.2.116), temporarily denoted by $\widetilde{RHS}(z,k,k_0)$, satisfies

$$
\widetilde{T}(z,k+1)^{-1}\widetilde{RHS}(z,k+1,k_0) = \widetilde{RHS}(z,k,k_0), \quad k>k_0, \tag{1.2.119}
$$

$$\widetilde{T}(z,k_0+1)^{-1}\widetilde{RHS}(z,k_0+1,k_0) = \begin{pmatrix} s_+(z,k_0,k_0) \\ \widetilde{q}_+(z,k_0,k_0) \end{pmatrix} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}. \tag{1.2.120}$$

At this point one can follow the first part of the proof replacing T by $\widetilde{T}$, $\left(\begin{smallmatrix} p_+ \\ r_+ \end{smallmatrix}\right)$ by $\left(\begin{smallmatrix} r_+ \\ \widetilde{p}_+ \end{smallmatrix}\right)$, $\left(\begin{smallmatrix} q_+ \\ s_+ \end{smallmatrix}\right)$ by $\left(\begin{smallmatrix} s_+ \\ \widetilde{q}_+ \end{smallmatrix}\right)$, etc.

The result for the remaining polynomials $\widetilde{p}_-(z,k,k_0)$, $r_-(z,k,k_0)$, $\widetilde{q}_-(z,k,k_0)$, and $s_-(z,k,k_0)$ follows similarly. $\square$

Corollary 1.2.14. *Let $k_0 \in \mathbb{Z}$. Then the sets of two-dimensional Laurent polynomials $\left(\begin{smallmatrix} p_\pm(z,k,k_0) \\ r_\pm(z,k,k_0) \end{smallmatrix}\right)_{k \gtreqless k_0}$ and $\left(\begin{smallmatrix} q_\pm(z,k,k_0) \\ s_\pm(z,k,k_0) \end{smallmatrix}\right)_{k \gtreqless k_0}$ satisfy the relation*

$$\begin{pmatrix} q_\pm(z,\cdot,k_0) \\ s_\pm(z,\cdot,k_0) \end{pmatrix} + m_\pm(z,k_0)\begin{pmatrix} p_\pm(z,\cdot,k_0) \\ r_\pm(z,\cdot,k_0) \end{pmatrix} \in \ell^2([k_0,\pm\infty)\cap\mathbb{Z})^2, \quad z \in \mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\}), \tag{1.2.121}$$

for some coefficients $m_\pm(z,k_0)$ given by

$$\begin{aligned} m_\pm(z,k_0) &= \pm(\delta_{k_0}, (U_{\pm,k_0}+zI)(U_{\pm,k_0}-zI)^{-1}\delta_{k_0})_{\ell^2([k_0,\pm\infty)\cap\mathbb{Z})} && (1.2.122) \\ &= \pm \oint_{\partial\mathbb{D}} d\mu_\pm(\zeta,k_0)\,\frac{\zeta+z}{\zeta-z}, \quad z \in \mathbb{C}\backslash\partial\mathbb{D} && (1.2.123) \end{aligned}$$

with

$$m_\pm(0,k_0) = \pm \oint_{\partial\mathbb{D}} d\mu_\pm(\zeta,k_0) = \pm 1. \tag{1.2.124}$$

Proof. Consider the operator

$$C_{\pm,k_0}(z) = \begin{cases} \begin{pmatrix} I & 0 \\ 0 & \pm I \end{pmatrix} ((\mathbb{U}_{\pm,k_0})^\top + zI)((\mathbb{U}_{\pm,k_0})^\top - zI)^{-1}, & k_0 \text{ odd}, \\ \begin{pmatrix} \pm I & 0 \\ 0 & I \end{pmatrix} ((\mathbb{U}_{\pm,k_0})^\top + zI)((\mathbb{U}_{\pm,k_0})^\top - zI)^{-1}, & k_0 \text{ even}, \end{cases} \quad z \in \mathbb{C}\backslash\partial\mathbb{D}, \tag{1.2.125}$$

on $\ell^2(\mathbb{Z})^2$. Since $C_{\pm,k_0}(z)$ is bounded for $z \in \mathbb{C}\backslash\partial\mathbb{D}$ one has

$$\left\{\left(\begin{pmatrix}\delta_{k_0}\\ \delta_{k_0}\end{pmatrix}, C_{\pm,k_0}(z)\begin{pmatrix}\delta_k\\ \delta_k\end{pmatrix}\right)\right\}_{k\in\mathbb{Z}} = \left\{\left(C_{\pm,k_0}(z)^*\begin{pmatrix}\delta_{k_0}\\ \delta_{k_0}\end{pmatrix}, \begin{pmatrix}\delta_k\\ \delta_k\end{pmatrix}\right)\right\}_{k\in\mathbb{Z}} \in \ell^2(\mathbb{Z})^2. \tag{1.2.126}$$

Using the spectral representation for the operator $C_{\pm,k_0}(z)$, Lemma 1.2.13, and equalities (1.2.59)–(1.2.62) one obtains

$$\begin{aligned}\left(\begin{pmatrix}\delta_{k_0}\\ \delta_{k_0}\end{pmatrix}, C_{\pm,k_0}(z)\begin{pmatrix}\delta_k\\ \delta_k\end{pmatrix}\right) &= \oint_{\partial\mathbb{D}} d\mu_\pm(\zeta,k_0)\,\frac{\zeta+z}{\zeta-z}\begin{pmatrix}\widetilde{p}_\pm(\zeta,k,k_0)\\ r_\pm(\zeta,k,k_0)\end{pmatrix}\\ &= \pm\left[\begin{pmatrix}\widetilde{q}_\pm(z,k,k_0)\\ s_\pm(z,k,k_0)\end{pmatrix} + m_\pm(z,k_0)\begin{pmatrix}\widetilde{p}_\pm(z,k,k_0)\\ r_\pm(z,k,k_0)\end{pmatrix}\right], \quad k \gtrless k_0,\end{aligned} \tag{1.2.127}$$

where $m_\pm(z,k_0) = \pm\int_{\partial\mathbb{D}} d\mu_\pm(\zeta,k_0)\,\frac{\zeta+z}{\zeta-z}$. $\square$

Lemma 1.2.15. *Let $k_0 \in \mathbb{Z}$. Then relation* (1.2.121) *uniquely determines the functions $m_\pm(\cdot,k_0)$ on $\mathbb{C}\backslash\partial\mathbb{D}$.*

Proof. We will prove the lemma by contradiction. Assume that there are two functions $m_+(z,k_0)$ and $\widetilde{m}_+(z,k_0)$ satisfying (1.2.121) such that $m_+(z_0,k_0) \neq \widetilde{m}_+(z_0,k_0)$ for some $z_0 \in \mathbb{C}\backslash\partial\mathbb{D}$. Then there are $\lambda_1, \lambda_2 \in \mathbb{C}$ such that the following vector

$$\begin{pmatrix}w_1(z_0,\cdot,k_0)\\ w_2(z_0,\cdot,k_0)\end{pmatrix} = (\lambda_1 m_+(z_0,k_0) + \lambda_2\widetilde{m}_+(z_0,k_0))\begin{pmatrix}p_+(z_0,\cdot,k_0\\ r_+(z_0,\cdot,k_0)\end{pmatrix} \tag{1.2.128}$$

$$+ (\lambda_1+\lambda_2)\begin{pmatrix}q_+(z_0,\cdot,k_0)\\ s_+(z_0,\cdot,k_0)\end{pmatrix} \in \ell^2([k_0,\infty)\cap\mathbb{Z})^2 \tag{1.2.129}$$

is nonzero and satisfies

$$w_1(z_0,k_0,k_0) = \begin{cases} z_0 w_2(z_0,k_0,k_0), & k_0 \text{ odd},\\ w_2(z_0,k_0,k_0), & k_0 \text{ even}.\end{cases} \tag{1.2.130}$$

By Lemma 1.2.3, $\big(w_1(z_0,k,k_0)\big)_{k\geq k_0}$ is an eigenvector of the operator U_{+,k_0} and $z_0 \in \mathbb{C}\backslash\partial\mathbb{D}$ is the corresponding eigenvalue which is impossible since U_{+,k_0} is unitary.

Similarly, one proves the result for $m_-(z,k_0)$. $\square$

Corollary 1.2.16. *There are solutions* $\begin{pmatrix} \psi_\pm(z,k) \\ \chi_\pm(z,k) \end{pmatrix}_{k\in\mathbb{Z}}$ *of* (1.2.17)*, unique up to constant multiples, so that for some* (*and hence for all*) $k_1 \in \mathbb{Z}$*,*

$$\begin{pmatrix} \psi_\pm(z,\cdot) \\ \chi_\pm(z,\cdot) \end{pmatrix} \in \ell^2([k_1,\pm\infty)\cap\mathbb{Z})^2, \quad z \in \mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\}). \tag{1.2.131}$$

Proof. Since any solution of (1.2.17) can be expressed as a linear combination of the polynomials $\begin{pmatrix} p_\pm(z,k,k_0) \\ r_\pm(z,k,k_0) \end{pmatrix}_{k\in\mathbb{Z}}$ and $\begin{pmatrix} q_\pm(z,k,k_0) \\ s_\pm(z,k,k_0) \end{pmatrix}_{k\in\mathbb{Z}}$, existence and uniqueness of the solutions $\begin{pmatrix} \psi_\pm(z,\cdot) \\ \chi_\pm(z,\cdot) \end{pmatrix}_{k\in\mathbb{Z}}$ follow from Corollary 1.2.14 and Lemma 1.2.15, respectively.

□

Lemma 1.2.17. *Let* $z \in \mathbb{C}\backslash\{0\}$ *and* $k_0 \in \mathbb{Z}$*. Then the two-dimensional Laurent polynomials* $\begin{pmatrix} p_+(z,k,k_0) \\ r_+(z,k,k_0) \end{pmatrix}_{k\in\mathbb{Z}}$, $\begin{pmatrix} q_+(z,k,k_0) \\ s_+(z,k,k_0) \end{pmatrix}_{k\in\mathbb{Z}}$, $\begin{pmatrix} p_-(z,k,k_0-1) \\ r_-(z,k,k_0-1) \end{pmatrix}_{k\in\mathbb{Z}}$, $\begin{pmatrix} q_-(z,k,k_0-1) \\ s_-(z,k,k_0-1) \end{pmatrix}_{k\in\mathbb{Z}}$ *satisfy the following relations for all* $k \in \mathbb{Z}$*,*

$$\begin{pmatrix} p_-(z,k,k_0-1) \\ r_-(z,k,k_0-1) \end{pmatrix} = \frac{i\mathrm{Im}(b_{k_0})}{\rho_{k_0}} \begin{pmatrix} p_+(z,k,k_0) \\ r_+(z,k,k_0) \end{pmatrix} + \frac{\mathrm{Re}(b_{k_0})}{\rho_{k_0}} \begin{pmatrix} q_+(z,k,k_0) \\ s_+(z,k,k_0) \end{pmatrix}, \tag{1.2.132}$$
$$\begin{pmatrix} q_-(z,k,k_0-1) \\ s_-(z,k,k_0-1) \end{pmatrix} = \frac{\mathrm{Re}(a_{k_0})}{\rho_{k_0}} \begin{pmatrix} p_+(z,k,k_0) \\ r_+(z,k,k_0) \end{pmatrix} + \frac{i\mathrm{Im}(a_{k_0})}{\rho_{k_0}} \begin{pmatrix} q_+(z,k,k_0) \\ s_+(z,k,k_0) \end{pmatrix}. \tag{1.2.133}$$

Proof. It follows from Definition 1.2.4 that the left- and right-hand sides of (1.2.132) and (1.2.133) satisfy the same recursion relation (1.2.17). Hence, it suffices to check (1.2.132) and (1.2.133) at one point, say, the point $k = k_0$. Using (1.2.4), (1.2.5), (1.2.17), and (1.2.58), one finds the following expressions for the left-hand sides of (1.2.132) and (1.2.133),

$$\begin{pmatrix} p_-(z,k_0,k_0-1) \\ r_-(z,k_0,k_0-1) \end{pmatrix} = \frac{1}{\rho_{k_0}} \begin{pmatrix} zb_{k_0} \\ -\overline{b_{k_0}} \end{pmatrix}, \quad \underbrace{\begin{pmatrix} q_-(z,k_0,k_0-1) \\ s_-(z,k_0,k_0-1) \end{pmatrix} = \frac{1}{\rho_{k_0}} \begin{pmatrix} za_{k_0} \\ \overline{a_{k_0}} \end{pmatrix}}_{k_0 \text{ odd}}, \tag{1.2.134}$$

and

$$\begin{pmatrix} p_-(z,k_0,k_0-1) \\ r_-(z,k_0,k_0-1) \end{pmatrix} = \frac{1}{\rho_{k_0}} \begin{pmatrix} -\overline{b_{k_0}} \\ b_{k_0} \end{pmatrix}, \quad \begin{pmatrix} q_-(z,k_0,k_0-1) \\ s_-(z,k_0,k_0-1) \end{pmatrix} = \frac{1}{\rho_{k_0}} \begin{pmatrix} \overline{a_{k_0}} \\ a_{k_0} \end{pmatrix}, \quad k_0 \text{ even.} \tag{1.2.135}$$

The same result also follows for the right-hand side of (1.2.132), (1.2.133) using (1.2.4), (1.2.5), and the initial conditions (1.2.57). □

Theorem 1.2.18. *Let $k_0 \in \mathbb{Z}$. Then there exist unique functions $M_\pm(\cdot, k_0)$ such that*

$$\begin{pmatrix} u_\pm(z,\cdot,k_0) \\ v_\pm(z,\cdot,k_0) \end{pmatrix} = \begin{pmatrix} q_+(z,\cdot,k_0) \\ s_+(z,\cdot,k_0) \end{pmatrix} + M_\pm(z,k_0) \begin{pmatrix} p_+(z,\cdot,k_0) \\ r_+(z,\cdot,k_0) \end{pmatrix} \in \ell^2([k_0,\pm\infty)\cap\mathbb{Z})^2, \quad z \in \mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\}). \tag{1.2.136}$$

Proof. Assertion (1.2.136) follows from equalities (1.2.59)–(1.2.62), Corollaries 1.2.14 and 1.2.16, and Lemmas 1.2.15 and 1.2.17. □

We will call $u_\pm(z,\cdot,k_0)$ (resp., $v_\pm(z,\cdot,k_0)$) *Weyl–Titchmarsh solutions* of U (resp., $U^\top$). By Corollary 1.2.16, $u_\pm(z,\cdot,k_0)$ and $v_\pm(z,\cdot,k_0)$ are constant multiples of solutions $\psi_\pm(z,\cdot,k_0)$ and $\chi_\pm(z,\cdot,k_0)$. Similarly, we will call $m_\pm(z,k_0)$ as well as $M_\pm(z,k_0)$ the *half-lattice Weyl–Titchmarsh m-functions* associated with $U_{\pm,k_0}$. (See also [169] for a comparison of various alternative notions of Weyl–Titchmarsh m-functions for U_{+,k_0}.)

It follows from Corollary 1.2.14 and 1.2.16 and Lemma 1.2.17 that

$$M_+(z,k_0) = m_+(z,k_0), \quad z \in \mathbb{C}\backslash\partial\mathbb{D}, \tag{1.2.137}$$

$$M_+(0,k_0) = 1, \tag{1.2.138}$$

$$M_-(z,k_0) = \frac{\mathrm{Re}(a_{k_0}) + i\mathrm{Im}(b_{k_0})m_-(z,k_0-1)}{i\mathrm{Im}(a_{k_0}) + \mathrm{Re}(b_{k_0})m_-(z,k_0-1)}, \quad z \in \mathbb{C}\backslash\partial\mathbb{D}, \tag{1.2.139}$$

$$M_-(0,k_0) = \frac{\alpha_{k_0}+1}{\alpha_{k_0}-1}. \tag{1.2.140}$$

In particular, one infers that $M_\pm$ are analytic at $z=0$.

Since (1.2.136) singles out $p_+(z,\cdot,k_0)$, $q_+(z,\cdot,k_0)$, $r_+(z,\cdot,k_0)$, and $s_+(z,\cdot,k_0)$, we now add the following observation.

Remark 1.2.19. One can also define functions $\widehat{M}_\pm(\cdot,k_0)$ such that the following relation holds

$$\begin{pmatrix}\widehat{u}_\pm(z,\cdot,k_0)\\ \widehat{v}_\pm(z,\cdot,k_0)\end{pmatrix} = \begin{pmatrix}q_-(z,\cdot,k_0)\\ s_-(z,\cdot,k_0)\end{pmatrix} + \widehat{M}_\pm(z,k_0)\begin{pmatrix}p_-(z,\cdot,k_0)\\ r_-(z,\cdot,k_0)\end{pmatrix} \in \ell^2([k_0,\pm\infty)\cap\mathbb{Z})^2,$$
$$z\in\mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\}). \tag{1.2.141}$$

Applying Corollary 1.2.16, $\widehat{u}_\pm(z,\cdot,k_0)$ and $\widehat{v}_\pm(z,\cdot,k_0)$ are also constant multiples of $\psi_\pm(z,\cdot,k_0)$ and $\chi_\pm(z,\cdot,k_0)$ (hence they are constant multiples of $u_\pm(z,\cdot,k_0)$ and $v_\pm(z,\cdot,k_0)$). It follows from Corollaries 1.2.14 and 1.2.16 and Lemmas 1.2.15 and 1.2.17, that $\widehat{M}_\pm(\cdot,k_0)$ are uniquely defined and satisfy the relations

$$\widehat{M}_+(z,k_0-1) = \frac{\mathrm{Re}(a_{k_0}) - i\mathrm{Im}(a_{k_0})m_+(z,k_0)}{-i\mathrm{Im}(b_{k_0}) + \mathrm{Re}(b_{k_0})m_+(z,k_0)}, \quad z\in\mathbb{C}\backslash\partial\mathbb{D}, \tag{1.2.142}$$
$$\widehat{M}_-(z,k_0) = m_-(z,k_0), \quad z\in\mathbb{C}\backslash\partial\mathbb{D}. \tag{1.2.143}$$

Moreover, one derives from (1.2.139) and (1.2.143) that

$$M_\pm(z,k_0) = \frac{\mathrm{Re}(a_{k_0}) + i\mathrm{Im}(b_{k_0})\widehat{M}_\pm(z,k_0-1)}{i\mathrm{Im}(a_{k_0}) + \mathrm{Re}(b_{k_0})\widehat{M}_\pm(z,k_0-1)}, \quad z\in\mathbb{C}\backslash\partial\mathbb{D}. \tag{1.2.144}$$

In this chapter we will only use $\left(\begin{smallmatrix}u_\pm(z,\cdot,k_0)\\ v_\pm(z,\cdot,k_0)\end{smallmatrix}\right)$ and $M_\pm(z,k_0)$.

Lemma 1.2.20. *Let $k \in \mathbb{Z}$. Then the functions $M_+(\cdot,k)|_{\mathbb{D}}$ (resp., $M_-(\cdot,k)|_{\mathbb{D}}$) are Caratheodory (resp., anti-Caratheodory) functions. Moreover, $M_\pm$ satisfy the following Riccati-type equation*

$$
\begin{aligned}
&(z\overline{b_k} - b_k)M_\pm(z,k-1)M_\pm(z,k) + (z\overline{b_k} + b_k)M_\pm(z,k) - (z\overline{a_k} + a_k)M_\pm(z,k-1) \\
&\quad = z\overline{a_k} - a_k, \quad z \in \mathbb{C}\backslash\partial\mathbb{D}. \qquad (1.2.145)
\end{aligned}
$$

Proof. It follows from (1.2.123) and Theorem A.2 that $m_\pm(z,k_0)$ are Caratheodory and anti-Caratheodory functions, respectively. From (1.2.137) one concludes that $M_+(z,k_0)$ is also a Caratheodory function. Using (1.2.139) one verifies that $M_-(z,k_0)$ is analytic in $\mathbb{D}$ since $\mathrm{Re}(m_-(z,k_0)) < 0$ and that

$$
\begin{aligned}
\mathrm{Re}(M_-(z,k_0)) &= \mathrm{Re}\left(\frac{\mathrm{Re}(a_{k_0}) + i\mathrm{Im}(b_{k_0})m_-(z,k_0-1)}{i\mathrm{Im}(a_{k_0}) + \mathrm{Re}(b_{k_0})m_-(z,k_0-1)}\right) \\
&= \frac{\mathrm{Re}(a_{k_0})\mathrm{Re}(b_{k_0}) + \mathrm{Im}(a_{k_0})\mathrm{Im}(b_{k_0})}{|i\mathrm{Im}(a_{k_0}) + \mathrm{Re}(b_{k_0})m_-(z,k_0-1)|^2}\mathrm{Re}(m_-(z,k_0-1)) \\
&= \frac{\rho_{k_0}^2\mathrm{Re}(m_-(z,k_0-1))}{|i\mathrm{Im}(a_{k_0}) + \mathrm{Re}(b_{k_0})m_-(z,k_0-1)|^2} < 0. \qquad (1.2.146)
\end{aligned}
$$

Hence, $M_-(z,k_0)$ is an anti-Caratheodory function.

Next, consider the 2×2 matrix

$$
D(z,k_0) = \big(d_{\ell,\ell'}(z,k_0)\big)_{\ell,\ell'=1,2} = \frac{1}{2\rho_{k_0}}\begin{cases}\begin{pmatrix}\overline{a_{k_0}} + a_{k_0}/z & \overline{a_{k_0}} - a_{k_0}/z \\ \overline{b_{k_0}} - b_{k_0}/z & \overline{b_{k_0}} + b_{k_0}/z\end{pmatrix}, & k_0 \text{ odd}, \\ \begin{pmatrix}z\overline{a_{k_0}} + a_{k_0} & z\overline{a_{k_0}} - a_{k_0} \\ z\overline{b_{k_0}} - b_{k_0} & z\overline{b_{k_0}} + b_{k_0}\end{pmatrix}, & k_0 \text{ even},\end{cases}
$$
$$
z \in \mathbb{C}\backslash\{0\},\ k_0 \in \mathbb{Z}. \qquad (1.2.147)
$$

It follows from (1.2.4), (1.2.5), and Definition 1.2.4 that $D(z,k_0)$ satisfies

$$
\begin{pmatrix}p_+(z,\cdot,k_0-1) & q_+(z,\cdot,k_0-1) \\ r_+(z,\cdot,k_0-1) & s_+(z,\cdot,k_0-1)\end{pmatrix} = \begin{pmatrix}p_+(z,\cdot,k_0) & q_+(z,\cdot,k_0) \\ r_+(z,\cdot,k_0) & s_+(z,\cdot,k_0)\end{pmatrix} D(z,k_0). \quad (1.2.148)
$$

Thus, using Theorem 1.2.18 one finds

$$M_\pm(z,k_0) = \frac{d_{1,2}(z,k_0) + d_{1,1}(z,k_0)M_\pm(z,k_0-1)}{d_{2,2}(z,k_0) + d_{2,1}(z,k_0)M_\pm(z,k_0-1)}. \tag{1.2.149}$$

□

In addition, we introduce the functions $\Phi_\pm(\cdot,k)$, $k \in \mathbb{Z}$, by

$$\Phi_\pm(z,k) = \frac{M_\pm(z,k)-1}{M_\pm(z,k)+1}, \quad z \in \mathbb{C}\backslash\partial\mathbb{D}. \tag{1.2.150}$$

One then verifies,

$$M_\pm(z,k) = \frac{1+\Phi_\pm(z,k)}{1-\Phi_\pm(z,k)}, \quad z \in \mathbb{C}\backslash\partial\mathbb{D}. \tag{1.2.151}$$

Moreover, we extend these functions to the unit circle $\partial\mathbb{D}$ by taking the radial limits which exist and are finite for μ_0-almost every $\zeta \in \partial\mathbb{D}$,

$$M_\pm(\zeta,k) = \lim_{r\uparrow 1} M_\pm(r\zeta,k), \tag{1.2.152}$$

$$\Phi_\pm(\zeta,k) = \lim_{r\uparrow 1} \Phi_\pm(r\zeta,k), \quad k \in \mathbb{Z}. \tag{1.2.153}$$

Lemma 1.2.21. *Let $z \in \mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\})$, $k_0, k \in \mathbb{Z}$. Then the functions $\Phi_\pm(\cdot,k)$ satisfy*

$$\Phi_\pm(z,k) = \begin{cases} z\frac{v_\pm(z,k,k_0)}{u_\pm(z,k,k_0)}, & k \text{ odd}, \\ \frac{u_\pm(z,k,k_0)}{v_\pm(z,k,k_0)}, & k \text{ even}, \end{cases} \tag{1.2.154}$$

where $u_\pm(\cdot,k,k_0)$ and $v_\pm(\cdot,k,k_0)$ are the polynomials defined in (1.2.136).

Proof. Using Corollary 1.2.16 it suffices to assume $k = k_0$. Then the statement follows immediately from (1.2.57) and (1.2.150). □

Lemma 1.2.22. *Let $k \in \mathbb{Z}$. Then the functions $\Phi_+(\cdot,k)|_{\mathbb{D}}$ (resp., $\Phi_-(\cdot,k)|_{\mathbb{D}}$) are Schur (resp., anti-Schur) functions. Moreover, $\Phi_\pm$ satisfy the following Riccati-type* *equation*

$$\alpha_k \Phi_\pm(z,k-1)\Phi_\pm(z,k) - \Phi_\pm(z,k-1) + z\Phi_\pm(z,k) = \overline{\alpha_k} z, \quad z \in \mathbb{C}\backslash\partial\mathbb{D},\ k \in \mathbb{Z}. \tag{1.2.155}$$

Proof. It follows from Lemma 1.2.20 and (1.2.150) that the functions $\Phi_+(\cdot,k)|_{\mathbb{D}}$ (resp., $\Phi_-(\cdot,k)|_{\mathbb{D}}$) are Schur (resp., anti-Schur) functions.

Let k be odd. Then applying Lemma 1.2.21 and the recursion relation (1.2.17) one obtains

$$\begin{aligned}\Phi_\pm(z,k) &= \frac{z v_\pm(z,k,k_0)}{u_\pm(z,k,k_0)} = \frac{u_\pm(z,k-1,k_0) + z\overline{\alpha_k} v_\pm(z,k-1,k_0)}{\alpha_k u_\pm(z,k-1,k_0) + z v_\pm(z,k-1,k_0)} \\ &= \frac{\Phi_\pm(z,k-1) + z\overline{\alpha_k}}{\alpha_k \Phi_\pm(z,k-1) + z}.\end{aligned} \tag{1.2.156}$$

For k even, one similarly obtains

$$\begin{aligned}\Phi_\pm(z,k) &= \frac{u_\pm(z,k,k_0)}{v_\pm(z,k,k_0)} = \frac{\overline{\alpha_k} u_\pm(z,k-1,k_0) + v_\pm(z,k-1,k_0)}{u_\pm(z,k-1,k_0) + \alpha_k v_\pm(z,k-1,k_0)} \\ &= \frac{z\overline{\alpha_k} + \Phi_\pm(z,k-1)}{z + \alpha_k \Phi_\pm(z,k-1)}.\end{aligned} \tag{1.2.157}$$

□

Remark 1.2.23. (i) In the special case $\alpha = \{\alpha_k\}_{k\in\mathbb{Z}} = 0$, one obtains

$$M_\pm(z,k) = \pm 1, \quad \Phi_+(z,k) = 0, \quad 1/\Phi_-(z,k) = 0, \quad z \in \mathbb{C},\ k \in \mathbb{Z}. \tag{1.2.158}$$

Thus, strictly speaking, one should always consider $1/\Phi_-$ rather than Φ_- and hence refer to the Riccati-type equation of $1/\Phi_-$,

$$\overline{\alpha_k} z \frac{1}{\Phi_-(z,k-1)} \frac{1}{\Phi_-(z,k)} + \frac{1}{\Phi_-(z,k)} - z\frac{1}{\Phi_-(z,k-1)} = \alpha_k, \quad z \in \mathbb{C}\backslash\partial\mathbb{D},\ k \in \mathbb{Z}, \tag{1.2.159}$$

rather than that of Φ_-, etc. For simplicity of notation, we will avoid this distinction between Φ_- and $1/\Phi_-$ and usually just invoke Φ_- whenever confusions are unlikely.

(ii) We note that $M_\pm(z,k)$ and $\Phi_\pm(z,k)$, $z \in \partial\mathbb{D}$, $k \in \mathbb{Z}$, have nontangential limits to $\partial\mathbb{D}$ μ_0-a.e. In particular, the Riccati-type equations (1.2.145), (1.2.155), and (1.2.159) extend to $\partial\mathbb{D}$ μ_0-a.e.

The Riccati-type equation for the Caratheodory function Φ_+ implies the following absolutely convergent expansion,

$$\Phi_+(z,k) = \sum_{j=1}^{\infty} \phi_{+,j}(k) z^j, \quad z \in \mathbb{D},\ k \in \mathbb{Z}, \tag{1.2.160}$$

$$\begin{aligned} \phi_{+,1}(k) &= -\overline{\alpha_{k+1}}, \\ \phi_{+,2}(k) &= -\rho_{k+1}^2\, \overline{\alpha_{k+2}}, \\ \phi_{+,j}(k) &= \alpha_{k+1} \sum_{\ell=1}^{j} \phi_{+,j-\ell}(k+1)\phi_{+,\ell}(k) + \phi_{+,j-1}(k+1),\ j \geq 3. \end{aligned} \tag{1.2.161}$$

The corresponding Riccati-type equation for the Caratheodory function $1/\Phi_-(z,k)$ implies the absolutely convergent expansion

$$1/\Phi_-(z,k) = \sum_{j=0}^{\infty} [1/\phi_{-,j}(k)] z^j, \quad z \in \mathbb{D},\ k \in \mathbb{Z}, \tag{1.2.162}$$

$$\begin{aligned} 1/\phi_{-,0}(k) &= \alpha_k, \\ 1/\phi_{-,1}(k) &= \rho_k^2\, \alpha_{k-1}, \\ 1/\phi_{-,j}(k) &= -\overline{\alpha_k} \sum_{\ell=0}^{j-1} [1/\phi_{-,j-1-\ell}(k-1)][1/\phi_{-,\ell}(k)] + [1/\phi_{-,j-1}(k-1)],\ j \geq 2. \end{aligned} \tag{1.2.163}$$

Next, we introduce the following notation for the half-open arc on the unit circle,

$$\operatorname{Arc}\big(\big(e^{i\theta_1}, e^{i\theta_2}\big]\big) = \big\{e^{i\theta} \in \partial\mathbb{D} \,|\, \theta_1 < \theta \leq \theta_2\big\}, \quad \theta_1 \in [0, 2\pi),\ \theta_1 < \theta_2 \leq \theta_1 + 2\pi. \tag{1.2.164}$$

In the same manner we also introduce open and closed arcs on $\partial\mathbb{D}$, $\mathrm{Arc}\big(\big(e^{i\theta_1}, e^{i\theta_2}\big)\big)$ and $\mathrm{Arc}\big(\big[e^{i\theta_1}, e^{i\theta_2}\big]\big)$, respectively. Moreover, we identify the unit circle $\partial\mathbb{D}$ with the arcs of the form $\mathrm{Arc}\big(\big(e^{i\theta_1}, e^{i\theta_1+2\pi}\big]\big)$, $\theta_1 \in [0, 2\pi)$.

The following result is the unitary operator analog of a version of Stone's formula relating resolvents of self-adjoint operators with spectral projections in the weak sense (cf., e.g., [43, p. 1203]).

Lemma 1.2.24. *Let U be a unitary operator in a complex separable Hilbert space $\mathcal{H}$ (with scalar product denoted by $(\cdot,\cdot)_{\mathcal{H}}$, linear in the second factor), $f, g \in \mathcal{H}$, and denote by $\{E_U(\zeta)\}_{\zeta\in\partial\mathbb{D}}$ the family of self-adjoint right-continuous spectral projections associated with U, that is, $(f, Ug)_{\mathcal{H}} = \int_{\partial\mathbb{D}} d(f, E_U(\zeta)g)_{\mathcal{H}}\, \zeta$. Moreover, let $\theta_1 \in [0, 2\pi)$, $\theta_1 < \theta_2 \leq \theta_1 + 2\pi$, $F \in C(\partial\mathbb{D})$, and denote by $C(U, z)$ the operator*

$$C(U, z) = (U + zI_{\mathcal{H}})(U - zI_{\mathcal{H}})^{-1} = I_{\mathcal{H}} + 2z(U - zI_{\mathcal{H}})^{-1}, \quad z \in \mathbb{C}\backslash\sigma(U) \quad (1.2.165)$$

with $I_{\mathcal{H}}$ the identity operator in $\mathcal{H}$. Then,

$$\begin{aligned} &\big(f, F(U)E_U\big(\mathrm{Arc}\big(\big(e^{i\theta_1}, e^{i\theta_2}\big]\big)\big)g\big)_{\mathcal{H}} \\ &\quad = \lim_{\delta\downarrow 0}\lim_{r\uparrow 1} \int_{\theta_1+\delta}^{\theta_2+\delta} \frac{d\theta}{4\pi}\, F\big(e^{i\theta}\big)\big[\big(f, C\big(U, re^{i\theta}\big)g\big)_{\mathcal{H}} - \big(f, C\big(U, r^{-1}e^{i\theta}\big)g\big)_{\mathcal{H}}\big]. \end{aligned} \quad (1.2.166)$$

Similar formulas hold for $\mathrm{Arc}\big(\big(e^{i\theta_1}, e^{i\theta_2}\big)\big)$ and $\mathrm{Arc}\big(\big[e^{i\theta_1}, e^{i\theta_2}\big]\big)$.

Proof. First one notices that

$$C\big(U, re^{i\theta}\big)^* = -C\big(U, r^{-1}e^{i\theta}\big), \quad r \in (0, \infty)\backslash\{1\},\ \theta \in [0, 2\pi]. \quad (1.2.167)$$

Next, introducing the characteristic function χ_A of a set $A \subseteq \partial\mathbb{D}$ and assuming $F \geq 0$, one obtains that

$$
\begin{aligned}
&\big(F(U)^{1/2}E_U\big(\mathrm{Arc}\big(\big(e^{i\theta_1},e^{i\theta_2}\big]\big)\big)f, C(U,z)F(U)^{1/2}E_U\big(\mathrm{Arc}\big(\big(e^{i\theta_1},e^{i\theta_2}\big]\big)\big)f\big)_{\mathcal{H}} \\
&\quad = \int_{\partial\mathbb{D}} d\big(f,E_U\big(e^{i\theta}\big)f\big)_{\mathcal{H}}\, F\big(e^{i\theta}\big)\chi_{(e^{i\theta_1},e^{i\theta_2}]}\big(e^{i\theta}\big)\frac{e^{i\theta}+z}{e^{i\theta}-z} \\
&\quad = \int_{\partial\mathbb{D}} d\Big(F(U)^{1/2}\chi_{(e^{i\theta_1},e^{i\theta_2}]}(U)f, E_U\big(e^{i\theta}\big)F(U)^{1/2}\chi_{(e^{i\theta_1},e^{i\theta_2}]}(U)f\Big)_{\mathcal{H}}\frac{e^{i\theta}+z}{e^{i\theta}-z}, \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad z\in\partial\mathbb{D}
\end{aligned} \tag{1.2.168}
$$

is a Caratheodory function and hence (1.2.166) for $g=f$ follows from (A.5). If F is not nonnegative, one decomposes F as $F=(F_1-F_2)+i(F_3-F_4)$ with $F_j\geq 0$ and applies (1.2.168) to each F_j, $j\in\{1,2,3,4\}$. The general case $g\neq f$ then follows from the special case $g=f$ by polarization. $\square$

Next, in addition to the definition of $\widetilde{p}_\pm$ and $\widetilde{q}_\pm$ in (1.2.59)–(1.2.62) we introduce $\widetilde{u}_+$ by

$$
\begin{pmatrix}\widetilde{u}_+(z,\cdot,k_0)\\ v_+(z,\cdot,k_0)\end{pmatrix} = \begin{pmatrix}\widetilde{q}_+(z,\cdot,k_0)\\ s_+(z,\cdot,k_0)\end{pmatrix} + m_+(z,k_0)\begin{pmatrix}\widetilde{p}_+(z,\cdot,k_0)\\ r_+(z,\cdot,k_0)\end{pmatrix}\in\ell^2([k_0,\infty)\cap\mathbb{Z})^2, \quad z\in\mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\}) \tag{1.2.169}
$$

and the functions $\widetilde{t}_-$ and w_- by

$$
\begin{pmatrix}\widetilde{t}_-(z,\cdot,k_0)\\ w_-(z,\cdot,k_0)\end{pmatrix} = \begin{pmatrix}\widetilde{q}_-(z,\cdot,k_0)\\ s_-(z,\cdot,k_0)\end{pmatrix} + m_-(z,k_0)\begin{pmatrix}\widetilde{p}_-(z,\cdot,k_0)\\ r_-(z,\cdot,k_0)\end{pmatrix}\in\ell^2((-\infty,k_0]\cap\mathbb{Z})^2, \quad z\in\mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\}). \tag{1.2.170}
$$

One then computes for the resolvent of $U_{\pm,k_0}$ in terms of its matrix representation in the standard basis of $\ell^2([k_0,\pm\infty)\cap\mathbb{Z})$,

$$
(U_{+,k_0}-zI)^{-1}(k,k') = \frac{1}{2z}\begin{cases}\widetilde{p}_+(z,k,k_0)v_+(z,k',k_0), & k<k' \text{ and } k=k' \text{ odd},\\ r_+(z,k',k_0)\widetilde{u}_+(z,k,k_0), & k'<k \text{ and } k=k' \text{ even},\end{cases}
$$

$$z \in \mathbb{C}\backslash(\partial\mathbb{D} \cup \{0\}),\ k_0 \in \mathbb{Z},\ k, k' \in [k_0, \infty) \cap \mathbb{Z}, \tag{1.2.171}$$

$$(U_{-,k_0} - zI)^{-1}(k, k') = \frac{1}{2z}\begin{cases} \widetilde{t}_-(z, k, k_0) r_-(z, k', k_0), & k < k' \text{ and } k = k' \text{ odd}, \\ w_-(z, k', k_0) \widetilde{p}_-(z, k, k_0), & k' < k \text{ and } k = k' \text{ even}, \end{cases}$$

$$z \in \mathbb{C}\backslash(\partial\mathbb{D} \cup \{0\}),\ k_0 \in \mathbb{Z},\ k, k' \in (-\infty, k_0] \cap \mathbb{Z}. \tag{1.2.172}$$

The proof of these formulas repeats the proof of the analogous result, Lemma 1.3.1, for the full-lattice CMV operator U and hence we omit it here.

We finish this section with an explicit connection between the family of spectral projections of $U_{\pm,k_0}$ and the spectral function $\mu_\pm(\cdot, k_0)$, supplementing relation (1.2.70).

Lemma 1.2.25. *Let $f, g \in \ell_0^\infty([k_0, \pm\infty) \cap \mathbb{Z})$, $F \in C(\partial\mathbb{D})$, and $\theta_1 \in [0, 2\pi)$, $\theta_1 < \theta_2 \leq \theta_1 + 2\pi$. Then,*

$$\begin{aligned} &\big(f, F(U_{\pm,k_0}) E_{U_{\pm,k_0}}\big(\mathrm{Arc}\big(\big(e^{i\theta_1}, e^{i\theta_2}\big]\big)\big) g\big)_{\ell^2([k_0,\pm\infty)\cap\mathbb{Z})} \\ &\quad = \big(\widehat{f}_\pm(\cdot, k_0), M_F M_{\chi_{\mathrm{Arc}((e^{i\theta_1}, e^{i\theta_2}])}} \widehat{g}_\pm(\cdot, k_0)\big)_{L^2(\partial\mathbb{D}; d\mu_\pm(\cdot, k_0))}, \end{aligned} \tag{1.2.173}$$

where we introduced the notation

$$\widehat{h}_\pm(\zeta, k_0) = \sum_{k=k_0}^{\pm\infty} r_\pm(\zeta, k, k_0) h(k), \quad \zeta \in \partial\mathbb{D},\ h \in \ell_0^\infty([k_0, \pm\infty) \cap \mathbb{Z}), \tag{1.2.174}$$

and M_G denotes the maximally defined operator of multiplication by the $d\mu_\pm(\cdot, k_0)$-measurable function G in the Hilbert space $L^2(\partial\mathbb{D}; d\mu_\pm(\cdot, k_0))$,

$$\begin{aligned} &(M_G \widehat{h})(\zeta) = G(\zeta) \widehat{h}(\zeta) \text{ for a.e. } \zeta \in \partial\mathbb{D}, \\ &\widehat{h} \in \mathrm{dom}(M_G) = \{\widehat{k} \in L^2(\partial\mathbb{D}; d\mu_\pm(\cdot, k_0)) \,|\, G\widehat{k} \in L^2(\partial\mathbb{D}; d\mu_\pm(\cdot, k_0))\}. \end{aligned} \tag{1.2.175}$$

Proof. It suffices to consider U_{+,k_0} only. Inserting (1.2.171) into (1.2.166) and observing (1.2.169) leads to

$$\big(f, F(U_{+,k_0}) E_{U_{+,k_0}}\big(\mathrm{Arc}\big(\big(e^{i\theta_1}, e^{i\theta_2}\big]\big)\big) g\big)_{\ell^2([k_0,\infty)\cap\mathbb{Z})}$$

$$
\begin{aligned}
&= \lim_{\delta\downarrow 0}\lim_{r\uparrow 1}\int_{\theta_1+\delta}^{\theta_2+\delta}\frac{d\theta}{4\pi}\,F\big(e^{i\theta}\big)\bigg[\sum_{k=k_0}^{\infty}\sum_{k'=k_0}^{\infty}\overline{f(k)}g(k')[C\big(U_{+,k_0},re^{i\theta}\big)(k,k') \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad - C\big(U_{+,k_0},r^{-1}e^{i\theta}\big)(k,k')\bigg] \\
&= \sum_{k=k_0}^{\infty}\overline{f(k)}\bigg\{\sum_{\substack{k_0\le k'<k\\ k'=k\,\text{even}}} g(k')\lim_{\delta\downarrow 0}\lim_{r\uparrow 1}\frac{1}{4\pi}\int_{\theta_1+\delta}^{\theta_2+\delta} d\theta\,F\big(e^{i\theta}\big)\widetilde{p}_+\big(e^{i\theta},k,k_0\big) \\
&\qquad\qquad\qquad \times r_+\big(e^{i\theta},k',k_0\big)\big[m_+\big(re^{i\theta},k_0\big)-m_+\big(r^{-1}e^{i\theta},k_0\big)\big] \\
&\qquad \sum_{\substack{k_0\le k<k'\\ k'=k\,\text{odd}}} g(k')\lim_{\delta\downarrow 0}\lim_{r\uparrow 1}\frac{1}{4\pi}\int_{\theta_1+\delta}^{\theta_2+\delta} d\theta\,F\big(e^{i\theta}\big)\widetilde{p}_+\big(e^{i\theta},k,k_0\big) \\
&\qquad\qquad\qquad \times r_+\big(e^{i\theta},k',k_0\big)\big[m_+\big(re^{i\theta},k_0\big)-m_+\big(r^{-1}e^{i\theta},k_0\big)\big]\bigg\}.
\end{aligned}
\tag{1.2.176}
$$

Here we freely interchanged the θ-integral with the sums over k and k' (the latter are finite) and also replaced $\widetilde{p}_+\big(r^{\pm 1}e^{i\theta},k,k_0\big)$ and $r_+\big(r^{\pm 1}e^{i\theta},k,k_0\big)$ by $\widetilde{p}_+\big(e^{i\theta},k,k_0\big)$ and $r_+\big(e^{i\theta},k,k_0\big)$. The latter is permissible since by (A.16),

$$
\big|\big(1-r^{\pm 1}\big)\mathrm{Re}\big(m_+\big(r^{\pm 1}e^{i\theta}\big)\big)\big| \underset{r\to 1}{=} O(1), \quad \big|\big(1-r^{\pm 1}\big)\mathrm{Im}\big(m_+\big(r^{\pm 1}e^{i\theta}\big)\big)\big| \underset{r\to 1}{=} o(1).
\tag{1.2.177}
$$

Finally, since $\widetilde{p}_+(\zeta,k,k_0) = \overline{r_+(\zeta,k,k_0)}$, $\zeta\in\partial\mathbb{D}$ by (1.2.63) and $m_+(re^{i\theta},k_0) = -\overline{m_+(\frac{1}{r}e^{i\theta},k_0)}$ by (A.19), one infers

$$
\begin{aligned}
&\big(f,F(U_{+,k_0})E_{U_{+,k_0}}\big(\mathrm{Arc}\big(\big(e^{i\theta_1},e^{i\theta_2}\big]\big)\big)g\big)_{\ell^2([k_0,\infty)\cap\mathbb{Z})} \\
&\quad = \sum_{k=k_0}^{\infty}\sum_{k'=k_0}^{\infty}\overline{f(k)}g(k')\lim_{\delta\downarrow 0}\lim_{r\uparrow 1}\int_{\theta_1+\delta}^{\theta_2+\delta}\frac{d\theta}{2\pi}\,F\big(e^{i\theta}\big)\widetilde{p}_+\big(e^{i\theta},k,k_0\big)r_+\big(e^{i\theta},k',k_0\big) \\
&\qquad\qquad\qquad\qquad\qquad\qquad \times \mathrm{Re}\big(m_+\big(re^{i\theta},k_0\big)\big) \\
&\quad = \sum_{k=k_0}^{\infty}\sum_{k'=k_0}^{\infty}\overline{f(k)}g(k')\int_{(\theta_1,\theta_2]} d\mu_+\big(e^{i\theta},k_0\big)\,F\big(e^{i\theta}\big)\overline{r_+\big(e^{i\theta},k,k_0\big)}r_+\big(e^{i\theta},k',k_0\big) \\
&\quad = \int_{(\theta_1,\theta_2]} d\mu_+\big(e^{i\theta},k_0\big)\,F\big(e^{i\theta}\big)\overline{\widehat{f}_+\big(e^{i\theta},k_0\big)}\widehat{g}_+\big(e^{i\theta},k_0\big)
\end{aligned}
$$

$$= \left(\widehat{f}_+(\cdot,k_0), M_F M_{\chi_{\mathrm{Arc}((e^{i\theta_1},e^{i\theta_2}])}} \widehat{g}_+(\cdot,k_0)\right)_{L^2(\partial\mathbb{D};d\mu_+(\cdot,k_0))}, \tag{1.2.178}$$

interchanging the (finite) sums over k and k' and the $d\mu(\cdot,k_0)$-integral once more. $\square$

Finally, this section would not be complete if we wouldn't briefly mention the analogs of Weyl disks for finite interval problems and their behavior in the limit where the finite interval tends to a half-lattice. Before starting the analysis, we note the following geometric fact: Let $p,q,r,s \in \mathbb{C}$, $|p| \neq |r|$. Then, the set of points $m(\theta) \in \mathbb{C}$ given by

$$m(\theta) = -\frac{q + se^{i\theta}}{p + re^{i\theta}}, \quad \theta \in [0,2\pi), \tag{1.2.179}$$

describes a circle in $\mathbb{C}$ with radius $R > 0$ and center $C \in \mathbb{C}$ given by

$$R = \frac{|qr - ps|}{\big||p|^2 - |r|^2\big|}, \quad C = -\frac{s}{r} - \frac{\overline{p}}{r}\frac{qr - ps}{|p|^2 - |r|^2}. \tag{1.2.180}$$

To introduce the analog of $\mathbb{U}_{+,k_0}^{(s)}$ and $\big(\mathbb{U}_{+,k_0}^{(s)}\big)^\top$ on a finite interval $[k_0,k_1] \cap \mathbb{Z}$, we choose $\alpha_{k_0} = e^{is_0}$, $\alpha_{k_1+1} = e^{is_1}$, $s_0, s_1 \in [0,2\pi)$. Then the operator $\mathbb{U}_{+,k_0}^{(s_0)}$ splits into a direct sum of two operators $\mathbb{U}_{[k_0,k_1]}^{(s_0,s_1)}$ and $\mathbb{U}_{+,k_1+1}^{(s_1)}$

$$\mathbb{U}_{+,k_0}^{(s_0)} = \mathbb{U}_{[k_0,k_1]}^{(s_0,s_1)} \oplus \mathbb{U}_{+,k_1+1}^{(s_1)} \tag{1.2.181}$$

acting on $\ell^2([k_0,k_1] \cap \mathbb{Z})$ and $\ell^2([k_1+1,\infty) \cap \mathbb{Z})$, respectively. Then, repeating the proof of Lemma 1.2.3 one obtains the following result for the CMV operator $\mathbb{U}_{[k_0,k_1]}^{(s_0,s_1)}$:

$$\mathbb{U}_{[k_0,k_1]}^{(s_0,s_1)} \begin{pmatrix} u(z,\cdot) \\ v(z,\cdot) \end{pmatrix} = z \begin{pmatrix} u(z,\cdot) \\ v(z,\cdot) \end{pmatrix}, \quad z \in \mathbb{C}\backslash\{0\} \tag{1.2.182}$$

is satisfied by $\left(\begin{smallmatrix} u(z,k) \\ v(z,k) \end{smallmatrix}\right)_{k \in [k_0,k_1] \cap \mathbb{Z}}$ such that

$$\begin{pmatrix} u(z,k) \\ v(z,k) \end{pmatrix} = T(z,k) \begin{pmatrix} u(z,k-1) \\ v(z,k-1) \end{pmatrix}, \quad k \in [k_0+1,k_1] \cap \mathbb{Z}, \tag{1.2.183}$$

$$u(z,k_0) = \begin{cases} z e^{is_0} v(z,k_0), & k_0 \text{ odd}, \\ e^{-is_0} v(z,k_0), & k_0 \text{ even}, \end{cases} \tag{1.2.184}$$

$$u(z,k_1) = \begin{cases} -e^{is_1} v(z,k_1), & k_1 \text{ odd}, \\ -z e^{-is_1} v(z,k_1), & k_1 \text{ even}. \end{cases} \tag{1.2.185}$$

To simplify matters we now put $s_0 = 0$ in the following. Moreover, we first treat the case k_0 even and k_1 odd. Then $\left(\begin{smallmatrix} p_+(z,k,k_0) \\ r_+(z,k,k_0) \end{smallmatrix}\right)$ satisfies (1.2.183) and (1.2.184) and hence there exists a coefficient $m_{+,s_1}(z,k_1,k_0)$ such that

$$\begin{pmatrix} q_+(z,k,k_0) \\ s_+(z,k,k_0) \end{pmatrix} + m_{+,s_1}(z,k_0,k_1) \begin{pmatrix} p_+(z,k,k_0) \\ r_+(z,k,k_0) \end{pmatrix} \tag{1.2.186}$$

satisfies (1.2.185). One computes

$$m_{+,s_1}(z,k_1,k_0) = -\frac{q_+(z,k_1,k_0) + s_+(z,k_1,k_0) e^{is_1}}{p_+(z,k_1,k_0) + r_+(z,k_1,k_0) e^{is_1}}. \tag{1.2.187}$$

By (1.2.179), this describes a (Weyl–Titchmarsh) circle as s_1 varies in $[0, 2\pi)$ of radius

$$\begin{aligned} R(z,k_1) &= \frac{|q_+(z,k_1,k_0) r_+(z,k_1,k_0) - p_+(z,k_1,k_0) s_+(z,k_1,k_0))|}{\big| |p_+(z,k_1,k_0)|^2 - |r_+(z,k_1,k_0)|^2 \big|} \\ &= \frac{2}{\big| |p_+(z,k_1,k_0)|^2 - |r_+(z,k_1,k_0)|^2 \big|} \end{aligned} \tag{1.2.188}$$

since

$$W\Bigg(\begin{pmatrix} p_+(z,k_1,k_0) \\ r_+(z,k_1,k_0) \end{pmatrix} \begin{pmatrix} q_+(z,k_1,k_0) \\ s_+(z,k_1,k_0) \end{pmatrix} \Bigg) = 2 \tag{1.2.189}$$

if k_0 is even and k_1 is odd (cf. also (1.3.3)).

Thus far our computations are subject to $|p_+(z,k_1,k_0)| \neq |r_+(z,k_1.k_0)|$. To clarify this point we now state the following result.

Lemma 1.2.26. *Let $z \in \mathbb{C}\backslash(\partial\mathbb{D} \cup \{0\})$ and $k_0, k_1 \in \mathbb{Z}$, $k_1 > k_0$. Then,*

$$\big(1 - |z|^{-2}\big) \sum_{k=k_0}^{k_1} |p_+(z,k,k_0)|^2 = \begin{cases} |p_+(z,k_1,k_0)|^2 - |r_+(z,k_1.k_0)|^2, & k_1 \ \textit{odd}, \\ |r_+(z,k_1.k_0)|^2 - |z|^{-2} |p_+(z,k_1,k_0)|^2, & k_1 \ \textit{even}. \end{cases} \tag{1.2.190}$$

Proof. It suffices to prove the case k_1 odd. The computation

$$\begin{aligned}
\overline{z}\sum_{k=k_0}^{k_1}|p_+(z,k,k_0)|^2 &= \sum_{k=k_0}^{k_1}\overline{(U_{+,k_0}p_+(z,\cdot,k_0))(k)}p_+(z,k,k_0)\\
&= \sum_{k=k_0}^{k_1-1}\overline{(V_{+,k_0}W_{+,k_0}p_+(z,\cdot,k_0))(k)}p_+(z,k,k_0)+\overline{z}|p_+(z,k_1,k_0)|^2\\
&= \sum_{k=k_0}^{k_1-1}\overline{(W_{+,k_0}p_+(z,\cdot,k_0))(k)}(V_{+,k_0}^*p_+(z,\cdot,k_0))(k)+\overline{z}|p_+(z,k_1,k_0)|^2\\
&= \sum_{k=k_0}^{k_1}\overline{p_+(z,k,k_0)}(W_{+,k_0}^*V_{+,k_0}^*p_+(z,\cdot,k_0))(k)\\
&\quad -\overline{(W_{+,k_0}p_+(z,\cdot,k_0))(k_1)}(V_{+,k_0}^*p_+(z,\cdot,k_0))(k_1)+\overline{z}|p_+(z,k_1,k_0)|^2\\
&= \sum_{k=k_0}^{k_1}\overline{p_+(z,k,k_0)}(U_{+,k_0}^*p_+(z,\cdot,k_0))(k)-\overline{z}|r_+(z,k_1,k_0))|^2+\overline{z}|p_+(z,k_1,k_0)|^2\\
&= z^{-1}\sum_{k=k_0}^{k_1}|p_+(z,k,k_0)|^2-\overline{z}|r_+(z,k_1,k_0))|^2+\overline{z}|p_+(z,k_1,k_0)|^2 \qquad (1.2.191)
\end{aligned}$$

proves (1.2.190) for k_1 odd. $\square$

A systematic investigation of all even/odd possibilities for k_0 and k_1 then yields the following result.

Theorem 1.2.27. *Let $z\in\mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\})$ and $k_0,k_1\in\mathbb{Z}$, $k_1>k_0$. Then,*

$$m_{+,s_1}(z,k_1,k_0)=\begin{cases}-\frac{q_+(z,k_1,k_0)+s_+(z,k_1,k_0)e^{is_1}}{p_+(z,k_1,k_0)+r_+(z,k_1,k_0)e^{is_1}}, & k_1 \text{ odd},\\ -\frac{z^{-1}q_+(z,k_1,k_0)+s_+(z,k_1,k_0)e^{-is_1}}{z^{-1}p_+(z,k_1,k_0)+r_+(z,k_1,k_0)e^{-is_1}}, & k_1 \text{ even}\end{cases} \qquad (1.2.192)$$

lies on a circle of radius

$$R(z,k_1,k_0)=\left[\big|1-|z|^{-2}\big|\sum_{k=k_0}^{k_1}|p_+(z,k_1,k_0)|^2\right]^{-1}\begin{cases}2|z|, & k_0 \text{ odd, } k_1 \text{ odd},\\ 2, & k_0 \text{ even, } k_1 \text{ odd},\\ 2, & k_0 \text{ odd, } k_1 \text{ even},\\ 2|z|^{-1}, & k_0 \text{ even, } k_1 \text{ even}\end{cases} \qquad (1.2.193)$$

with center

$$C(z,k_1,k_0)=\begin{cases} -\frac{s_+(z,k_1,k_0)}{r_+(z,k_1,k_0)}-\frac{\overline{p_+(z,k_1,k_0)}}{r_+(z,k_1,k_0)} & \\ \quad\times\frac{2z}{|p_+(z,k_1,k_0)|^2-|r_+(z,k_1,k_0)|^2}, & k_0 \text{ odd, } k_1 \text{ odd,}\\ -\frac{s_+(z,k_1,k_0)}{r_+(z,k_1,k_0)}-\frac{\overline{p_+(z,k_1,k_0)}}{r_+(z,k_1,k_0)} & \\ \quad\times\frac{2}{|p_+(z,k_1,k_0)|^2-|r_+(z,k_1,k_0)|^2}, & k_0 \text{ even, } k_1 \text{ odd,}\\ -\frac{s_+(z,k_1,k_0)}{r_+(z,k_1,k_0)}-\frac{\overline{z^{-1}p_+(z,k_1,k_0)}}{r_+(z,k_1,k_0)} & \\ \quad\times\frac{-2}{|z|^{-2}|p_+(z,k_1,k_0)|^2-|r_+(z,k_1,k_0)|^2}, & k_0 \text{ odd, } k_1 \text{ even,}\\ -\frac{s_+(z,k_1,k_0)}{r_+(z,k_1,k_0)}-\frac{\overline{z^{-1}p_+(z,k_1,k_0)}}{r_+(z,k_1,k_0)} & \\ \quad\times\frac{-2z^{-1}}{|z|^{-2}|p_+(z,k_1,k_0)|^2-|r_+(z,k_1,k_0)|^2}, & k_0 \text{ even, } k_1 \text{ even.} \end{cases} \tag{1.2.194}$$

In particular, the limit point case holds at $+\infty$ since

$$\lim_{k_1\uparrow\infty} R(z,k_1,k_0)=0. \tag{1.2.195}$$

Proof. The case k_0 even, k_1 odd has been discussed explicitly in (1.2.186)–(1.2.190). The remaining cases follow similarly using Lemma 1.2.26 for k_1 even and the Wronski relations (1.3.3). Relation (1.2.195) follows since $p_+(z,\cdot,k_0)\notin\ell^2([k_0,\infty)\cap\mathbb{Z})$, $z\in\mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\})$. The latter follows from $(U_{+,k_0}p(z,\cdot,k_0))(k)=zp_+(z,k,k_0)$, $z\in\mathbb{C}\backslash\{0\}$, in the weak sense (cf. Remark 1.2.6) and the fact that U_{+,k_0} is unitary. $\square$

1.3 Weyl–Titchmarsh Theory for CMV Operators on $\mathbb{Z}$

In this section we describe the Weyl–Titchmarsh theory for the CMV operator U on $\mathbb{Z}$. We note that in a context different from orthogonal polynomials on the unit circle, Bourget, Howland, and Joye [25] introduced a set of doubly infinite family of matrices with three sets of parameters which for special choices of the parameters reduces to two-sided CMV matrices on $\mathbb{Z}$.

We denote by

$$W\left(\begin{pmatrix} u_1(z,k,k_0) \\ v_1(z,k,k_0)\end{pmatrix}, \begin{pmatrix} u_2(z,k,k_0) \\ v_2(z,k,k_0)\end{pmatrix}\right) = \det\left(\begin{pmatrix} u_1(z,k,k_0) & u_2(z,k,k_0) \\ v_1(z,k,k_0) & v_2(z,k,k_0)\end{pmatrix}\right), \quad k \in \mathbb{Z}, \tag{1.3.1}$$

the Wronskian of two solutions $\begin{pmatrix} u_1(z,\cdot,k_0) \\ v_1(z,\cdot,k_0)\end{pmatrix}$ and $\begin{pmatrix} u_2(z,\cdot,k_0) \\ v_2(z,\cdot,k_0)\end{pmatrix}$ of (1.2.17) for $z \in \mathbb{C}\backslash\{0\}$. Then, since

$$\det(T(z,k)) = -1, \quad k \in \mathbb{Z}, \tag{1.3.2}$$

it follows from Definition 1.2.4 that

$$W\left(\begin{pmatrix} p_+(z,k,k_0) \\ r_+(z,k,k_0)\end{pmatrix}, \begin{pmatrix} q_+(z,k,k_0) \\ s_+(z,k,k_0)\end{pmatrix}\right) = (-1)^k \begin{cases} 2z, & k_0 \text{ odd}, \\ 2, & k_0 \text{ even}, \end{cases} \tag{1.3.3}$$

$$W\left(\begin{pmatrix} p_-(z,k,k_0) \\ r_-(z,k,k_0)\end{pmatrix}, \begin{pmatrix} q_-(z,k,k_0) \\ s_-(z,k,k_0)\end{pmatrix}\right) = (-1)^{k+1} \begin{cases} 2, & k_0 \text{ odd}, \\ 2z, & k_0 \text{ even}, \end{cases} \quad z \in \mathbb{C}\backslash\{0\},\ k \in \mathbb{Z}. \tag{1.3.4}$$

Next, in order to compute the resolvent of U, we introduce in addition to $\widetilde{p}_\pm$ and $\widetilde{q}_\pm$ in (1.2.59)–(1.2.62) the functions $\widetilde{u}_\pm$ by

$$\begin{pmatrix} \widetilde{u}_\pm(z,\cdot,k_0) \\ v_\pm(z,\cdot,k_0)\end{pmatrix} = \begin{pmatrix} \widetilde{q}_+(z,\cdot,k_0) \\ s_+(z,\cdot,k_0)\end{pmatrix} + M_\pm(z,k_0)\begin{pmatrix} \widetilde{p}_+(z,\cdot,k_0) \\ r_+(z,\cdot,k_0)\end{pmatrix} \in \ell^2([k_0,\pm\infty)\cap\mathbb{Z})^2, \quad z \in \mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\}). \tag{1.3.5}$$

Lemma 1.3.1. *Let $z \in \mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\})$ and fix $k_0, k_1 \in \mathbb{Z}$. Then the resolvent $(U-zI)^{-1}$ of the unitary CMV operator U on $\ell^2(\mathbb{Z})$ is given in terms of its matrix representation in the standard basis of $\ell^2(\mathbb{Z})$ by*

$$(U-zI)^{-1}(k,k') = \frac{(-1)^{k_1+1}}{zW\left(\begin{pmatrix} u_+(z,k_1,k_0) \\ v_+(z,k_1,k_0)\end{pmatrix}, \begin{pmatrix} u_-(z,k_1,k_0) \\ v_-(z,k_1,k_0)\end{pmatrix}\right)}$$

$$\times \begin{cases} u_-(z,k,k_0)v_+(z,k',k_0), & k<k' \text{ and } k=k' \text{ odd}, \\ v_-(z,k',k_0)u_+(z,k,k_0), & k'<k \text{ and } k=k' \text{ even}, \end{cases} \quad k,k'\in\mathbb{Z}, \tag{1.3.6}$$

$$= \frac{-1}{2z[M_+(z,k_0)-M_-(z,k_0)]}$$

$$\times \begin{cases} \widetilde{u}_-(z,k,k_0)v_+(z,k',k_0), & k<k' \text{ and } k=k' \text{ odd}, \\ v_-(z,k',k_0)\widetilde{u}_+(z,k,k_0), & k'<k \text{ and } k=k' \text{ even}, \end{cases} \quad k,k'\in\mathbb{Z}, \tag{1.3.7}$$

where

$$W\left(\begin{pmatrix} u_+(z,k_1,k_0) \\ v_+(z,k_1,k_0)\end{pmatrix}, \begin{pmatrix} u_-(z,k_1,k_0) \\ v_-(z,k_1,k_0)\end{pmatrix}\right) = \det\left(\begin{pmatrix} u_+(z,k_1,k_0) & u_-(z,k_1,k_0) \\ v_+(z,k_1,k_0) & v_-(z,k_1,k_0)\end{pmatrix}\right)$$

$$= (-1)^{k_1}[M_+(z,k_0)-M_-(z,k_0)] \begin{cases} 2z, & k_0 \text{ odd}, \\ 2, & k_0 \text{ even}, \end{cases} \tag{1.3.8}$$

and

$$W\left(\begin{pmatrix} \widetilde{u}_+(z,k_1,k_0) \\ v_+(z,k_1,k_0)\end{pmatrix}, \begin{pmatrix} \widetilde{u}_-(z,k_1,k_0) \\ v_-(z,k_1,k_0)\end{pmatrix}\right) = 2(-1)^{k_1}[M_+(z,k_0)-M_-(z,k_0)]. \tag{1.3.9}$$

Moreover, since $0\in\mathbb{C}\backslash\sigma(U)$*,* (1.3.6) *and* (1.3.7) *analytically extend to* $z=0$*.*

Proof. Denote

$$w(z,k,k',k_0) = \begin{cases} u_-(z,k,k_0)v_+(z,k',k_0), & k<k',\ k=k' \text{ odd}, \\ u_+(z,k,k_0)v_-(z,k',k_0), & k'<k,\ k=k' \text{ even}, \end{cases} \tag{1.3.10}$$
$$k,k',k_0\in\mathbb{Z}.$$

We will prove that

$$(U-zI)w(z,\cdot,k',k_0) = (-1)^{k'+1}z\det\left(\begin{pmatrix} u_+(z,k',k_0) & u_-(z,k',k_0) \\ v_+(z,k',k_0) & v_-(z,k',k_0)\end{pmatrix}\right)\delta_{k'}, \tag{1.3.11}$$
$$k',k_0\in\mathbb{Z},$$

and hence, using (1.3.2), one obtains

$$(U-zI)w(z,\cdot,k',k_0) = (-1)^{k_1+1}z\det\left(\begin{pmatrix} u_+(z,k_1,k_0) & u_-(z,k_1,k_0) \\ v_+(z,k_1,k_0) & v_-(z,k_1,k_0)\end{pmatrix}\right)\delta_{k'},$$

$$k', k_0, k_1 \in \mathbb{Z}. \tag{1.3.12}$$

First, let $k_0 \in \mathbb{Z}$ and assume k' to be odd. Then,

$$\big((U - zI)w(z, \cdot, k', k_0)\big)(\ell) = \big((VW - zI)w(z, \cdot, k', k_0)\big)(\ell) = 0,$$
$$\ell \in \mathbb{Z}\backslash\{k', k'+1\} \tag{1.3.13}$$

and

$$\begin{aligned}
&\begin{pmatrix} ((U - zI)w(z, \cdot, k', k_0))(k') \\ ((U - zI)w(z, \cdot, k', k_0))(k'+1) \end{pmatrix} = \begin{pmatrix} ((VW - zI)w(z, \cdot, k', k_0))(k') \\ ((VW - zI)w(z, \cdot, k', k_0))(k'+1) \end{pmatrix} \\
&\quad = \theta_{k'+1} z \begin{pmatrix} (v_+(z, k', k_0)v_-(z, \cdot, k_0))(k') \\ (v_-(z, k', k_0)v_+(z, \cdot, k_0))(k'+1) \end{pmatrix} - z \begin{pmatrix} w(z, k', k', k_0) \\ w(z, k'+1, k', k_0) \end{pmatrix} \\
&\quad = z v_-(z, k', k_0) \begin{pmatrix} u_+(z, k', k_0) \\ u_+(z, k'+1, k_0) \end{pmatrix} - z \begin{pmatrix} v_+(z, k', k_0)u_-(z, k', k_0) \\ v_-(z, k', k_0)u_+(z, k'+1, k_0) \end{pmatrix} \\
&\quad = z \begin{pmatrix} \det\left(\begin{pmatrix} u_+(z, k', k_0) & u_-(z, k', k_0) \\ v_+(z, k', k_0) & v_-(z, k', k_0) \end{pmatrix}\right) \\ 0 \end{pmatrix}.
\end{aligned} \tag{1.3.14}$$

Next, assume k' to be even. Then,

$$\big((U - zI)w(z, \cdot, k', k_0)\big)(\ell) = \big((VW - zI)w(z, \cdot, k', k_0)\big)(\ell) = 0,$$
$$\ell \in \mathbb{Z}\backslash\{k'-1, k'\} \tag{1.3.15}$$

and

$$\begin{aligned}
&\begin{pmatrix} ((U - zI)w(z, \cdot, k', k_0))(k'-1) \\ ((U - zI)w(z, \cdot, k', k_0))(k') \end{pmatrix} = \begin{pmatrix} ((VW - zI)w(z, \cdot, k', k_0))(k'-1) \\ ((VW - zI)w(z, \cdot, k', k_0))(k') \end{pmatrix} \\
&\quad = \theta_{k'} z \begin{pmatrix} (v_+(z, k', k_0)v_-(z, \cdot, k_0))(k'-1) \\ (v_-(z, k', k_0)v_+(z, \cdot, k_0))(k') \end{pmatrix} - z \begin{pmatrix} w(z, k'-1, k', k_0) \\ w(z, k', k', k_0) \end{pmatrix} \\
&\quad = z v_+(z, k', k_0) \begin{pmatrix} u_-(z, k'-1, k_0) \\ u_-(z, k', k_0) \end{pmatrix} - z \begin{pmatrix} v_+(z, k', k_0)u_-(z, k'-1, k_0) \\ v_-(z, k', k_0)u_+(z, k', k_0) \end{pmatrix} \\
&\quad = z \begin{pmatrix} 0 \\ -\det\left(\begin{pmatrix} u_+(z, k', k_0) & u_-(z, k', k_0) \\ v_+(z, k', k_0) & v_-(z, k', k_0) \end{pmatrix}\right) \end{pmatrix}.
\end{aligned} \tag{1.3.16}$$

Thus, one obtains (1.3.11). $\square$

Next, we denote by $d\Omega(\cdot,k)$, $k\in\mathbb{Z}$, the 2×2 matrix-valued measure,

$$\begin{aligned}
d\Omega(\zeta,k) &= d\begin{pmatrix} \Omega_{0,0}(\zeta,k) & \Omega_{0,1}(\zeta,k) \\ \Omega_{1,0}(\zeta,k) & \Omega_{1,1}(\zeta,k) \end{pmatrix} \\
&= d\begin{pmatrix} (\delta_{k-1}, E_U(\zeta)\delta_{k-1})_{\ell^2(\mathbb{Z})} & (\delta_{k-1}, E_U(\zeta)\delta_k)_{\ell^2(\mathbb{Z})} \\ (\delta_k, E_U(\zeta)\delta_{k-1})_{\ell^2(\mathbb{Z})} & (\delta_k, E_U(\zeta)\delta_k)_{\ell^2(\mathbb{Z})} \end{pmatrix}, \quad \zeta\in\partial\mathbb{D}, \qquad (1.3.17)
\end{aligned}$$

where $dE_U(\cdot)$ denotes the operator-valued spectral measure of the unitary CMV operator U on $\ell^2(\mathbb{Z})$,

$$U = \oint_{\partial\mathbb{D}} dE_U(\zeta)\,\zeta. \qquad (1.3.18)$$

We note that by (1.3.17) $d\Omega_{0,0}(\cdot,k)$ and $d\Omega_{1,1}(\cdot,k)$ are nonnegative measures on $\partial\mathbb{D}$ and $d\Omega_{0,1}(\cdot,k)$ and $d\Omega_{1,0}(\cdot,k)$ are complex-valued measures on $\partial\mathbb{D}$.

We also introduce the 2×2 matrix-valued function $\mathcal{M}(\cdot,k)$, $k\in\mathbb{Z}$, by

$$\begin{aligned}
\mathcal{M}(z,k) &= \begin{pmatrix} M_{0,0}(z,k) & M_{0,1}(z,k) \\ M_{1,0}(z,k) & M_{1,1}(z,k) \end{pmatrix} \\
&= \begin{pmatrix} (\delta_{k-1}, (U+zI)(U-zI)^{-1}\delta_{k-1})_{\ell^2(\mathbb{Z})} & (\delta_{k-1}, (U+zI)(U-zI)^{-1}\delta_k)_{\ell^2(\mathbb{Z})} \\ (\delta_k, (U+zI)(U-zI)^{-1}\delta_{k-1})_{\ell^2(\mathbb{Z})} & (\delta_k, (U+zI)(U-zI)^{-1}\delta_k)_{\ell^2(\mathbb{Z})} \end{pmatrix} \\
&= \oint_{\partial\mathbb{D}} d\Omega(\zeta,k)\,\frac{\zeta+z}{\zeta-z}, \quad z\in\mathbb{C}\backslash\partial\mathbb{D}. \qquad (1.3.19)
\end{aligned}$$

We note that,

$$M_{0,0}(\cdot,k+1) = M_{1,1}(\cdot,k), \quad k\in\mathbb{Z} \qquad (1.3.20)$$

and

$$\begin{aligned}
M_{1,1}(z,k) &= (\delta_k, (U+zI)(U-zI)^{-1}\delta_k)_{\ell^2(\mathbb{Z})} \qquad (1.3.21) \\
&= \oint_{\partial\mathbb{D}} d\Omega_{1,1}(\zeta,k)\,\frac{\zeta+z}{\zeta-z}, \quad z\in\mathbb{C}\backslash\partial\mathbb{D},\ k\in\mathbb{Z}, \qquad (1.3.22)
\end{aligned}$$

where

$$d\Omega_{1,1}(\zeta,k) = d(\delta_k, E_U(\zeta)\delta_k)_{\ell^2(\mathbb{Z})}, \quad \zeta\in\partial\mathbb{D}. \qquad (1.3.23)$$

Thus, $M_{0,0}|_{\mathbb{D}}$ and $M_{1,1}|_{\mathbb{D}}$ are Caratheodory functions. Moreover, by (1.3.21) one infers that

$$M_{1,1}(0,k) = 1, \quad k \in \mathbb{Z}. \tag{1.3.24}$$

Lemma 1.3.2. *Let $z \in \mathbb{C}\backslash\partial\mathbb{D}$. Then the functions $M_{1,1}(\cdot,k)$ and $M_{\pm}(\cdot,k)$, $k \in \mathbb{Z}$, satisfy the following relations*

$$M_{0,0}(z,k) = 1 + \frac{[\overline{a_k} - \overline{b_k}M_+(z,k)][a_k + b_k M_-(z,k)]}{\rho_k^2[M_+(z,k) - M_-(z,k)]}, \tag{1.3.25}$$

$$M_{1,1}(z,k) = \frac{1 - M_+(z,k)M_-(z,k)}{M_+(z,k) - M_-(z,k)}, \tag{1.3.26}$$

$$M_{0,1}(z,k) = \frac{-1}{\rho_k[M_+(z,k) - M_-(z,k)]}\begin{cases} [1 - M_+(z,k)][\overline{a_k} - \overline{b_k}M_-(z,k)], \\ \hfill k \ \textit{odd}, \\ [1 + M_+(z,k)][a_k + b_k M_-(z,k)], \\ \hfill k \ \textit{even}, \end{cases} \tag{1.3.27}$$

$$M_{1,0}(z,k) = \frac{-1}{\rho_k[M_+(z,k) - M_-(z,k)]}\begin{cases} [1 + M_+(z,k)][a_k + b_k M_-(z,k)], \\ \hfill k \ \textit{odd}, \\ [1 - M_+(z,k)][\overline{a_k} - \overline{b_k}M_-(z,k)], \\ \hfill k \ \textit{even}. \end{cases} \tag{1.3.28}$$

Proof. Using (1.2.4), (1.2.5), (1.2.17), and (1.2.57) one finds

$$\begin{pmatrix} p_+(z,k_0-1,k_0) \\ r_+(z,k_0-1,k_0) \end{pmatrix} = \begin{cases} \frac{1}{\rho_{k_0}}\begin{pmatrix} z\overline{b_{k_0}} \\ b_{k_0} \end{pmatrix}, & k_0 \text{ odd}, \\ \frac{1}{\rho_{k_0}}\begin{pmatrix} b_{k_0} \\ \overline{b_{k_0}} \end{pmatrix}, & k_0 \text{ even}, \end{cases} \tag{1.3.29}$$

$$\begin{pmatrix} q_+(z,k_0-1,k_0) \\ s_+(z,k_0-1,k_0) \end{pmatrix} = \begin{cases} \frac{1}{\rho_{k_0}}\begin{pmatrix} -z\overline{a_{k_0}} \\ a_{k_0} \end{pmatrix}, & k_0 \text{ odd}, \\ \frac{1}{\rho_{k_0}}\begin{pmatrix} a_{k_0} \\ -\overline{a_{k_0}} \end{pmatrix}, & k_0 \text{ even}. \end{cases} \tag{1.3.30}$$

It follows from (1.3.19) that

$$M_{\ell,\ell'}(z,k_0) = \delta_{\ell,\ell'} + 2z\big(\delta_{k_0+\ell-1}, (U - zI)^{-1}\delta_{k_0+\ell'-1}\big)_{\ell^2(\mathbb{Z})}$$

$$= \delta_{\ell,\ell'} + 2z(U - zI)^{-1}(k_0 + \ell - 1, k_0 + \ell' - 1), \quad \ell, \ell' = 0, 1. \tag{1.3.31}$$

Thus, by Lemma 1.3.1 and equalities (1.2.57), (1.2.136), (1.3.29), and (1.3.30), one finds

$$(U - zI)^{-1}(k_0, k_0) = \frac{[1 - M_+(z, k_0)][1 + M_-(z, k_0)]}{2z[M_+(z, k_0) - M_-(z, k_0)]}, \tag{1.3.32}$$

$$(U - zI)^{-1}(k_0 - 1, k_0 - 1) = \frac{[\overline{a_{k_0}} - \overline{b_{k_0}} M_+(z, k_0)][a_{k_0} + b_{k_0} M_-(z, k_0)]}{2z\rho_{k_0}^2 [M_+(z, k_0) - M_-(z, k_0)]}, \tag{1.3.33}$$

$$(U - zI)^{-1}(k_0 - 1, k_0) = -\frac{\begin{cases} [1 - M_+(z, k_0)][\overline{a_{k_0}} - \overline{b_{k_0}} M_-(z, k_0)], & k_0 \text{ odd}, \\ [1 + M_+(z, k_0)][a_{k_0} + b_{k_0} M_-(z, k_0)], & k_0 \text{ even}, \end{cases}}{2z\rho_{k_0} [M_+(z, k_0) - M_-(z, k_0)]}, \tag{1.3.34}$$

$$(U - zI)^{-1}(k_0, k_0 - 1) = -\frac{\begin{cases} [1 + M_+(z, k_0)][a_{k_0} + b_{k_0} M_-(z, k_0)], & k_0 \text{ odd}, \\ [1 - M_+(z, k_0)][\overline{a_{k_0}} - \overline{b_{k_0}} M_-(z, k_0)], & k_0 \text{ even}, \end{cases}}{2z\rho_{k_0} [M_+(z, k_0) - M_-(z, k_0)]}, \tag{1.3.35}$$

and hence (1.3.25)–(1.3.28). □

Finally, introducing the functions $\Phi_{1,1}(\cdot, k)$, $k \in \mathbb{Z}$, by

$$\Phi_{1,1}(z, k) = \frac{M_{1,1}(z, k) - 1}{M_{1,1}(z, k) + 1}, \quad z \in \mathbb{C} \backslash \partial \mathbb{D}, \tag{1.3.36}$$

then,

$$M_{1,1}(z, k) = \frac{1 + \Phi_{1,1}(z, k)}{1 - \Phi_{1,1}(z, k)}, \quad z \in \mathbb{C} \backslash \partial \mathbb{D}. \tag{1.3.37}$$

Both, $M_{1,1}(z, k)$ and $\Phi_{1,1}(z, k)$, $z \in \mathbb{C} \backslash \partial \mathbb{D}$, $k \in \mathbb{Z}$, have nontangential limits to $\partial \mathbb{D}$ μ_0-a.e.

Lemma 1.3.3. *The function $\Phi_{1,1}|_{\mathbb{D}}$ is a Schur function and $\Phi_{1,1}$ is related to $\Phi_\pm$ by*

$$\Phi_{1,1}(z, k) = \frac{\Phi_+(z, k)}{\Phi_-(z, k)}, \quad z \in \mathbb{C} \backslash \partial \mathbb{D}, \ k \in \mathbb{Z}. \tag{1.3.38}$$

Proof. The assertion follows from (1.2.150), (1.3.36) and Lemma 1.3.2. $\square$

Lemma 1.3.4. *Let $\zeta \in \partial\mathbb{D}$ and $k_0 \in \mathbb{Z}$. Then the following sets of two-dimensional Laurent polynomials $\{P(\zeta,k,k_0)\}_{k\in\mathbb{Z}}$ and $\{R(\zeta,k,k_0)\}_{k\in\mathbb{Z}}$,*

$$P(\zeta,k,k_0) = \begin{pmatrix} P_0(\zeta,k,k_0) \\ P_1(\zeta,k,k_0) \end{pmatrix} = \begin{cases} \frac{1}{2\zeta}\begin{pmatrix} -\rho_{k_0} & \rho_{k_0} \\ \overline{b_{k_0}} & \overline{a_{k_0}} \end{pmatrix} \begin{pmatrix} q_+(\zeta,k,k_0) \\ p_+(\zeta,k,k_0) \end{pmatrix}, & k_0 \text{ odd}, \\ \frac{1}{2}\begin{pmatrix} \rho_{k_0} & \rho_{k_0} \\ -b_{k_0} & a_{k_0} \end{pmatrix} \begin{pmatrix} q_+(\zeta,k,k_0) \\ p_+(\zeta,k,k_0) \end{pmatrix}, & k_0 \text{ even}, \end{cases} \tag{1.3.39}$$

$$R(\zeta,k,k_0) = \begin{pmatrix} R_0(\zeta,k,k_0) \\ R_1(\zeta,k,k_0) \end{pmatrix} = \begin{cases} \frac{1}{2}\begin{pmatrix} \rho_{k_0} & \rho_{k_0} \\ -b_{k_0} & a_{k_0} \end{pmatrix} \begin{pmatrix} s_+(\zeta,k,k_0) \\ r_+(\zeta,k,k_0) \end{pmatrix}, & k_0 \text{ odd}, \\ \frac{1}{2}\begin{pmatrix} -\rho_{k_0} & \rho_{k_0} \\ \overline{b_{k_0}} & \overline{a_{k_0}} \end{pmatrix} \begin{pmatrix} s_+(\zeta,k,k_0) \\ r_+(\zeta,k,k_0) \end{pmatrix}, & k_0 \text{ even} \end{cases} \tag{1.3.40}$$

form complete orthonormal systems in $L^2(\partial\mathbb{D}; d\Omega(\cdot,k_0)^\top)$ and $L^2(\partial\mathbb{D}; d\Omega(\cdot,k_0))$, respectively.

Proof. Consider the following relation,

$$U^\top \delta_k = \sum_{j\in\mathbb{Z}} U^\top(j,k)\delta_j = \sum_{j\in\mathbb{Z}} U(k,j)\delta_j, \quad k \in \mathbb{Z}. \tag{1.3.41}$$

By Lemma 1.2.2 any solution u of

$$zu(z,k,k_0) = \sum_{j\in\mathbb{Z}} U(k,j)u(z,j,k_0), \quad k \in \mathbb{Z}, \tag{1.3.42}$$

is a linear combination of $p_+(z,\cdot,k_0)$ and $q_+(z,\cdot,k_0)$, and hence, (1.3.42) has a unique solution $\{u(z,k,k_0)\}_{k\in\mathbb{Z}}$ with prescribed values at k_0-1 and k_0,

$$u(z,\cdot,k_0) = P_0(z,\cdot,k_0)u(z,k_0-1,k_0) + P_1(z,\cdot,k_0)u(z,k_0,k_0). \tag{1.3.43}$$

Due to the algebraic nature of the proof of Lemma 1.2.2 and the algebraic similarity of equations (1.3.41) and (1.3.42), one concludes from (1.3.43) that

$$\delta_k = P_0(U^\top,k,k_0)\delta_{k_0-1} + P_1(U^\top,k,k_0)\delta_{k_0}, \quad k \in \mathbb{Z}. \tag{1.3.44}$$

Using the spectral representation for the operator $U^\top$ one then obtains

$$P_\ell(U^\top, k, k_0) = \oint_{\partial\mathbb{D}} dE_{U^\top}(\zeta)\, P_\ell(\zeta, k, k_0), \quad \ell = 0, 1 \tag{1.3.45}$$

and by (1.3.44),

$$\begin{aligned}(\delta_k, \delta_{k'})_{\ell^2(\mathbb{Z})} &= \sum_{\ell,\ell'=0}^{1} \Big(P_\ell(U^\top, k, k_0)\delta_{k_0+\ell-1}, P_{\ell'}(U^\top, k', k_0)\delta_{k_0+\ell'-1}\Big)_{\ell^2(\mathbb{Z})} \\ &= \oint_{\partial\mathbb{D}} P(\zeta, k, k_0)^*\, d\Omega(\zeta, k_0)^\top P(\zeta, k', k_0). \end{aligned} \tag{1.3.46}$$

Similarly, one obtains the orthonormality relation for the two-dimensional Laurent polynomials $\{R(\zeta, k, k_0)\}_{k\in\mathbb{Z}}$ in $L^2(\partial\mathbb{D}; d\Omega(\cdot, k_0))$.

To prove completeness of $\{P(\zeta, k, k_0)\}_{k\in\mathbb{Z}}$ we first note the following fact,

$$\begin{aligned}\operatorname{span}\{P(z, k, k_0)\}_{k\in\mathbb{Z}} &= \operatorname{span}\left\{\begin{pmatrix} z^k \\ z^{k-1}\end{pmatrix}, \begin{pmatrix} z^{k-1} \\ z^k\end{pmatrix}, \begin{pmatrix} 1 \\ 0\end{pmatrix}, \begin{pmatrix} 0 \\ 1\end{pmatrix}\right\}_{k\in\mathbb{Z}} \\ &= \operatorname{span}\left\{\begin{pmatrix} z^k \\ 0\end{pmatrix}, \begin{pmatrix} 0 \\ z^k\end{pmatrix}\right\}_{k\in\mathbb{Z}}, \quad k_0 \in \mathbb{Z}. \end{aligned} \tag{1.3.47}$$

This follows by investigating the leading coefficients of $p_+(z, k, k_0)$ and $q_+(z, k, k_0)$. Thus, it suffices to prove that $\left\{\binom{\zeta^k}{0}, \binom{0}{\zeta^k}\right\}_{k\in\mathbb{Z}}$ form a basis in $L^2(\partial\mathbb{D}; d\Omega(\cdot, k_0)^\top)$ for all $k_0 \in \mathbb{Z}$.

Let $k_0 \in \mathbb{Z}$ and suppose that $F = \binom{f_0}{f_1} \in L^2(\partial\mathbb{D}; d\Omega(\cdot, k_0)^\top)$ is orthogonal to $\left\{\binom{\zeta^k}{0}, \binom{0}{\zeta^k}\right\}_{k\in\mathbb{Z}}$ in $L^2(\partial\mathbb{D}; d\Omega(\cdot, k_0)^\top)$, that is,

$$0 = \oint_{\partial\mathbb{D}} \overline{\begin{pmatrix}\zeta^k & 0\end{pmatrix}}\, d\Omega(\zeta, k_0)^\top F(\zeta) = \oint_{\partial\mathbb{D}} \overline{\zeta^k}\, [f_0(\zeta) d\Omega_{0,0}(\zeta, k_0) + f_1(\zeta) d\Omega_{1,0}(\zeta, k_0)] \tag{1.3.48}$$

and

$$0 = \oint_{\partial\mathbb{D}} \overline{\begin{pmatrix}0 & \zeta^k\end{pmatrix}}\, d\Omega(\zeta, k_0)^\top F(\zeta) = \oint_{\partial\mathbb{D}} \overline{\zeta^k}\, [f_0(\zeta) d\Omega_{0,1}(\zeta, k_0) + f_1(\zeta) d\Omega_{1,1}(\zeta, k_0)] \tag{1.3.49}$$

for all $k \in \mathbb{Z}$. Hence (cf., e.g., [44, p. 24]),

$$f_0 d\Omega_{0,0} + f_1 d\Omega_{1,0} = 0, \tag{1.3.50}$$

$$f_0 d\Omega_{0,1} + f_1 d\Omega_{1,1} = 0. \tag{1.3.51}$$

Multiplying (1.3.50) by $\overline{f_0}$ and (1.3.51) by $\overline{f_1}$ then yields

$$|f_0|^2 d\Omega_{0,0} + \overline{f_0} f_1 d\Omega_{1,0} + \overline{f_1} f_0 d\Omega_{0,1} + |f_1|^2 d\Omega_{1,1} = 0 \tag{1.3.52}$$

and hence

$$\|F\|^2_{L^2(\partial\mathbb{D}; d\Omega(\cdot,k_0)^\top)} = \oint_{\partial\mathbb{D}} F(\zeta)^* \, d\Omega(\zeta,k_0)^\top F(\zeta) = 0. \tag{1.3.53}$$

Similarly, one proves completeness of $\{R(\zeta,k,k_0)\}_{k\in\mathbb{Z}}$ in $L^2(\partial\mathbb{D}; d\Omega(\cdot,k_0))$. $\square$

Denoting by I_2 the identity operator in $\mathbb{C}^2$, we state the following result.

Corollary 1.3.5. *Let $k_0 \in \mathbb{Z}$. Then the operators U and $U^\top$ are unitarily equivalent to the operator of multiplication by $I_2 id$ (where $id(\zeta) = \zeta$) on $L^2(\partial\mathbb{D}; d\Omega(\cdot,k_0))$ and $L^2(\partial\mathbb{D}; d\Omega(\cdot,k_0)^\top)$, respectively. Thus,*

$$\sigma(U) = \operatorname{supp}(d\Omega(\cdot,k_0)) = \operatorname{supp}(d\Omega^{\mathrm{tr}}(\cdot,k_0)) = \operatorname{supp}(d\Omega(\cdot,k_0)^\top) = \sigma(U^\top), \tag{1.3.54}$$

where

$$d\Omega^{\mathrm{tr}}(\cdot,k_0) = d\Omega_{0,0}(\cdot,k_0) + d\Omega_{1,1}(\cdot,k_0) \tag{1.3.55}$$

denotes the trace measure of $d\Omega(\cdot,k_0)$.

Proof. Consider the linear map $\dot{\mathcal{U}}$ from $\ell^\infty_0(\mathbb{Z})$ into the set of two-dimensional Laurent polynomials on $\partial\mathbb{D}$ defined by,

$$(\dot{\mathcal{U}} f)(\zeta) = \sum_{k\in\mathbb{Z}} R(\zeta,k,k_0) f(k), \quad f \in \ell^\infty_0(\mathbb{Z}). \tag{1.3.56}$$

A simple calculation for $F(\zeta) = (\dot{\mathcal{U}} f)(\zeta)$, $f \in \ell_0^\infty(\mathbb{Z})$, shows that

$$\sum_{k\in\mathbb{Z}} |f(k)|^2 = \oint_{\partial\mathbb{D}} F(\zeta)^* d\Omega(\zeta, k_0) F(\zeta). \tag{1.3.57}$$

Since $\ell_0^\infty(\mathbb{Z})$ is dense in $\ell^2(\mathbb{Z})$, $\mathcal{U}$ extends to a bounded linear operator $\mathcal{U}\colon \ell^2(\mathbb{Z}) \to L^2(\partial\mathbb{D}; d\Omega(\cdot, k_0))$. By Lemma 1.3.4, $\mathcal{U}$ is onto and one verifies that

$$(\mathcal{U}^{-1} F)(k) = \oint_{\partial\mathbb{D}} R(\zeta, k, k_0)^* d\Omega(\zeta, k_0) F(\zeta). \tag{1.3.58}$$

In particular, $\mathcal{U}$ is unitary. Moreover, we claim that $\mathcal{U}$ maps the operator U on $\ell^2(\mathbb{Z})$ to the operator of multiplication by $id(\zeta) = \zeta$, $\zeta \in \partial\mathbb{D}$, denoted by $M(id)$, on $L^2(\partial\mathbb{D}; d\Omega(\cdot, k_0))$,

$$\mathcal{U} U \mathcal{U}^{-1} = M(id), \tag{1.3.59}$$

where

$$(M(id)F)(\zeta) = \zeta F(\zeta), \quad F \in L^2(\partial\mathbb{D}; d\Omega(\cdot, k_0)). \tag{1.3.60}$$

Indeed,

$$\begin{aligned}
(\mathcal{U} U \mathcal{U}^{-1} F(\cdot))(\zeta) &= (\mathcal{U} U f(\cdot))(\zeta) \\
&= \sum_{k\in\mathbb{Z}} (U f(\cdot))(k) R(\zeta, k, k_0) = \sum_{k\in\mathbb{Z}} (U^\top R(\zeta, \cdot, k_0))(k) f(k) \\
&= \sum_{k\in\mathbb{Z}} \zeta R(\zeta, k, k_0) f(k) = \zeta F(\zeta) \\
&= (M(id)F(\cdot))(\zeta), \quad F \in L^2(\partial\mathbb{D}; d\Omega(\cdot, k_0)).
\end{aligned} \tag{1.3.61}$$

The result for the operator $U^\top$ is proved analogously. $\square$

Finally, we note an alternative approach to (a variant of) the 2×2 matrix-valued spectral function $\Omega(\cdot,k_0)$ associated with U.

First we introduce $\widetilde{\mathcal{M}}(z,k)$, $z\in\mathbb{C}\backslash\partial\mathbb{D}$, $k\in\mathbb{Z}$, defined by

$$\begin{aligned}
\widetilde{\mathcal{M}}(z,k) &= \begin{pmatrix} \widetilde{M}_{0,0}(z,k) & \widetilde{M}_{0,1}(z,k) \\ \widetilde{M}_{1,0}(z,k) & \widetilde{M}_{1,1}(z,k) \end{pmatrix} \\
&= \begin{cases} \frac{1}{4}\begin{pmatrix} \rho_k & \rho_k \\ -b_k & a_k \end{pmatrix}^* \mathcal{M}(z,k) \begin{pmatrix} \rho_k & \rho_k \\ -b_k & a_k \end{pmatrix}, & k \text{ odd}, \\ \frac{1}{4}\begin{pmatrix} -\rho_k & \rho_k \\ \overline{b_k} & \overline{a_k} \end{pmatrix}^* \mathcal{M}(z,k) \begin{pmatrix} -\rho_k & \rho_k \\ \overline{b_k} & \overline{a_k} \end{pmatrix}, & k \text{ even}, \end{cases} \\
&= \begin{pmatrix} \frac{1}{M_+(z,k)-M_-(z,k)} + \frac{i}{2}\mathrm{Im}(\alpha_k) & \frac{1}{2}\frac{M_+(z,k)+M_-(z,k)}{M_+(z,k)-M_-(z,k)} + \frac{1}{2}\mathrm{Re}(\alpha_k) \\ -\frac{1}{2}\frac{M_+(z,k)+M_-(z,k)}{M_+(z,k)-M_-(z,k)} - \frac{1}{2}\mathrm{Re}(\alpha_k) & -\frac{M_+(z,k)M_-(z,k)}{M_+(z,k)-M_-(z,k)} - \frac{i}{2}\mathrm{Im}(\alpha_k) \end{pmatrix} \\
&\qquad\qquad z\in\mathbb{C}\backslash\partial\mathbb{D},\ k\in\mathbb{Z}. \qquad (1.3.62)
\end{aligned}$$

Clearly, $\mathcal{M}(\cdot,k)$, and hence, $\widetilde{\mathcal{M}}(\cdot,k)$, $k\in\mathbb{Z}$, are 2×2 matrix-valued Caratheodory functions. Since by (1.3.19) $\mathcal{M}(0,k)=I$, $k\in\mathbb{Z}$, one computes

$$\widetilde{\mathcal{M}}(0,k) = \frac{1}{4}\begin{pmatrix} \rho_k^2+|b_k|^2 & -2i\mathrm{Im}(\alpha_k) \\ 2i\mathrm{Im}(\alpha_k) & \rho_k^2+|a_k|^2 \end{pmatrix} = [\widetilde{\mathcal{M}}(0,k)]^*, \quad k\in\mathbb{Z}. \qquad (1.3.63)$$

Hence, the Herglotz representation of $\widetilde{\mathcal{M}}(\cdot,k)$ is given by

$$\widetilde{\mathcal{M}}(z,k) = \int_{\partial\mathbb{D}} d\widetilde{\Omega}(\zeta,k)\,\frac{\zeta+z}{\zeta-z}, \quad z\in\mathbb{C}\backslash\partial\mathbb{D},\ k\in\mathbb{Z}, \qquad (1.3.64)$$

where the measure $d\widetilde{\Omega}(\cdot,k)$ can be reconstructed from the boundary values of the function $\mathrm{Re}(\widetilde{\mathcal{M}}(\cdot,k))$ via

$$\begin{aligned}
\widetilde{\Omega}\big(\big(e^{i\theta_1},e^{i\theta_2}\big],k\big) &= \lim_{\delta\downarrow 0}\lim_{r\uparrow 1}\frac{1}{2\pi}\int_{\theta_1+\delta}^{\theta_2+\delta} d\theta \\
&\times \begin{pmatrix} \mathrm{Re}\left(\frac{1}{M_+(re^{i\theta},k)-M_-(re^{i\theta},k)}\right) & \frac{i}{2}\mathrm{Im}\left(\frac{M_+(re^{i\theta},k)+M_-(re^{i\theta},k)}{M_+(re^{i\theta},k)-M_-(re^{i\theta},k)}\right) \\ -\frac{i}{2}\mathrm{Im}\left(\frac{M_+(re^{i\theta},k)+M_-(re^{i\theta},k)}{M_+(re^{i\theta},k)-M_-(re^{i\theta},k)}\right) & -\mathrm{Re}\left(\frac{M_+(re^{i\theta},k)M_-(re^{i\theta},k)}{M_+(re^{i\theta},k)-M_-(re^{i\theta},k)}\right) \end{pmatrix}, \qquad (1.3.65)
\end{aligned}$$

$$\theta_1 \in [0, 2\pi),\ \theta_1 < \theta_2 < \theta_1 + 2\pi,\ k \in \mathbb{Z}.$$

Finally, the analog of Lemma 1.2.25 in the full-lattice context reads as follows.

Lemma 1.3.6. *Let $f, g \in \ell_0^\infty(\mathbb{Z})$, $F \in C(\partial\mathbb{D})$, and $\theta_1 \in [0, 2\pi)$, $\theta_1 < \theta_2 \leq \theta_1 + 2\pi$. Then,*

$$\begin{aligned} &\big(f, F(U)E_U\big(\mathrm{Arc}\big((e^{i\theta_1}, e^{i\theta_2}]\big)\big)g\big)_{\ell^2(\mathbb{Z})} \\ &\quad = \big(\widehat{f}(\cdot, k_0), M_F M_{\chi_{\mathrm{Arc}((e^{i\theta_1}, e^{i\theta_2}])}} \widehat{g}(\cdot, k_0)\big)_{L^2(\partial\mathbb{D}; d\widetilde{\Omega}_\pm(\cdot, k_0))}, \end{aligned} \tag{1.3.66}$$

where we introduced the notation

$$\widehat{h}(\zeta, k_0) = \sum_{k\in\mathbb{Z}} \begin{pmatrix} s_+(\zeta, k, k_0) \\ r_+(\zeta, k, k_0) \end{pmatrix} h(k), \quad \zeta \in \partial\mathbb{D},\ h \in \ell_0^\infty(\mathbb{Z}), \tag{1.3.67}$$

and M_G denotes the maximally defined operator of multiplication by the $d\widetilde{\Omega}(\cdot, k_0)$-measurable function G in the Hilbert space $L^2(\partial\mathbb{D}; d\widetilde{\Omega}(\cdot, k_0))$,

$$\begin{aligned} &(M_G\widehat{h})(\zeta) = G(\zeta)\widehat{h}(\zeta) \ \text{ for a.e. } \zeta \in \partial\mathbb{D}, \\ &\widehat{h} \in \mathrm{dom}(M_G) = \{\widehat{k} \in L^2(\partial\mathbb{D}; d\widetilde{\Omega}(\cdot, k_0)) \,|\, G\widehat{k} \in L^2(\partial\mathbb{D}; d\widetilde{\Omega}(\cdot, k_0))\} \end{aligned} \tag{1.3.68}$$

Using Lemma 1.2.24, (1.2.63), (1.2.64), (1.2.169), and (1.3.7) one can follow the proof of Lemma 1.2.25 step by step and so we omit the details (cf. also Theorem 3.2.12).

Finally, Weyl–Titchmarsh circles associated with finite intervals $[k_-, k_+] \cap \mathbb{Z}$ and the ensuing limits $k_\pm \to \pm\infty$ can be discussed in analogy to the half-lattice case at the end of Section 1.2. Without entering into details, we mention that U is of course in the limit point case at $\pm\infty$.

Chapter 2

A Borg-Type Theorem Associated with Orthogonal Polynomials on the Unit Circle

2.1 Introduction

The aim of this chapter is to prove a Borg-type uniqueness theorem for a special class of unitary doubly infinite five-diagonal matrices (cf. (1.1.1)) introduced in the previous Chapter. The corresponding unitary semi-infinite five-diagonal matrices were first introduced by Cantero, Moral, and Velázquez (CMV) in [28]. In [171, Sects. 4.5, 10.5], Simon introduced the corresponding notion of unitary doubly infinite five-diagonal matrices. We note that in a context different from orthogonal polynomials on the unit circle, Bourget, Howland, and Joye [25] introduced a set of doubly infinite family of matrices with three sets of parameters which for special choices of the parameters reduces to two-sided CMV matrices on $\mathbb{Z}$.

We now turn to Borg-type uniqueness theorems. From the outset, Borg-type theorems are inverse spectral theory assertions which typically prescribe a connected interval (or arc) as the spectrum of a self-adjoint (or unitary) differential or difference operator, and under a reflectionless condition imposed on the operator (one may think of a periodicity condition on the (potential) coefficients of the differential or difference operator) infers the explicit form of the coefficients of the operator in question. Typically, the form of the coefficients determined in this context is fairly simple and usually given by constants or functions of exponential type.

Next, we briefly describe the history of Borg-type theorems relevant to this chapter. In 1946, Borg [24] proved, among a variety of other inverse spectral theorems, the following result for one-dimensional Schrödinger operators. (Throughout this chapter we denote by $\sigma(\cdot)$ and $\sigma_{\text{ess}}(\cdot)$ the spectrum and essential spectrum of a densely defined closed linear operator in a complex separable Hilbert space.)

Theorem 2.1.1 ([24]).
Let $q \in L^1_{\text{loc}}(\mathbb{R})$ be real-valued and periodic. Let $H = -\frac{d^2}{dx^2} + q$ be the associated self-adjoint Schrödinger operator in $L^2(\mathbb{R})$ and suppose that

$$\sigma(H) = [e_0, \infty) \text{ for some } e_0 \in \mathbb{R}. \tag{2.1.1}$$

Then q is of the form,

$$q(x) = e_0 \text{ for a.e. } x \in \mathbb{R}. \tag{2.1.2}$$

Traditionally, uniqueness results such as Theorem 2.1.1 are called Borg-type theorems. However, this terminology is not uniquely adopted and hence a bit unfortunate. Indeed, inverse spectral results on finite intervals in which the coefficient(s) in the underlying differential or difference expression are recovered from two spectra, were also pioneered by Borg in his celebrated paper [24], and hence are also coined Borg-type theorems in the literature, see, for instance, [127], [128].

A closer examination of the proof of Theorem 2.1.1 in [30] shows that periodicity of q is not the point for the uniqueness result (2.1.2). The key ingredient (besides $\sigma(H) = [e_0, \infty)$ and q real-valued) is the fact that

$$\text{for all } x \in \mathbb{R}, \ \xi(\lambda, x) = 1/2 \ \text{ for a.e. } \lambda \in \sigma_{\mathrm{ess}}(h). \tag{2.1.3}$$

Here $\xi(\lambda, x)$, the argument of the boundary value $g(\lambda + i0, x)$ of the diagonal Green's function of H on the real axis (where $g(z, x) = (H - zI)^{-1}(x, x)$, $z \in \mathbb{C}\backslash\sigma(h)$, $x \in \mathbb{R}$), is defined by

$$\xi(\lambda, x) = \pi^{-1} \lim_{\varepsilon \downarrow 0} \mathrm{Im}(\ln(g(\lambda + i\varepsilon, x))) \ \text{ for a.e. } \lambda \in \mathbb{R} \text{ and all } x \in \mathbb{R}. \tag{2.1.4}$$

Real-valued periodic potentials are known to satisfy (2.1.3), but so do certain classes of real-valued quasi-periodic and almost-periodic potentials q. In particular, the class of real-valued algebro-geometric finite-gap KdV potentials q (a subclass of the set of real-valued quasi-periodic potentials) is a prime example satisfying (2.1.3) without necessarily being periodic. Traditionally, potentials q satisfying (2.1.3) are called *reflectionless* (see [31], [30] and the references therein).

The extension of Borg's Theorem 2.1.1 to periodic matrix-valued Schrödinger operators was proved by Dépres [39]. A new strategy of the proof based on exponential Herglotz representations and a trace formula (cf. [76]) for such potentials, as well as the extension to reflectionless matrix-valued potentials, was obtained in [30].

The direct analog of Borg's Theorem 2.1.1 for periodic Jacobi operators was proved by Flaschka [51] in 1975.

Theorem 2.1.2 ([51]).

Suppose $a = \{a_k\}_{k\in\mathbb{Z}}$ and $b = \{b_k\}_{k\in\mathbb{Z}}$ are periodic real-valued sequences in $\ell^\infty(\mathbb{Z})$ with the same period and $a_k > 0$, $k \in \mathbb{Z}$. Let $H = aS^+ + a^- S^- + b$ be the associated self-adjoint Jacobi operator on $\ell^2(\mathbb{Z})$ and suppose that

$$\sigma(H) = [E_-, E_+] \text{ for some } E_- < E_+. \tag{2.1.5}$$

Then $a = \{a_k\}_{k\in\mathbb{Z}}$ and $b = \{b_k\}_{k\in\mathbb{Z}}$ are of the form,

$$a_k = (E_+ - E_-)/4, \quad b_k = (E_- + E_+)/2, \quad k \in \mathbb{Z}. \tag{2.1.6}$$

Here $S^\pm$ denote the shift operators $(S^\pm f)(n) = f(n \pm 1)$, $n \in \mathbb{Z}$, $f \in \ell^\infty(\mathbb{Z})$.

The extension of Theorem 2.1.2 to reflectionless scalar Jacobi operators is due to Teschl [182, Corollary 6.3] (see also [183, Corollary 8.6]). The extension of Theorem 2.1.2 to matrix-valued reflectionless Jacobi operators (and a corresponding result for Dirac-type difference operators) has recently been obtained in [32].

The following very recent result of Simon is the first in connection with orthogonal polynomials on the unit circle.

Theorem 2.1.3 ([171], Sect. 11.14).

Suppose $\alpha = \{\alpha_k\}_{k\in\mathbb{Z}} \subset \mathbb{D}$ is a periodic sequence. Let U be the associated unitary CMV operator (2.2.1) (*cf. also* (1.2.10)) *on $\ell^2(\mathbb{Z})$ and suppose that*

$$\sigma(U) = \partial\mathbb{D}. \tag{2.1.7}$$

Then $\alpha = \{\alpha_k\}_{k\in\mathbb{Z}}$ is of the form,

$$\alpha_k = 0, \quad k \in \mathbb{Z}. \tag{2.1.8}$$

We will extend Simon's result to reflectionless Verblunsky coefficients corresponding to a CMV operator with spectrum a connected arc on the unit circle in our principal Section 2.5.

In Section 2.2 we prove an infinite sequence of trace formulas connected with CMV operators U using Weyl–Titchmarsh functions (and their exponential Herglotz representations) associated with U. Section 2.3 proves certain scaling results for Schur functions associated with U using a Riccati-type equation for the Verblunsky coefficients α. The notion of reflectionless CMV operators U is introduced in Section 2.4 and a variety of necessary conditions (many of them also sufficient) for U to be reflectionless are established. In our principal Section 2.5 we extend Simon's Borg-type result, Theorem 2.1.3, from periodic to reflectionless Verblunsky coefficients, and then we prove our main new result, a Borg-type theorem for reflectionless CMV operators whose spectrum consists of a connected subarc of the unit circle $\partial\mathbb{D}$.

2.2 Trace Formulas

In this section we discuss trace formulas associated with the CMV operator U on $\ell^2(\mathbb{Z})$. We freely use the notation established in Chapter 1 and Appendix A.

As discussed in (1.2.6)–(1.2.10), the unitary CMV operator U on $\ell^2(\mathbb{Z})$ can be written as a special five-diagonal doubly infinite matrix in the standard basis of $\ell^2(\mathbb{Z})$

(cf. [171, Sects. 4.5, 10.5]) as,

$$U = \begin{pmatrix} \ddots & \ddots & \ddots & \ddots & \ddots & & & & \textbf{0} & \\ & 0 & -\alpha_0\rho_{-1} & -\overline{\alpha_{-1}}\alpha_0 & -\alpha_1\rho_0 & \rho_0\rho_1 & & & & \\ & & \rho_{-1}\rho_0 & \overline{\alpha_{-1}}\rho_0 & -\overline{\alpha_0}\alpha_1 & \overline{\alpha_0}\rho_1 & 0 & & & \\ & & & 0 & -\alpha_2\rho_1 & -\overline{\alpha_1}\alpha_2 & -\alpha_3\rho_2 & \rho_2\rho_3 & & \\ & \textbf{0} & & & \rho_1\rho_2 & \overline{\alpha_1}\rho_2 & -\overline{\alpha_2}\alpha_3 & \overline{\alpha_2}\rho_3 & 0 & \\ & & & & & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}. \tag{2.2.1}$$

Here terms of the form $-\overline{\alpha_k}\alpha_{k+1}$, $k \in \mathbb{Z}$, represent the diagonal entries in the infinite matrix (2.2.1), specifically, $-\overline{\alpha_k}\alpha_{k+1}$ is the (k,k) diagonal entry. The half-lattice (i.e., semi-infinite) version of U was first introduced by Cantero, Moral, and Velázquez [28].

Next, we recall the half-lattice Weyl–Titchmarsh functions $M_\pm(\cdot,k)$ associated with U (cf. (1.2.136)–(1.2.140)) and the Caratheodory function $M_{1,1}(\cdot,k)$ in (1.3.21). By Theorem A.4 and the fact that $M_{1,1}(0,k) = 1$ by (1.3.24), one then obtains for the exponential Herglotz representation of $M_{1,1}(\cdot,k)$, $k \in \mathbb{Z}$,

$$-i\ln[iM_{1,1}(z,k)] = \oint_{\partial\mathbb{D}} d\mu_0(\zeta)\,\Upsilon_{1,1}(\zeta,k)\frac{\zeta+z}{\zeta-z}, \quad z \in \mathbb{D}, \tag{2.2.2}$$

$$0 \leq \Upsilon_{1,1}(\zeta,k) \leq \pi \text{ for } \mu_0\text{-a.e. } \zeta \in \partial\mathbb{D}. \tag{2.2.3}$$

For our present purpose it is more convenient to rewrite (2.2.2) in the form ($k \in \mathbb{Z}$)

$$\ln[M_{1,1}(z,k)] = i\oint_{\partial\mathbb{D}} d\mu_0(\zeta)\,\Xi_{1,1}(\zeta,k)\frac{\zeta+z}{\zeta-z}, \quad z \in \mathbb{D}, \tag{2.2.4}$$

$$-\pi/2 \leq \Xi_{1,1}(\zeta,k) \leq \pi/2 \text{ for } \mu_0\text{-a.e. } \zeta \in \partial\mathbb{D}, \tag{2.2.5}$$

where

$$\Xi_{1,1}(\zeta,k) = \lim_{r\uparrow 1} \mathrm{Im}[\ln(M_{1,1}(r\zeta))] \tag{2.2.6}$$

$$= \Upsilon_{1,1}(\zeta,k) - (\pi/2) \text{ for } \mu_0\text{-a.e. } \zeta \in \partial\mathbb{D}. \tag{2.2.7}$$

We note that $M_{1,1}(0,k)=1$ also implies

$$\oint_{\partial\mathbb{D}} d\mu_0(\zeta)\,\Xi_{1,1}(\zeta,k)=0, \quad k\in\mathbb{Z}. \tag{2.2.8}$$

To derive trace formulas for U we now expand $M_{1,1}(z,k)$ near $z=0$. Using (1.3.21) one obtains

$$\begin{aligned} M_{1,1}(z,k) &= (\delta_k,(U+zI)(U-zI)^{-1}\delta_k)_{\ell^2(\mathbb{Z})} \\ &= 1+2(\delta_k, zU^*(I-zU^*)^{-1}\delta_k)_{\ell^2(\mathbb{Z})} \\ &= 1+\sum_{j=1}^{\infty} M_j(U,k)z^j, \quad z\in\mathbb{D}, \end{aligned} \tag{2.2.9}$$

where

$$M_j(U,k)=2(\delta_k,(U^*)^j\delta_k)_{\ell^2(\mathbb{Z})}, \quad j\in\mathbb{N},\ k\in\mathbb{Z} \tag{2.2.10}$$

and (2.2.10) represents a convergent expansion in $\mathcal{B}(\ell^2(\mathbb{Z}))$. (Here $\mathcal{B}(\mathcal{H})$ denotes the Banach space of bounded linear operators mapping the Hilbert space $\mathcal{H}$ into itself.) Explicitly, one computes

$$M_1(U,k)=-2\alpha_k\overline{\alpha_{k+1}}, \quad k\in\mathbb{Z}. \tag{2.2.11}$$

Next, we recall the well-known fact that the convergent Taylor expansion

$$g(z)=1+\sum_{j=1}^{\infty} c_j z^j, \quad z\in\mathbb{D} \tag{2.2.12}$$

implies the absolutely convergent expansion

$$\ln[g(z)]=\sum_{j=1}^{\infty} d_j z^j, \quad |z|<\varepsilon \tag{2.2.13}$$

(for $\varepsilon = \varepsilon(g)$ sufficiently small), where d_j can be recursivly computed via

$$d_1 = c_1, \quad d_j = c_j - \sum_{\ell=1}^{j-1} (\ell/j) c_{j-\ell}\, d_\ell, \quad j = 2, 3, \dots . \tag{2.2.14}$$

Thus, one obtains

$$\ln(M_{1,1}(z,k)) = \sum_{j=1}^{\infty} L_j(U,k) z^j, \ \ |z| \text{ sufficiently small}, \ k \in \mathbb{Z}, \tag{2.2.15}$$

where

$$\begin{aligned} &L_1(U,k) = M_1(U,k), \\ &L_j(U,k) = M_j(U,k) - \sum_{\ell=1}^{j-1} (\ell/j) M_{j-\ell}(U,k) L_\ell(U,k), \quad j = 2, 3, \dots, \ k \in \mathbb{Z}. \end{aligned} \tag{2.2.16}$$

Theorem 2.2.1. *Let $\alpha = \{\alpha_k\}_{k\in\mathbb{Z}} \subset \mathbb{D}$ and $k \in \mathbb{Z}$. Then,*

$$L_j(U,k) = 2i \oint_{\partial\mathbb{D}} d\mu_0(\zeta)\, \Xi_{1,1}(\zeta,k)\, \overline{\zeta}^j, \quad j \in \mathbb{N}. \tag{2.2.17}$$

In particular,

$$L_1(U,k) = -2\alpha_k \overline{\alpha_{k+1}} = 2i \oint_{\partial\mathbb{D}} d\mu_0(\zeta)\, \Xi_{1,1}(\zeta,k)\, \overline{\zeta}. \tag{2.2.18}$$

Proof. Let $z \in \mathbb{D}$, $k \in \mathbb{Z}$. Since

$$\frac{\zeta + z}{\zeta - z} = 1 + 2\sum_{j=1}^{\infty} (\overline{\zeta} z)^j, \quad \zeta \in \partial\mathbb{D}, \tag{2.2.19}$$

(2.2.4) implies

$$\ln[M_{1,1}(z,k)] = 2i \sum_{j=1}^{\infty} \oint_{\partial\mathbb{D}} d\mu_0(\zeta)\, \Xi_{1,1}(\zeta,k) \overline{\zeta}^j z^j, \ \ |z| \text{ sufficiently small}. \tag{2.2.20}$$

A comparison of coefficients of z^j in (2.2.15) and (2.2.20) then proves (2.2.17). (2.2.18) is then clear from (2.2.11) and (2.2.16). □

2.3 Scaling Considerations

In this section we prove some facts about the scaling behavior of the Schur functions $\Phi_\pm$ and $\Phi_{1,1}$ and use that to obtain spectral results for U. Again we freely use the notation established in Chapter 1 and Appendix A.

Throughout this section we suppose that the sequence α satisfies Hypothesis 1.2.1, that is, $\alpha = \{\alpha_k\}_{k\in\mathbb{Z}} \subset \mathbb{D}$.

We start by recalling the Riccati-type equation (1.2.155) satisfied by $\Phi_\pm$ (cf. Remark 1.2.23),

$$\alpha_k \Phi_\pm(z,k-1)\Phi_\pm(z,k) - \Phi_\pm(z,k-1) + z\Phi_\pm(z,k) = \overline{\alpha_k} z, \quad z \in \mathbb{C}\backslash\partial\mathbb{D},\ k \in \mathbb{Z}. \tag{2.3.1}$$

In the following it is convenient to indicate explicitly the α-dependence of $\Phi_\pm$ and $\Phi_{1,1}$ and we will thus temporarily write $\Phi_\pm(z,k;\alpha)$ and $\Phi_{1,1}(z,k;\alpha)$, etc.

Lemma 2.3.1. *Let $z \in \mathbb{C}\backslash\partial\mathbb{D}$ and $k \in \mathbb{Z}$. Suppose $\alpha = \{\alpha_k\}_{k\in\mathbb{Z}} \subset \mathbb{D}$ and assume $\{\gamma_0, \gamma_1\} \subset \partial\mathbb{D}$. Define $\beta = \{\gamma_0\gamma_1^k \alpha_k\}_{k\in\mathbb{Z}}$. Then,*

$$\Phi_\pm(z,k;\alpha) = \gamma_0\gamma_1^k \Phi_\pm(\gamma_1 z,k;\beta), \tag{2.3.2}$$

$$\Phi_{1,1}(z,k;\alpha) = \Phi_{1,1}(\gamma_1 z,k;\beta). \tag{2.3.3}$$

Proof. We recall that

$$\Phi_+(\cdot,k)\colon \mathbb{D} \to \mathbb{D}, \quad 1/\Phi_-(\cdot,k)\colon \mathbb{D} \to \mathbb{D}, \quad k \in \mathbb{Z}, \tag{2.3.4}$$

are analytic, with unique Taylor coefficients at $z = 0$, and hence $\Phi_\pm$ are the unique solutions of the Riccati-type equation (2.3.1) satisfying (2.3.4). Since the right-hand side of (2.3.2) also shares the mapping properties (2.3.4), it suffices to show that the right-hand side of (2.3.2) satisfies the Riccati-type equation (2.3.1). Multiplying

$$\beta_k \Phi_\pm(z,k-1;\beta)\Phi_\pm(z,k;\beta) - \Phi_\pm(z,k-1;\beta) + z\Phi_\pm(z,k;\beta) - z\overline{\beta_k} = 0 \qquad (2.3.5)$$

by $\gamma_0\gamma_1^{k-1}$, one infers

$$\begin{aligned}&\beta_k\gamma_0^{-1}\gamma_1^{-k}\big[\gamma_0\gamma_1^{k-1}\Phi_\pm(z,k-1;\beta)\big]\big[\gamma_0\gamma_1^{k}\Phi_\pm(z,k;\beta)\big] - \big[\gamma_0\gamma_1^{k-1}\Phi_\pm(z,k-1;\beta)\big]\\ &\quad + z\gamma_1^{-1}\big[\gamma_0\gamma_1^{k}\Phi_\pm(z,k;\beta)\big] - z\gamma_1^{-1}\big[\overline{\beta_k\gamma_0^{-1}\gamma_1^{-k}}\big] = 0. \qquad (2.3.6)\end{aligned}$$

This proves (2.3.2). Since $\Phi_{1,1} = \Phi_+/\Phi_-$ by (1.3.38), (2.3.2) implies (2.3.3). $\square$

Next, we also indicate the explicit α-dependence of $U_{\pm,k_0}$ and U by $U_{\pm,k_0;\alpha}$ and U_α, respectively. Similarly, we write $M_\pm(z,k;\alpha)$, $M_{\ell,\ell'}(z,k;\alpha)$, $\ell,\ell'=0,1$, and $\mathcal{M}(z,k;\alpha)$.

Corollary 2.3.2. *Let $k_0\in\mathbb{Z}$. Suppose $\alpha=\{\alpha_k\}_{k\in\mathbb{Z}}\subset\mathbb{D}$ and assume $\{\gamma_0,\gamma_1\}\subset\partial\mathbb{D}$. Define $\beta=\{\gamma_0\gamma_1^k\alpha_k\}_{k\in\mathbb{Z}}$. Then,*

$$\sigma_{\mathrm{ac}}(U_{\pm,k_0;\alpha}) = \gamma_1^{-1}\sigma_{\mathrm{ac}}(U_{\pm,k_0;\beta}), \qquad (2.3.7)$$

$$\sigma(U_\alpha) = \gamma_1^{-1}\sigma(U_\beta). \qquad (2.3.8)$$

Moreover, the operators U_α and $\gamma_1^{-1}U_\beta$ are unitarily equivalent.

Proof. Since by (1.2.151), $\pm\mathrm{Re}(M_\pm)>0$ is equivalent to $|\Phi_\pm^{\pm1}|<1$ and $\pm\mathrm{Re}(M_\pm)>0$ is equivalent to $\pm\mathrm{Re}(m_\pm)>0$ by (1.2.137) and (1.2.139), and $\{\gamma_0,\gamma_1\}\subset\partial\mathbb{D}$, (2.3.7) follows from (2.3.2), (A.12), and (A.14).

By (1.3.20), (1.3.37), (2.3.3), and (A.18),

$$d\Omega_{0,0}(\zeta,k;\alpha) = d\Omega_{0,0}(\gamma_1\zeta,k;\beta), \quad \zeta\in\partial\mathbb{D},\ k\in\mathbb{Z}, \qquad (2.3.9)$$

$$d\Omega_{1,1}(\zeta,k;\alpha) = d\Omega_{1,1}(\gamma_1\zeta,k;\beta), \quad \zeta\in\partial\mathbb{D},\ k\in\mathbb{Z}. \tag{2.3.10}$$

Applying Corollary 1.3.5 then proves (2.3.8).

Finally, we prove the unitary equivalence of U_α and $\gamma_1^{-1}U_\beta$. We fix a reference point $k\in\mathbb{Z}$. By (2.3.3) and (1.3.37) one then infers

$$M_{1,1}(z,k;\alpha) = M_{1,1}(z,k;\beta), \quad z\in\mathbb{C}\backslash\partial\mathbb{D} \tag{2.3.11}$$

and hence also

$$M_{0,0}(z,k;\alpha) = M_{0,0}(z,k;\beta), \quad z\in\mathbb{C}\backslash\partial\mathbb{D}, \tag{2.3.12}$$

using (1.3.20). Next, using (2.3.2) and (1.2.151) one computes

$$M_\pm(z,k;\alpha) = \frac{(1+\gamma_0\gamma_1^k)M_\pm(\gamma_1 z,k;\beta)+1-\gamma_0\gamma_1^k}{(1-\gamma_0\gamma_1^k)M_\pm(\gamma_1 z,k;\beta)+1+\gamma_0\gamma_1^k}, \quad z\in\mathbb{C}\backslash\partial\mathbb{D}. \tag{2.3.13}$$

Insertion of (2.3.13) into (1.3.25)–(1.3.28) then yields

$$\begin{aligned} M_{0,1}(z,k;\alpha) &= \begin{cases} \gamma_0\gamma_1^k M_{0,1}(\gamma_1 z,k;\beta), & k \text{ odd},\\ \gamma_0^{-1}\gamma_1^{-k} M_{0,1}(\gamma_1 z,k;\beta), & k \text{ even},\end{cases}\\ M_{1,0}(z,k;\alpha) &= \begin{cases} \gamma_0^{-1}\gamma_1^{-k} M_{1,0}(\gamma_1 z,k;\beta), & k \text{ odd},\\ \gamma_0\gamma_1^k M_{1,0}(\gamma_1 z,k;\beta), & k \text{ even}.\end{cases} \end{aligned} \tag{2.3.14}$$

Thus,

$$\mathcal{M}(z,k;\alpha) = \begin{cases} \mathcal{A}_k\mathcal{M}(\gamma_1 z,k;\beta)\mathcal{A}_k^{-1}, & k \text{ odd},\\ \mathcal{A}_k^{-1}\mathcal{M}(\gamma_1 z,k;\beta)\mathcal{A}_k, & k \text{ even},\end{cases} \tag{2.3.15}$$
$$z\in\mathbb{C}\backslash\partial\mathbb{D},$$

where

$$\mathcal{A}_k = \begin{pmatrix} (\gamma_0\gamma_1^k)^{-1/2} & 0\\ 0 & (\gamma_0\gamma_1^k)^{1/2}\end{pmatrix}, \quad k\in\mathbb{Z}. \tag{2.3.16}$$

Since $\gamma_0,\gamma_1\in\partial\mathbb{D}$, $\mathcal{M}(z,k;\alpha)$ and $\mathcal{M}(\gamma_1 z,k;\beta)$ are unitarily equivalent, this implies the unitary equivalence of U_α and $\gamma_1^{-1}U_\beta$ by (1.3.19), Corollary 1.3.5, and Theorem A.6. $\square$

2.4 Reflectionless Verblunsky Coefficients

In this section we discuss a variety of equivalent conditions for the Verblunsky coefficients α (resp., the CMV operator U) to be reflectionless.

We denote by $M_{\pm}(\zeta, k)$, $M_{1,1}(\zeta, k)$, $\Phi_{\pm}(\zeta, k)$, and $\Phi_{1,1}(\zeta, k)$, $\zeta \in \partial\mathbb{D}$, $k \in \mathbb{Z}$, etc., the radial limits to the unit circle of the corresponding functions,

$$M_{\pm}(\zeta, k) = \lim_{r \uparrow 1} M_{\pm}(r\zeta, k), \quad M_{1,1}(\zeta, k) = \lim_{r \uparrow 1} M_{1,1}(r\zeta, k), \tag{2.4.1}$$

$$\Phi_{\pm}(\zeta, k) = \lim_{r \uparrow 1} \Phi_{\pm}(r\zeta, k), \quad \Phi_{1,1}(\zeta, k) = \lim_{r \uparrow 1} \Phi_{1,1}(r\zeta, k), \quad \zeta \in \partial\mathbb{D}, \ k \in \mathbb{Z}. \tag{2.4.2}$$

These limits are known to exist μ_0-almost everywhere. The following definition of reflectionless Verblunsky coefficients represents the analog of reflectionless coefficients in Schrödinger, Dirac, and Jacobi operators (cf., e.g. [31], [30], [34], [35], [70], [76], [82], [83], [103], [115]–[117], [173], [174], [182], [183]).

Definition 2.4.1. Let $\alpha = \{\alpha_k\}_{k \in \mathbb{Z}} \subset \mathbb{D}$ and denote by U the associated unitary CMV operator U on $\ell^2(\mathbb{Z})$. Then α (resp., U) is called *reflectionless*, if

$$\text{for all } k \in \mathbb{Z}, \ M_+(\zeta, k) = -\overline{M_-(\zeta, k)} \ \text{ for } \mu_0\text{-a.e. } \zeta \in \sigma_{\text{ess}}(U). \tag{2.4.3}$$

The following result provides a variety of equivalent criteria for α (resp., U) to be reflectionless.

Theorem 2.4.2. *Let $\alpha = \{\alpha_k\}_{k \in \mathbb{Z}} \subset \mathbb{D}$ and denote by U the associated unitary CMV operator U on $\ell^2(\mathbb{Z})$. Then the following assertions (i)–(vi) are equivalent:*

(i) $\alpha = \{\alpha_k\}_{k \in \mathbb{Z}}$ is reflectionless.

(ii) Let $\gamma \in \partial\mathbb{D}$. Then $\beta = \{\gamma\alpha_k\}_{k \in \mathbb{Z}}$ is reflectionless.

(iii) For all $k \in \mathbb{Z}$, $M_+(\zeta, k) = -\overline{M_-(\zeta, k)}$ *for* μ_0*-a.e.* $\zeta \in \sigma_{\text{ess}}(U)$.

(iv) For some $k_0 \in \mathbb{Z}$, $M_+(\zeta, k_0) = -\overline{M_-(\zeta, k_0)}$ *for* μ_0*-a.e.* $\zeta \in \sigma_{\text{ess}}(U)$.

(v) For all $k \in \mathbb{Z}$, $\Phi_+(\zeta, k) = 1/\overline{\Phi_-(\zeta, k)}$ *for* μ_0*-a.e.* $\zeta \in \sigma_{\text{ess}}(U)$.

(vi) For some $k_0 \in \mathbb{Z}$, $\Phi_+(\zeta, k_0) = 1/\overline{\Phi_-(\zeta, k_0)}$ *for* μ_0*-a.e.* $\zeta \in \sigma_{\text{ess}}(U)$.

Moreover, conditions (i)–(vi) imply the following equivalent assertions (vii)–(ix):

(vii) For all $k \in \mathbb{Z}$, $\Xi_{1,1}(\zeta, k) = 0$ *for* μ_0*-a.e.* $\zeta \in \sigma_{\text{ess}}(U)$.

(viii) For all $k \in \mathbb{Z}$, $M_{1,1}(\zeta, k) > 0$ *for* μ_0*-a.e.* $\zeta \in \sigma_{\text{ess}}(U)$.

(ix) For all $k \in \mathbb{Z}$, $\Phi_{1,1}(\zeta, k) \in (-1, 1)$ *for* μ_0*-a.e.* $\zeta \in \sigma_{\text{ess}}(U)$.

Proof. We will prove the following diagram:

$$
\begin{array}{ccc}
 & (ii) & \\
 & \Updownarrow & \\
(i) \Leftrightarrow (iii) \Leftrightarrow & (v) & \Leftrightarrow (vi) \Leftrightarrow (iv) \\
 & \Downarrow & \\
 & (ix) & \Leftrightarrow (viii) \Leftrightarrow (vii)
\end{array}
$$

(i) is equivalent to (iii) by Definition 2.4.1.

(iii) is equivalent to (v) and (vi) is equivalent to (iv) by (1.2.150) and (1.2.151).

$(v) \Leftrightarrow (ii)$: By Lemma 2.3.1,

$$\Phi_+(z, k; \alpha)\overline{\Phi_-(z, k; \alpha)} = \Phi_+(z, k; \beta)\overline{\Phi_-(z, k; \beta)}, \quad z \in \mathbb{C},\ k \in \mathbb{Z}, \tag{2.4.4}$$

hence the fact that (i) is equivalent to (v) implies that (v) is equivalent to (ii).

That (v) implies (vi) is clear.

$(vi) \Rightarrow (v)$: By (1.2.155),

$$\Phi_\pm(z,k+1) = \frac{z\overline{\alpha_{k+1}} + \Phi_\pm(z,k)}{\alpha_{k+1}\Phi_\pm(z,k) + z}, \tag{2.4.5}$$

$$\Phi_\pm(z,k-1) = \frac{z\overline{\alpha_k} - z\Phi_\pm(z,k)}{\alpha_k\Phi_\pm(z,k) - 1}, \quad z \in \mathbb{C}\backslash\partial\mathbb{D}, \ k \in \mathbb{Z}. \tag{2.4.6}$$

Taking into account (vi) at the point $k_0 \in \mathbb{Z}$,

$$\Phi_+(\zeta,k_0)\overline{\Phi_-(\zeta,k_0)} = 1 \ \text{ for } \mu_0\text{-a.e. } \zeta \in \sigma_{\text{ess}}(U), \tag{2.4.7}$$

one proves (vi) at the points $k_0 \pm 1$ as follows:

$$\begin{aligned}
\Phi_+(\zeta,k_0+1)\overline{\Phi_-(\zeta,k_0+1)} &= \frac{\zeta\overline{\alpha_{k_0+1}} + \Phi_+(\zeta,k_0)}{\alpha_{k_0+1}\Phi_+(\zeta,k_0) + \zeta}\ \frac{\overline{\zeta}\alpha_{k_0+1} + \overline{\Phi_-(\zeta,k_0)}}{\overline{\alpha_{k_0+1}}\,\overline{\Phi_-(\zeta,k_0)} + \overline{\zeta}} \\
&= \frac{1 + |\alpha_{k_0+1}|^2 + \overline{\zeta}\alpha_{k_0+1}\Phi_+(\zeta,k_0) + \zeta\overline{\alpha_{k_0+1}}\,\overline{\Phi_-(\zeta,k_0)}}{|\alpha_{k_0+1}|^2 + 1 + \overline{\zeta}\alpha_{k_0+1}\Phi_+(\zeta,k_0) + \zeta\overline{\alpha_{k_0+1}}\,\overline{\overline{\Phi_-(\zeta,k_0)}}} \\
&= 1 \text{ for } \mu_0\text{-a.e. } \zeta \in \sigma_{\text{ess}}(U),
\end{aligned} \tag{2.4.8}$$

$$\begin{aligned}
\Phi_+(\zeta,k_0-1)\overline{\Phi_-(\zeta,k_0-1)} &= |\zeta|^2\frac{\overline{\alpha_{k_0}} - \Phi_+(\zeta,k_0)}{\alpha_{k_0}\Phi_+(\zeta,k_0) - 1}\ \frac{\alpha_{k_0} - \overline{\Phi_-(\zeta,k_0)}}{\overline{\alpha_{k_0}}\,\overline{\Phi_-(\zeta,k_0)} - 1} \\
&= \frac{|\alpha_{k_0}|^2 + 1 - \alpha_{k_0}\Phi_+(\zeta,k_0) - \overline{\alpha_{k_0}}\,\overline{\Phi_-(\zeta,k_0)}}{|\alpha_{k_0}|^2 + 1 - \alpha_{k_0}\Phi_+(\zeta,k_0) - \overline{\alpha_{k_0}}\,\overline{\overline{\Phi_-(\zeta,k_0)}}} = 1 \ \text{ for } \mu_0\text{-a.e. } \zeta \in \sigma_{\text{ess}}(U).
\end{aligned} \tag{2.4.9}$$

Iterating this procedure implies (v).

(ix) is equivalent to $(viii)$ by (1.3.36) and (1.3.37).

$(viii)$ is equivalent to (vii) by (2.2.7).

$(v) \Rightarrow (ix)$: By (1.3.38),

$$\Phi_{1,1}(z,k) = \frac{\Phi_+(z,k)}{\Phi_-(z,k)} = \frac{\Phi_+(z,k)\overline{\Phi_-(z,k)}}{|\Phi_-(z,k)|^2}, \quad z \in \mathbb{C}\backslash\partial\mathbb{D}, \ k \in \mathbb{Z}, \tag{2.4.10}$$

and hence (v) implies (ix). $\square$

The next result shows that periodic Verblunsky coefficients are reflectionless.

Lemma 2.4.3. *Let $\alpha = \{\alpha_k\}_{k\in\mathbb{Z}}$ be a sequence of periodic Verblunsky coefficients. Then α is reflectionless.* (*This applies, in particular, to $\alpha = 0$.*)

Proof. Let $\omega \in \mathbb{N}$ denote the period of $\alpha = \{\alpha_k\}_{k\in\mathbb{Z}}$. Without loss of generality we may assume ω to be even. (If ω is odd, we can consider the even period 2ω.) Then,

$$\mathfrak{M}(z,k_0) = \begin{pmatrix} \mathfrak{M}_{1,1}(z,k_0) & \mathfrak{M}_{1,2}(z,k_0) \\ \mathfrak{M}_{2,1}(z,k_0) & \mathfrak{M}_{2,2}(z,k_0) \end{pmatrix} = \prod_{k=1}^{\omega} T(z,k_0+k),$$
$$z \in \mathbb{C}\backslash\{0\}, \; k_0 \in \mathbb{Z}, \tag{2.4.11}$$

represents the monodromy matrix of the CMV operator U associated with the sequence α. By $\Delta(z)$ we denote the corresponding Floquet discriminant,

$$\Delta(z) = \frac{1}{2}\operatorname{tr}(\mathfrak{M}(z,k_0)), \quad z \in \mathbb{C}\backslash\{0\}. \tag{2.4.12}$$

We note that $\Delta(z)$ does not depend on k_0. By (1.2.18) and (2.4.11),

$$\mathfrak{M}_{1,1}(\zeta,k_0) = \overline{\mathfrak{M}_{2,2}(\zeta,k_0)}, \tag{2.4.13}$$

$$\mathfrak{M}_{1,2}(\zeta,k_0) = \overline{\mathfrak{M}_{2,1}(\zeta,k_0)}, \quad \zeta \in \partial\mathbb{D}, \; k_0 \in \mathbb{Z}. \tag{2.4.14}$$

Thus, $\Delta(\zeta) = \operatorname{Re}(\mathfrak{M}_{1,1}(\zeta,k_0)) \in \mathbb{R}$ for all $\zeta \in \partial\mathbb{D}$. Moreover, since $\det(\mathfrak{M}(z,k_0)) = 1$, for all $k_0 \in \mathbb{Z}$, the eigenvalues of $\mathfrak{M}(z,k_0)$ are given by

$$\rho_\pm(z) = \Delta(z) \mp \sqrt{\Delta(z)^2 - 1}, \quad z \in \mathbb{C}\backslash\{0\}, \tag{2.4.15}$$

where the branch of the square root is chosen such that $|\rho_\pm(z)| \lessgtr 1$ for $z \in \mathbb{C}\backslash(\partial\mathbb{D} \cup \{0\})$, and hence,

$$\begin{pmatrix} u_\pm(z,k+\omega,k_0) \\ v_\pm(z,k+\omega,k_0) \end{pmatrix} = \rho_\pm(z) \begin{pmatrix} u_\pm(z,k,k_0) \\ v_\pm(z,k,k_0) \end{pmatrix}, \quad z \in \mathbb{C}\backslash\{0\}, \; k,k_0 \in \mathbb{Z}. \tag{2.4.16}$$

Thus, $\rho_\pm$ are the Floquet multipliers associated with U and consequently one obtains the following characterization of the spectrum of U,

$$\sigma(U) = \{\zeta \in \partial\mathbb{D} \,|\, |\rho_\pm(\zeta)| = 1\} = \{\zeta \in \partial\mathbb{D} \,|\, -1 \leq \Delta(\zeta) \leq 1\}. \tag{2.4.17}$$

Next, assume k to be even. Then (1.2.154) implies

$$\begin{aligned}\Phi_\pm(z,k) &= \frac{u_\pm(z,k,k_0)}{v_\pm(z,k,k_0)} = \frac{u_\pm(z,k+\omega,k_0)/\rho_\pm(z)}{v_\pm(z,k+\omega,k_0)/\rho_\pm(z)} \\ &= \frac{\mathfrak{M}_{1,1}(z,k)\Phi_\pm(z,k) + \mathfrak{M}_{1,2}(z,k)}{\mathfrak{M}_{2,1}(z,k)\Phi_\pm(z,k) + \mathfrak{M}_{2,2}(z,k)}, \quad z \in \mathbb{C}\backslash\{0\}.\end{aligned} \tag{2.4.18}$$

It follows that

$$\Phi_\pm(z,k) = \frac{\mathfrak{M}_{1,1}(z,k) - \mathfrak{M}_{2,2}(z,k) \pm 2\sqrt{\Delta(z)^2 - 1}}{2\,\mathfrak{M}_{2,1}(z,k)}, \quad z \in \mathbb{C}\backslash\{0\}, \tag{2.4.19}$$

and hence, by (2.4.13) and (2.4.17),

$$\Phi_\pm(\zeta,k) = i\frac{\mathrm{Im}(\mathfrak{M}_{1,1}(\zeta,k)) \pm \sqrt{1 - \mathrm{Re}(\mathfrak{M}_{1,1}(\zeta,k))^2}}{\mathfrak{M}_{2,1}(\zeta,k)}, \quad \zeta \in \sigma(U). \tag{2.4.20}$$

Thus, by (2.4.13), (2.4.14), and $\det(\mathfrak{M}(z,k)) = 1$ for all $z \in \mathbb{C}\backslash\{0\}$, $k \in \mathbb{Z}$,

$$\Phi_+(\zeta,k)\overline{\Phi_-(\zeta,k)} = \frac{|\mathfrak{M}_{1,1}(\zeta,k)|^2 - 1}{|\mathfrak{M}_{2,1}(\zeta,k)|^2} = 1, \quad \zeta \in \sigma(U), \tag{2.4.21}$$

and hence α is reflectionless by Theorem 2.4.2 (vi). $\square$

We conclude this section with another result concerning the reflectionless condition (2.4.3) on arcs of the unit circle. It is contained in Lemma 10.11.17 in [171]. The latter is based on results in [115] (see also [91], [116]). For completeness we include the following elementary proof (which only slightly differs from that in [171] in that no H^p-arguments are involved). To fix some notation we denote by f_+ and f_- a

Caratheodory and anti-Caratheodory function, respectivley, and by φ_+ and φ_- the corresponding Schur and anti-Schur function,

$$\varphi_\pm = \frac{f_\pm - 1}{f_\pm + 1}. \tag{2.4.22}$$

Moreover, we introduce the corresponding Herglotz representations of $f_\pm$ (cf. (A.3), (A.4))

$$f_\pm(z) = ic_\pm \pm \oint_{\partial\mathbb{D}} d\mu_\pm(\zeta)\,\frac{\zeta+z}{\zeta-z}, \quad z \in \mathbb{D},\ c_\pm \in \mathbb{R}. \tag{2.4.23}$$

We introduce the following notation for open arcs on the unit circle $\partial\mathbb{D}$,

$$\mathrm{Arc}\big(\big(e^{i\theta_1}, e^{i\theta_2}\big)\big) = \big\{e^{i\theta} \in \partial\mathbb{D} \,|\, \theta_1 < \theta < \theta_2\big\}, \quad \theta_1 \in [0,2\pi),\ \theta_1 < \theta_2 \le \theta_1 + 2\pi. \tag{2.4.24}$$

An open arc $\mathcal{A} \subseteq \partial\mathbb{D}$ then either coincides with $\mathrm{Arc}\big(\big(e^{i\theta_1}, e^{i\theta_2}\big)\big)$ for some $\theta_1 \in [0,2\pi)$, $\theta_1 < \theta_2 \le \theta_1 + 2\pi$, or else, $\mathcal{A} = \partial\mathbb{D}$.

Lemma 2.4.4. *Let $\mathcal{A} \subseteq \partial\mathbb{D}$ be an open arc and assume that f_+ (resp., f_-) is a Caratheodory (resp., anti-Caratheodory) function satisfying the reflectionless condition* (2.4.3) *μ_0-a.e. on $\mathcal{A}$, that is,*

$$\lim_{r\uparrow 1}\big[f_+(r\zeta) + \overline{f_-(r\zeta)}\big] = 0 \ \ \mu_0\text{-a.e. on } \mathcal{A}. \tag{2.4.25}$$

Then,

(i) $f_+(\zeta) = -\overline{f_-(\zeta)}$ for all $\zeta \in \mathcal{A}$.

(ii) For $z \in \mathbb{D}$, $-\overline{f_-(1/\overline{z})}$ is the analytic continuation of $f_+(z)$ through the arc $\mathcal{A}$.

(iii) $d\mu_\pm$ are purely absolutely continuous on A and

$$\frac{d\mu_\pm}{d\mu_0}(\zeta) = \mathrm{Re}(f_+(\zeta)) = -\mathrm{Re}(f_-(\zeta)), \quad \zeta \in \mathcal{A}. \tag{2.4.26}$$

Proof. By (2.4.22) and

$$\varphi_+(z) - \overline{1/\varphi_-(z)} = \frac{-2\big[f_+(z) + \overline{f_-(z)}\,\big]}{\big[f_+(z)+1\big]\big[\,\overline{f_-(z)}-1\big]}, \quad z \in \mathbb{D}, \tag{2.4.27}$$

equation (2.4.25) is equivalent to

$$\lim_{r\uparrow 1}\big[\varphi_+(r\zeta) - \overline{1/\varphi_-(r\zeta)}\,\big] = 0 \ \text{ for } \mu_0\text{-a.e. } \zeta \in \mathcal{A}. \tag{2.4.28}$$

Next, introducing

$$g_1(z) = [\varphi_+(z) - 1/\varphi_-(z)]/2, \quad g_2(z) = [\varphi_+(z) + 1/\varphi_-(z)]/(2i), \quad z \in \mathbb{D}, \tag{2.4.29}$$

then g_j, $j = 1, 2$, are Schur functions (since $z_1, z_2 \in \mathbb{D}$ implies $(z_1 \pm z_2)/2 \in \mathbb{D}$) and hence,

$$g_j + 1,\ j = 1, 2, \text{ are Caratheodory functions.} \tag{2.4.30}$$

Moreover, by (2.4.28),

$$\mathrm{Re}(g_j(\zeta)) = \lim_{r\uparrow 1}\mathrm{Re}(g_j(r\zeta)) = 0 \ \text{ for } \mu_0\text{-a.e. } \zeta \in \mathcal{A},\ j = 1, 2. \tag{2.4.31}$$

Since g_j, $j = 1, 2$, are Schur functions,

$$|g_j(z)| \leq 1, \quad z \in \mathbb{D},\ j = 1, 2, \tag{2.4.32}$$

and hence the measures $d\mu_j$ in the Herglotz representation of $g_j + 1$, $j = 1, 2$, are purely absolutely continuous by (A.15),

$$d\mu_j = d\mu_{j,\mathrm{ac}}, \quad d\mu_{j,\mathrm{s}} = 0, \quad j = 1, 2. \tag{2.4.33}$$

By (A.7) and (A.12) one thus obtains

$$g_j(z) + 1 = ic_j + \oint_{\partial\mathbb{D}} [\mathrm{Re}(g_j(\zeta)) + 1]d\mu_0(\zeta)\,\frac{\zeta + z}{\zeta - z},$$

$$= ic_j + 1 + \oint_{\partial\mathbb{D}} \mathrm{Re}(g_j(\zeta)) d\mu_0(\zeta) \, \frac{\zeta + z}{\zeta - z}, \quad z \in \mathbb{D}, \ j = 1, 2, \tag{2.4.34}$$

that is,

$$g_j(z) = ic_j + \oint_{\partial\mathbb{D}} \mathrm{Re}(g_j(\zeta)) d\mu_0(\zeta) \, \frac{\zeta + z}{\zeta - z}, \quad z \in \mathbb{D}, \ j = 1, 2. \tag{2.4.35}$$

By (2.4.31), the signed measure $\mathrm{Re}(g_j) d\mu_0$ has no support on the arc $\mathcal{A}$ and hence g_j, $j = 1, 2$, admit an analytic continuation through $\mathcal{A}$. Moreover, using (2.4.35) one computes

$$\overline{g_j(\zeta_0)} = -g_j(\zeta_0), \quad \zeta_0 \in \mathcal{A}, \ j = 1, 2. \tag{2.4.36}$$

Thus, the Schwarz symmetry principle yields

$$g_j(z) = -\overline{g_j(1/\overline{z})}, \quad z \in \mathbb{C} \backslash \mathbb{D}, \ j = 1, 2. \tag{2.4.37}$$

Since

$$\varphi_+ = g_1 + ig_2, \quad 1/\varphi_- = -g_1 + ig_2, \tag{2.4.38}$$

also φ_+ and $1/\varphi_-$ admit analytic continuations through the open arc $\mathcal{A}$ and because of (2.4.37) (and in agreement with (2.4.28)) one obtains

$$\varphi_+(z) = \overline{1/\varphi_-(1/\overline{z})}, \quad z \in \mathbb{C} \backslash \mathbb{D}. \tag{2.4.39}$$

Thus, one computes

$$f_+(z) = \frac{1 + \varphi_+(z)}{1 - \varphi_+(z)} = \frac{1 + \overline{1/\varphi_-(1/\overline{z})}}{1 - \overline{1/\varphi_-(1/\overline{z}))}} = \frac{\overline{\varphi_-(1/\overline{z})} + 1}{\overline{\varphi_-(1/\overline{z})} - 1} = -\overline{f_-(1/\overline{z})}, \quad z \in \mathbb{C} \backslash \mathbb{D}. \tag{2.4.40}$$

This proves items (*i*) and (*ii*). In particular, $\mathrm{Re}(f_\pm(\zeta))$ exists and is finite for all $\zeta \in \mathcal{A}$ and hence

$$S_{\mu_{\pm,\mathrm{s}}} \cap \mathcal{A} = \emptyset, \tag{2.4.41}$$

where $S_{\mu_{\pm,s}}$ denotes an essential support of $d\mu_{\pm,s}$. By (A.12) one thus computes

$$\frac{d\mu_\pm}{d\mu_0}(\zeta) = \mathrm{Re}(f_+(\zeta)) = -\mathrm{Re}(f_-(\zeta)), \quad \zeta \in \mathcal{A}, \tag{2.4.42}$$

proving item (iii). □

It is perhaps worth noting that this proof is based on the elementary fact that if g is any Schur function, then $g+1$ is a Caratheodory function with purely absolutely continuous measure in its Herglotz representation (cf. the first line of (2.4.34)). (In particular, the support of the measure in the Herglotz representation of $g+1$ equals $\partial\mathbb{D}$.) The rest are simple Schwarz symmetry considerations.

2.5 The Borg-type Theorem for CMV operators

We recall our notation for closed arcs on the unit circle $\partial\mathbb{D}$,

$$\mathrm{Arc}\big(\big[e^{i\theta_1}, e^{i\theta_2}\big]\big) = \big\{e^{i\theta} \in \partial\mathbb{D} \,|\, \theta_1 \le \theta \le \theta_2\big\}, \quad \theta_1 \in [0, 2\pi),\ \theta_1 \le \theta_2 \le \theta_1 + 2\pi \tag{2.5.1}$$

and similarly for open arcs (cf. (2.4.24)) and arcs open or closed at one endpoint (cf. (A.6)).

We start with a short proof of a recent result of Simon [171] in the case where α is a periodic sequence of Verblunsky coefficients, see Theorem 2.1.3. We will extend this result from the periodic to the reflectionless case.

Theorem 2.5.1. *Let $\alpha = \{\alpha_k\}_{k\in\mathbb{Z}} \subset \mathbb{D}$ be a reflectionless sequence of Verblunsky coefficients. Let U be the associated unitary CMV operator* (2.2.1) (*cf. also* (1.2.6)–(1.2.9)) *on $\ell^2(\mathbb{Z})$ and suppose that*

$$\sigma(U) = \partial\mathbb{D}. \tag{2.5.2}$$

Then $\alpha = \{\alpha_k\}_{k\in\mathbb{Z}}$ is of the form,

$$\alpha_k = 0, \quad k \in \mathbb{Z}. \tag{2.5.3}$$

Proof. Since by hypothesis U is reflectionless, one infers from Definition 2.4.1 that

$$\text{for all } k \in \mathbb{Z},\ M_+(\zeta, k) = -\overline{M_-(\zeta, k)} \text{ for } \mu_0\text{-a.e. } \zeta \in \partial\mathbb{D}. \tag{2.5.4}$$

Denote by $d\omega_\pm(\cdot, k)$ the measures associated with the Herglotz representation (A.3) of $M_\pm(\cdot, k)$, $k \in \mathbb{Z}$. (Of course, $d\omega_+ = d\mu_+$ by (1.2.137).) By Lemma 2.4.4, $d\omega_\pm(\cdot, k)$ are purely absolutely continuous for all $k \in \mathbb{Z}$,

$$d\omega_\pm(\cdot, k) = d\omega_{\pm,\mathrm{ac}}(\cdot, k), \quad k \in \mathbb{Z}. \tag{2.5.5}$$

Moreover, by (2.5.4), (2.5.5), and (A.12) one concludes that

$$d\omega_+(\cdot, k) = d\omega_-(\cdot, k), \quad k \in \mathbb{Z} \tag{2.5.6}$$

and hence that

$$M_+(z, k) = -M_-(z, k), \quad z \in \mathbb{C},\ k \in \mathbb{Z}. \tag{2.5.7}$$

Taking $z = 0$ in (2.5.7), and utilizing (1.2.138) and (1.2.140) then proves

$$1 = -\frac{\alpha_k + 1}{\alpha_k - 1}, \quad k \in \mathbb{Z} \tag{2.5.8}$$

and hence (2.5.3) holds. $\square$

Actually, still assuming the hypotheses of Theorem 2.5.1, one can go a bit further: In addition to (2.5.3) and (2.5.4), (2.5.2) and Theorem 2.4.2 (vii) yield that

$$\text{for all } k \in \mathbb{Z},\ \Xi_{1,1}(\zeta, k) = 0 \text{ for } \mu_0\text{-a.e. } \zeta \in \partial\mathbb{D} \tag{2.5.9}$$

and hence that

$$M_{1,1}(z,k) = 1, \quad z \in \mathbb{D},\ k \in \mathbb{Z}. \tag{2.5.10}$$

Moreover, (2.5.2), (2.5.4), and (1.3.26) yield

$$\text{for all } k \in \mathbb{Z},\ M_{\pm}(z,k) = \pm 1,\ z \in \mathbb{D}, \quad d\omega_{\pm}(\cdot,k) = d\mu_0. \tag{2.5.11}$$

Remark 2.5.2. The special case where α is periodic and $\sigma(U) = \partial\mathbb{D}$ and thus $\alpha = 0$ has originally been derived by Simon [171, Sect. 11.14] using different techniques based on Floquet theory (cf. Theorem 2.1.3).

The principal new result of this chapter then reads as follows.

Theorem 2.5.3. *Let $\alpha = \{\alpha_k\}_{k\in\mathbb{Z}} \subset \mathbb{D}$ be a reflectionless sequence of Verblunsky coefficients. Let U be the associated unitary CMV operator* (2.2.1) (*cf. also* (1.2.6)–(1.2.9)) *on $\ell^2(\mathbb{Z})$ and suppose that the spectrum of U consists of a connected arc of $\partial\mathbb{D}$,*

$$\sigma(U) = \mathrm{Arc}\big(\big[e^{i\theta_0}, e^{i\theta_1}\big]\big) \tag{2.5.12}$$

with $\theta_0 \in [0,2\pi]$, $\theta_0 < \theta_1 \leq \theta_0 + 2\pi$, and hence $e^{i(\theta_0+\theta_1)/2} \in \mathrm{Arc}\big(\big(e^{i\theta_0}, e^{i\theta_1}\big)\big)$. Then $\alpha = \{\alpha_k\}_{k\in\mathbb{Z}}$ is of the form,

$$\alpha_k = \alpha_0 g^k, \quad k \in \mathbb{Z}, \tag{2.5.13}$$

where

$$g = -\exp(i(\theta_0+\theta_1)/2) \ \text{ and } \ |\alpha_0| = \cos((\theta_1-\theta_0)/4). \tag{2.5.14}$$

Proof. By Theorem 2.4.2 (*vii*) (as a consequence of the reflectionless property of α) and the fact that $M_{1,1}(\cdot,k)$, $k \in \mathbb{Z}$, is purely imaginary on the spectral gap

$\mathrm{Arc}((e^{i\theta_1}, e^{i\theta_0+2\pi}))$ (since by Corollary 1.3.5 $\mathrm{supp}(d\Omega_{1,1}) \subseteq \sigma(U)$) and strictly monotone as described in (A.9) and (A.10), there exists a $\theta_*(k) \in [\theta_1, \theta_0 + 2\pi]$ such that $\Xi_{1,1}(\cdot, k)$, $k \in \mathbb{Z}$, is of the form

$$\Xi_{1,1}(\zeta, k) = \begin{cases} 0, & \zeta \in \mathrm{Arc}\big((e^{i\theta_0}, e^{i\theta_1})\big), \\ \pi/2, & \zeta \in \mathrm{Arc}\big((e^{i\theta_1}, e^{i\theta_*(k)})\big), \\ -\pi/2, & \zeta \in \mathrm{Arc}\big((e^{i\theta_*(k)}, e^{i(\theta_0+2\pi)})\big) \end{cases} \tag{2.5.15}$$

for μ_0-a.e. $\zeta \in \partial\mathbb{D}$, $k \in \mathbb{Z}$. Taking into account (2.2.8) then yields

$$\begin{aligned} 0 &= \oint_{\partial\mathbb{D}} d\mu_0(\zeta)\, \Xi_{1,1}(\zeta, k) = \frac{1}{4} \oint_{\theta_1}^{\theta_*(k)} d\theta - \frac{1}{4} \oint_{\theta_*(k)}^{\theta_0+2\pi} d\theta \\ &= \frac{1}{4}[2\theta_*(k) - \theta_0 - 2\pi - \theta_1], \quad k \in \mathbb{Z} \end{aligned} \tag{2.5.16}$$

and hence

$$\theta_*(k) = \frac{1}{2}(\theta_0 + \theta_1) + \pi, \quad k \in \mathbb{Z} \tag{2.5.17}$$

is in fact k-independent and denoted by θ_* in the following. As a result, $\Xi_{1,1}(\cdot, k) = \Xi_{1,1}(\cdot)$ in (2.5.15) is also k-independent.

By (2.2.18),

$$\begin{aligned} \alpha_k \overline{\alpha_{k+1}} &= -i \oint_{\partial\mathbb{D}} d\mu_0(\zeta)\, \Xi_{1,1}(\zeta)\, \overline{\zeta} = -i \oint_{\theta_1}^{\theta_*} \frac{\pi}{2} e^{-it} \frac{dt}{2\pi} + i \oint_{\theta_*}^{\theta_0+2\pi} \frac{\pi}{2} e^{-it} \frac{dt}{2\pi} \\ &= -\frac{1}{4} e^{-i(\theta_0+\theta_1)/2} \big(2 + 2\cos((\theta_1 - \theta_0)/2)\big) \\ &= -e^{-i(\theta_0+\theta_1)/2} \cos^2((\theta_1 - \theta_0)/4), \quad k \in \mathbb{Z}. \end{aligned} \tag{2.5.18}$$

Thus, $\alpha_{k_0} \overline{\alpha_{k_0+1}} = 0$ for some $k_0 \in \mathbb{Z}$ is equivalent to $\theta_1 = \theta_0 + 2\pi$ and hence the assertions (2.5.13) and (2.5.14) reduce to $\alpha = 0$ as in Theorem 2.5.1. (This is of course consistent with (2.5.13), (2.5.14), since $|\alpha_0| = 0$ in this case.) In the case $\alpha_k \overline{\alpha_{k+1}} \neq 0$ for all $k \in \mathbb{Z}$, it follows from (2.5.18) that,

$$\alpha_k = \gamma_0 \gamma_1^k |\alpha_k| \quad \text{and} \quad \cdots = |\alpha_1||\alpha_2| = |\alpha_2||\alpha_3| = |\alpha_3||\alpha_4| = |\alpha_4||\alpha_5| = \cdots$$

Hence,

$$\alpha_k = \gamma_0 \gamma_1^k \begin{cases} |\alpha_1|, & k \text{ odd}, \\ |\alpha_2|, & k \text{ even}, \end{cases} \tag{2.5.19}$$

where

$$\{\gamma_0 = \alpha_0/|\alpha_0|,\, \gamma_1 = -e^{i(\theta_0+\theta_1)/2}\} \subset \partial\mathbb{D} \text{ and } |\alpha_1||\alpha_2| = \cos^2((\theta_1 - \theta_0)/4). \tag{2.5.20}$$

Thus, it remains to show that $|\alpha_1| = |\alpha_2|$. We assume the contrary, $|\alpha_1| \neq |\alpha_2|$ and consider the sequence $|\alpha| = \{|\alpha_k|\}_{k\in\mathbb{Z}}$. Then $|\alpha|$ is a sequence of period 2 Verblunsky coefficients and by (2.4.12) the associated Floquet discriminant, denoted by $\Delta(\cdot;|\alpha|)$, is given by

$$\begin{aligned} \Delta(e^{i\theta};|\alpha|) &= \frac{1}{\rho_1\rho_2}\left[\frac{e^{i\theta}+e^{-i\theta}}{2} + \mathrm{Re}\Big(|\alpha_1|\overline{|\alpha_2|}\Big)\right] \\ &= \frac{1}{\sqrt{1-|\alpha_1|^2}\sqrt{1-|\alpha_2|^2}}\left[\cos(\theta) + |\alpha_1||\alpha_2|\right]. \end{aligned} \tag{2.5.21}$$

Since

$$\sigma(U_{|\alpha|}) = \big\{e^{i\theta} \in \partial\mathbb{D} \,\big|\, -1 \le \Delta\big(e^{i\theta};|\alpha|\big) \le 1\big\} = \big\{e^{i\theta} \in \partial\mathbb{D} \,\big|\, \lambda_- \le \cos(\theta) \le \lambda_+\big\}, \tag{2.5.22}$$

where

$$\lambda_\pm = -|\alpha_1||\alpha_2| \pm \sqrt{1-|\alpha_1|^2}\sqrt{1-|\alpha_2|^2}, \tag{2.5.23}$$

and $|\alpha_1| \neq |\alpha_2|$ is equivalent to $|\lambda_\pm| < 1$, $\sigma(U_{|\alpha|})$ consists of two arcs. Taking into account (2.5.19), it follows from Corollary 2.3.2 that $\sigma(U_\alpha)$ should also contain two arcs which contradicts the basic hypothesis of Theorem 2.5.3. Thus, $|\alpha_1| = |\alpha_2|$ and (2.5.19) implies (2.5.14). $\square$

Remark 2.5.4. By the last part of Corollary 2.3.2, the phase of α_0 in (2.5.13) is a unitary invariant and hence necessarily remains undetermined.

Chapter 3

On Spectral Theory for Schrödinger Operators with Strongly Singular Potentials

3.1 Introduction

The principal goal of this chapter is to study singular Schrödinger operators on a half-line $[a, \infty)$, $a \in \mathbb{R}$, with strongly singular potentials at the finite end point a in the sense that

$$V \in L^1_{\mathrm{loc}}((a, \infty); dx), \;\; V \text{ real-valued}, \; V \notin L^1([a, b]; dx), \quad b > a. \tag{3.1.1}$$

For previous studies of strongly singular Schrödinger operators we refer, for instance, to [6], [9]–[14], [26], [27], [48]–[50], [52]–[59], [69], [73], [75], [131], [137], [145], [155]–[158] and the references therein. (Many of these references treat, in fact, a discrete set of singularities on $\mathbb{R}$ or on (a, b), $-\infty \leq a < b \leq \infty$.) Quite recently, singular potentials became again a popular object of study from various points of views: Some groups study singular interactions in connections with scales of Hilbert spaces (see, e.g., [38], [98]–[101] and the references therein), while other groups study strongly singular interactions in the context of Pontryagin spaces (we refer, e.g., to [16], [37], [40], [41], [154] and the references therein).

Our point of departure in connection with strongly singular potentials is quite different: We focus on the derivation of the spectral function for strongly singular half-line Schrödinger operators starting from the resolvent (and hence the Green's function). In stark contrast to the standard situation of Schrödinger operators on a half-line $[a, \infty)$, $a \in \mathbb{R}$, with a regular end point a, where the associated spectral function generates the measure in the Herglotz representation of the Weyl–Titchmarsh coefficient, we show that half-line Schrödinger operators with strongly singular potentials at the endpoint a lead to spectral functions which are related to the analog of a Weyl–Titchmarsh coefficient which ceases to be a Herglotz function. In fact, the strongly singular potentials studied in this chapter are so singular at a that the associated maximally defined Schrödinger operator is self-adjoint (equivalently, the associated minimal Schrödinger operator is essentially self-adjoint) and hence no boundary condition is required at the finite endpoint a.

In Section 3.2 we recall the essential ingredients of standard spectral theory for self-adjoint Schrödinger operators on a half-line $[a, \infty)$, $a \in \mathbb{R}$, with a regular end point a and problems on the real line with locally integrable potentials. In either case the notion of a spectral function or 2×2 matrix spectral function is intimately connected with Herglotz functions and 2×2 Herglotz matrices representing the celebrated Weyl–Titchmarsh coefficients. This section is, in part, of an expository nature. In stark contrast to the half-line case with a regular finite endpoint a in Section 3.2, we will show in Section 3.3 in the case of strongly singular potentials V on (a, ∞) with singularity concentrated at the endpoint a, that the corresponding spectral functions are no longer derived from associated Herglotz functions (although, certain Herglotz functions still play an important role in this context). We present and contrast two approaches in Section 3.3: First we discuss the case where the reference point x_0 coincides with the singular endpoint a, leading to a scalar Weyl–Titchmarsh coefficient and a scalar spectral function. Alternatively, we treat the case where the reference point x_0 belongs to the interior of the interval (a, ∞), leading to a 2×2 matrix-valued Weyl–Titchmarsh and spectral function. Finally, in Section 3.4 we provide a detailed discussion of the explicitly solvable example $V(x) = [\gamma^2 - (1/4)]x^{-2}$, $x \in (0, \infty)$, $\gamma \in [1, \infty)$. Again we illustrate the two approaches with a choice of reference point $x_0 = 0$ and $x_0 \in (0, \infty)$.

3.2 Spectral Theory and Herglotz Functions

In this section we separately recall basic spectral theory for the case of half-line Schrödinger operators with a regular left endpoint and the case of full-line Schrödinger operators with locally integrable potentials and their relationship to Herglotz functions and matrices. The material of this section is standard and various parts of it can be found, for instance, in [17], [33, Ch. 9], [43, Sect. XIII.5], [45, Ch. 2], [47], [93, Ch. 10], [95], [110], [123], [125, Ch. 2], [135, Ch. VI], [146, Ch. 6], [184, Chs. II, III], [191, Sects. 7–10].

Starting with the half-line case (with a regular left endpoint) we introduce the following main assumption:

Hypothesis 3.2.1. (i) Let $a \in \mathbb{R}$ and assume that

$$V \in L^1([a,c];dx) \text{ for all } c \in (a,\infty), \ V \text{ real-valued.} \tag{3.2.1}$$

(ii) Introducing the differential expression τ_+ given by

$$\tau_+ = -\frac{d^2}{dx^2} + V(x), \quad x \in (a,\infty), \tag{3.2.2}$$

we assume τ_+ to be in the limit point case at $+\infty$.

Associated with the differential expression τ_+ one introduces the self-adjoint Schrödinger operator $H_{+,\alpha}$ in $L^2([a,\infty);dx)$ by

$$\begin{aligned} &H_{+,\alpha} f = \tau_+ f, \quad \alpha \in [0,\pi), \\ &f \in \mathrm{dom}(H_{+,\alpha}) = \Big\{ g \in L^2([a,\infty);dx) \,\Big|\, g, g' \in AC([a,c]) \text{ for all } c \in (a,\infty); \\ &\qquad \sin(\alpha) g'(a_+) + \cos(\alpha) g(a_+) = 0; \ \tau_+ g \in L^2([a,\infty);dx) \Big\}. \end{aligned} \tag{3.2.3}$$

Here (and in the remainder of this manuscript) $\prime$ denotes d/dx and $AC([c,d])$ denotes the class of absolutely continuous functions on the closed interval $[c,d]$.

Remark 3.2.2. For simplicity we chose the half-line $[a,\infty)$ rather than a finite interval $[a,b)$, $a < b < \infty$. Moreover, we chose the limit point hypothesis of τ_+ at the right end point to avoid having to consider any boundary conditions at that point. Both limitations can be removed.

Next, we introduce the standard fundamental system of solutions $\phi_\alpha(z,\cdot)$ and $\theta_\alpha(z,\cdot)$, $z \in \mathbb{C}$, of

$$(\tau_+ \psi)(z,x) = z\psi(z,x), \quad x \in [a,\infty), \tag{3.2.4}$$

satisfying the initial conditions at the point $x = a$,

$$\phi_\alpha(z,a) = -\theta'_\alpha(z,a) = -\sin(\alpha), \;\; \phi'_\alpha(z,a) = \theta_\alpha(z,a) = \cos(\alpha), \;\; \alpha \in [0,\pi). \quad (3.2.5)$$

For future purpose we emphasize that for any fixed $x \in [a,\infty)$, $\phi_\alpha(z,x)$ and $\theta_\alpha(z,x)$ are entire with respect to z and that

$$W(\theta_\alpha(z,\cdot),\phi_\alpha(z,\cdot))(x) = 1, \quad z \in \mathbb{C}, \tag{3.2.6}$$

where

$$W(f,g)(x) = f(x)g'(x) - f'(x)g(x) \tag{3.2.7}$$

denotes the Wronskian of f and g.

A particularly important special solution of (3.2.4) is the *Weyl–Titchmarsh solution* $\psi_{+,\alpha}(z,\cdot)$, $z \in \mathbb{C}\backslash\mathbb{R}$, uniquely characterized by

$$\psi_{+,\alpha}(z,\cdot) \in L^2([a,\infty);dx), \quad \sin(\alpha)\psi'_{+,\alpha}(z,a) + \cos(\alpha)\psi_{+,\alpha}(z,a) = 1, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{3.2.8}$$

The second condition in (3.2.8) just determines the normalization of $\psi_{+,\alpha}(z,\cdot)$ and defines it uniquely. The crucial condition in (3.2.8) is the L^2-property which uniquely determines $\psi_{+,\alpha}(z,\cdot)$ up to constant multiples by the limit point hypothesis of τ_+ at ∞. In particular, for $\alpha, \beta \in [0,\pi)$,

$$\psi_{+,\alpha}(z,\cdot) = C(z,\alpha,\beta)\psi_{+,\beta}(z,\cdot) \text{ for some coefficient } C(z,\alpha,\beta) \in \mathbb{C}. \tag{3.2.9}$$

The normalization in (3.2.8) shows that $\psi_{+,\alpha}(z,\cdot)$ is of the type

$$\psi_{+,\alpha}(z,x) = \theta_\alpha(z,x) + m_{+,\alpha}(z)\phi_\alpha(z,x), \quad z \in \mathbb{C}\backslash\mathbb{R}, \; x \in [a,\infty) \tag{3.2.10}$$

for some coefficient $m_{+,\alpha}(z)$, the *Weyl–Titchmarsh m-function* associated with τ_+ and α.

Next, we recall the fundamental identity

$$\int_a^\infty dx\, \psi_{+,\alpha}(z_1,x)\psi_{+,\alpha}(z_2,x) = \frac{m_{+,\alpha}(z_1) - m_{+,\alpha}(z_2)}{z_1 - z_2}, \quad z_1, z_2 \in \mathbb{C}\backslash\mathbb{R},\ z_1 \neq z_2. \tag{3.2.11}$$

It is a consequence of the elementary fact

$$\frac{d}{dx} W(\psi(z_1,\cdot),\psi(z_2,\cdot))(x) = (z_1 - z_2)\psi(z_1,x)\psi(z_2,x) \tag{3.2.12}$$

for solutions $\psi(z_j,\cdot)$, $j = 1,2$, of (3.2.4), and the fact that τ_+ is assumed to be in the limit point case at ∞ which implies

$$\lim_{x\uparrow\infty} W(\psi_{+,\alpha}(z_1,\cdot),\psi_{+,\alpha}(z_2,\cdot))(x) = 0. \tag{3.2.13}$$

Moreover, since $\overline{\psi_{+,\alpha}(z,\cdot)}$ is the unique solution of $\tau_+\psi(\overline{z},x) = \overline{z}\psi(\overline{z},x)$, $x \in [a,\infty)$, satisfying

$$\overline{\psi_{+,\alpha}(z,\cdot)} \in L^2([a,\infty);dx), \quad \sin(\alpha)\overline{\psi'_{+,\alpha}(z,a)} + \cos(\alpha)\overline{\psi_{+,\alpha}(z,a)} = 1, \tag{3.2.14}$$

and since

$$\overline{\phi_\alpha(z,x)} = \phi_\alpha(\overline{z},x), \quad \overline{\theta_\alpha(z,x)} = \theta_\alpha(\overline{z},x), \quad z \in \mathbb{C},\ x \in [a,\infty), \tag{3.2.15}$$

one concludes that $\overline{\psi_{+,\alpha}(z,\cdot)}$ is the Weyl–Titchmarsh solution of $\tau_+\psi(\overline{z},x) = \overline{z}\psi(\overline{z},x)$, $x \geq a$, and hence

$$\overline{m_{+,\alpha}(z)} = m_{+,\alpha}(\overline{z}), \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{3.2.16}$$

Thus, choosing $z_1 = z$, $z_2 = \overline{z}$ in (3.2.11), one infers

$$\int_a^\infty dx\, |\psi_{+,\alpha}(z,x)|^2 = \frac{\operatorname{Im}(m_{+,\alpha}(z))}{\operatorname{Im}(z)}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{3.2.17}$$

Before we turn to the proper interpretation of formulas (3.2.16) and (3.2.17), we briefly take a look at the Green's function $G_{+,\alpha}(z,x,x')$ of $H_{+,\alpha}$. Using (3.2.5), (3.2.6), and (3.2.8) one obtains,

$$G_{+,\alpha}(z,x,x') = \begin{cases} \phi_\alpha(z,x)\psi_{+,\alpha}(z,x'), & a \le x \le x', \\ \phi_\alpha(z,x')\psi_{+,\alpha}(z,x), & a \le x' \le x, \end{cases} \quad z \in \mathbb{C}\backslash\mathbb{R} \tag{3.2.18}$$

and thus,

$$((H_{+,\alpha} - zI)^{-1} f)(x) = \int_a^\infty dx'\, G_{+,\alpha}(z,x,x') f(x'), \tag{3.2.19}$$
$$z \in \mathbb{C}\backslash\mathbb{R},\ x \in [a,\infty),\ f \in L^2([a,\infty); dx).$$

Next we mention the following analyticity result (for the notion of Herglotz functions we refer to Appendix B). Here and in the remainder of this manuscript, $\chi_{\mathcal{M}}$ denotes the characteristic function of a set $\mathcal{M} \subset \mathbb{R}$.

Lemma 3.2.3. *Assume Hypothesis 3.2.1 and let $\alpha \in [0,\pi)$. Then $m_{+,\alpha}$ is analytic on $\mathbb{C}\backslash\sigma(H_{+,\alpha})$, moreover, $m_{+,\alpha}$ is a Herglotz function. In addition, for each $x \in [a,\infty)$, $\psi_{+,\alpha}(\cdot,x)$ and $\psi'_{+,\alpha}(\cdot,x)$ are analytic on $\mathbb{C}\backslash\sigma(H_{+,\alpha})$.*

Proof. Pick real numbers c and d such that $a \le c < d < \infty$. Then, using (3.2.18) and (3.2.19) one computes

$$\begin{aligned} \int_{\sigma(H_{+,\alpha})} \frac{d\big\|E_{H_{+,\alpha}}(\lambda)\chi_{[c,d]}\big\|^2_{L^2([a,\infty);dx)}}{\lambda - z} &= \big(\chi_{[c,d]}, (H_{+,\alpha} - zI)^{-1}\chi_{[c,d]}\big)_{L^2([a,\infty);dx)} \\ &= \int_c^d dx \int_c^x dx'\, \theta_\alpha(z,x)\phi_\alpha(z,x') + \int_c^d dx \int_x^d dx'\, \phi_\alpha(z,x)\theta_\alpha(z,x') \end{aligned} \tag{3.2.20}$$

$$+ m_{+,\alpha}(z)\bigg[\int_c^d dx\, \phi_\alpha(z,x)\bigg]^2, \quad z \in \mathbb{C}\backslash\sigma(H_{+,\alpha}).$$

Since the left-hand side of (3.2.20) is analytic with respect to z on $\mathbb{C}\backslash\sigma(H_{+,\alpha})$ and since $\phi_\alpha(\cdot,x)$ and $\theta_\alpha(\cdot,x)$ are entire for fixed $x \in [a,\infty)$ with $\phi_\alpha(z,\cdot)$, $\theta_\alpha(z,\cdot)$, and their first x-derivatives being absolutely continuous on each interval $[a,b]$, $b > a$, one concludes that $m_{+,\alpha}$ is analytic in a sufficiently small open neighborhood $\mathcal{N}_{z_0}$ of a given point $z_0 \in \mathbb{C}\backslash\sigma(H_{+,\alpha})$, as long as we can guarantee the existence of $c(z_0), d(z_0) \in [a,\infty)$ such that

$$\int_{c(z_0)}^{d(z_0)} dx\, \phi_\alpha(z,x) \neq 0, \quad z \in \mathcal{N}_{z_0}. \tag{3.2.21}$$

The latter is shown as follows: First, pick $z_0 \in \mathbb{C}\backslash\sigma(H_{+,\alpha})$. Then since $\phi_\alpha(z_0,\cdot)$ does not vanish identically, one can find $c(z_0), d(z_0) \in [a,\infty)$ such that

$$\int_{c(z_0)}^{d(z_0)} dx\, \phi_\alpha(z_0,x) \neq 0. \tag{3.2.22}$$

Since

$$\int_{c(z_0)}^{d(z_0)} dx\, \phi_\alpha(z,x) \tag{3.2.23}$$

is entire with respect to z, (3.2.22) guarantees the existence of an open neighborhood $\mathcal{N}_{z_0}$ of z_0 such that (3.2.21) holds. Since $z_0 \in \mathbb{C}\backslash\sigma(H_{+,\alpha})$ was chosen arbitrary, $m_{+,\alpha}$ is analytic on $\mathbb{C}\backslash\sigma(H_{+,\alpha})$. Together with (3.2.16) and (3.2.17) this proves that $m_{+,\alpha}$ is a Herglotz function. By (3.2.10) (and its x-derivative), $\psi_{+,\alpha}(\cdot,x)$ and $\psi'_{+,\alpha}(\cdot,x)$ are analytic on $\mathbb{C}\backslash\sigma(H_{+,\alpha})$ for each $x \in [a,\infty)$. $\square$

Remark 3.2.4. Traditionally, one proves analyticity of $m_{+,\alpha}$ on $\mathbb{C}\backslash\mathbb{R}$ by first restricting $H_{+,\alpha}$ to the interval $[a,b]$ (introducing a self-adjoint boundary condition at the endpoint b) and then controls the uniform limit of a sequence of meromorphic Weyl–Titchmarsh coefficients analytic on $\mathbb{C}\backslash\mathbb{R}$ as $b \uparrow \infty$. We chose the somewhat roundabout proof of Lemma 3.2.3 based on the fundamental identity (3.2.20) in view of Section 3.3, in which we consider strongly singular potentials at $x = a$, where the traditional approach leading to a Weyl–Titchmarsh coefficient m_+ possessing the Herglotz property is not applicable, but the current method of proof relying on the family of spectral projections $\{E_{H_{+,\alpha}}\}_{\lambda\in\mathbb{R}}$, the Green's function $G_{+,\alpha}(z,x,x')$ of $H_{+,\alpha}$, and identity (3.2.20), remains in effect.

Moreover, we recall the following well-known facts on $m_{+,\alpha}$:

$$\lim_{\epsilon\downarrow 0} i\epsilon\, m_{+,\alpha}(\lambda+i\epsilon) = \begin{cases} 0, & \phi_\alpha(\lambda,\,\cdot\,) \notin L^2([a,\infty);dx), \\ -\|\phi_\alpha(\lambda,\,\cdot\,)\|^{-2}_{L^2([a,\infty);dx)}, & \phi_\alpha(\lambda,\,\cdot\,) \in L^2([a,\infty);dx), \end{cases} \tag{3.2.24}$$
$$\lambda\in\mathbb{R},\ \alpha\in[0,\pi),$$

$$m_{+,\alpha_1}(z) = \frac{-\sin(\alpha_1-\alpha_2)+\cos(\alpha_1-\alpha_2)m_{+,\alpha_2}(z)}{\cos(\alpha_1-\alpha_2)+\sin(\alpha_1-\alpha_2)m_{+,\alpha_2}(z)}, \quad \alpha_1,\alpha_2\in[0,\pi), \tag{3.2.25}$$

$$m_{+,\alpha}(z) \underset{z\to i\infty}{=} \begin{cases} \cot(\alpha) + \frac{i}{\sin^2(\alpha)}\, z^{-1/2} - \frac{\cos(\alpha)}{\sin^3(\alpha)}\, z^{-1} + o(z^{-1}), & \alpha\in(0,\pi), \\ iz^{1/2} + o(1), & \alpha = 0. \end{cases} \tag{3.2.26}$$

The asymptotic behavior (3.2.26) then implies the Herglotz representation of $m_{+,\alpha}$ (cf. Theorem B.2 (iii)),

$$m_{+,\alpha}(z) = \begin{cases} c_{+,\alpha} + \int_{\mathbb{R}} d\rho_{+,\alpha}(\lambda)\left[\frac{1}{\lambda-z} - \frac{\lambda}{1+\lambda^2}\right], & \alpha\in[0,\pi), \\ \cot(\alpha) + \int_{\mathbb{R}} d\rho_{+,\alpha}(\lambda)\,(\lambda-z)^{-1}, & \alpha\in(0,\pi), \end{cases} \quad z\in\mathbb{C}\backslash\mathbb{R} \tag{3.2.27}$$

with

$$\int_{\mathbb{R}} \frac{d\rho_{+,\alpha}(\lambda)}{1+|\lambda|} \begin{cases} <\infty, & \alpha\in(0,\pi), \\ =\infty, & \alpha=0, \end{cases} \qquad \int_{\mathbb{R}} \frac{d\rho_{+,0}(\lambda)}{1+\lambda^2} < \infty. \tag{3.2.28}$$

We note that in formulas (3.2.10)–(3.2.27) one can of course replace $z\in\mathbb{C}\backslash\mathbb{R}$ by $z\in\mathbb{C}\backslash\sigma(H_{+,\alpha})$.

For future purposes we also note the following result, a version of Stone's formula in the weak sense (cf., e.g., [43, p. 1203]).

Lemma 3.2.5. *Let T be a self-adjoint operator in a complex separable Hilbert space $\mathcal{H}$ (with scalar product denoted by $(\cdot,\cdot)_{\mathcal{H}}$, linear in the second factor) and denote by $\{E_T(\lambda)\}_{\lambda\in\mathbb{R}}$ the family of self-adjoint right-continuous spectral projections associated with T, that is, $E_T(\lambda) = \chi_{(-\infty,\lambda]}(T)$, $\lambda \in \mathbb{R}$. Moreover, let $f, g \in \mathcal{H}$, $\lambda_1, \lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$, and $F \in C(\mathbb{R})$. Then,*

$$\begin{aligned}
&\big(f, F(T)E_T((\lambda_1,\lambda_2])g\big)_{\mathcal{H}} \\
&\quad = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, F(\lambda)\big[\big(f,(T-(\lambda+i\varepsilon)I_{\mathcal{H}})^{-1}g\big)_{\mathcal{H}} \\
&\qquad\qquad\qquad - \big(f,(T-(\lambda-i\varepsilon)I_{\mathcal{H}})^{-1}g\big)_{\mathcal{H}}\big]. \qquad (3.2.29)
\end{aligned}$$

Proof. First, assume $F \geq 0$. Then

$$\begin{aligned}
&\big(F(T)^{1/2}E_T((\lambda_1,\lambda_2])f, (T-zI_{\mathcal{H}})^{-1}F(T)^{1/2}E_T((\lambda_1,\lambda_2])f\big)_{\mathcal{H}} \\
&\quad = \int_{\mathbb{R}} d\big(f, E_T(\lambda)f\big)_{\mathcal{H}}\, F(\lambda)\chi_{(\lambda_1,\lambda_2]}(\lambda)(\lambda-z)^{-1} \\
&\quad = \int_{\mathbb{R}} \frac{d\big(F(T)^{1/2}\chi_{(\lambda_1,\lambda_2]}(T)f, E_T(\lambda)F(T)^{1/2}\chi_{(\lambda_1,\lambda_2]}(T)f\big)_{\mathcal{H}}}{(\lambda-z)}, \quad z\in\mathbb{C}_+ \qquad (3.2.30)
\end{aligned}$$

is a Herglotz function and hence (3.2.29) for $g = f$ follows from (B.4). If F is not nonnegative, one decomposes F as $F = (F_1 - F_2) + i(F_3 - F_4)$ with $F_j \geq 0$, $1 \leq j \leq 4$ and applies (3.2.30) to each $j \in \{1,2,3,4\}$. The general case $g \neq f$ then follows from the case $g = f$ by polarization. □

Next, we relate the family of spectral projections, $\{E_{H_{+,\alpha}}(\lambda)\}_{\lambda\in\mathbb{R}}$, of the self-adjoint operator $H_{+,\alpha}$ and the spectral function $\rho_{+,\alpha}(\lambda)$, $\lambda\in\mathbb{R}$, which generates the measure in the Herglotz representation (3.2.27) of $m_{+,\alpha}$.

We first note that for $F \in C(\mathbb{R})$,

$$\begin{aligned}
&\big(f, F(H_{+,\alpha})g\big)_{L^2([a,\infty);dx)} = \int_{\mathbb{R}} d\big(f, E_{H_{+,\alpha}}(\lambda)g\big)_{L^2([a,\infty);dx)}\, F(\lambda),\\
&f, g \in \operatorname{dom}(F(H_{+,\alpha})) \qquad\qquad (3.2.31)\\
&\quad = \bigg\{h \in L^2([a,\infty);dx) \,\bigg|\, \int_{\mathbb{R}} d\big\|E_{H_{+,\alpha}}(\lambda)h\big\|^2_{L^2([a,\infty);dx)}\, |F(\lambda)|^2 < \infty\bigg\}.
\end{aligned}$$

Equation (3.2.31) extends to measurable functions F and holds also in the strong sense, but the displayed weak version will suffice for our purpose.

In the following, $C_0^\infty((c,d))$, $-\infty \le c < d \le \infty$, denotes the usual space of infinitely differentiable functions of compact support contained in (c,d).

Theorem 3.2.6. *Let* $\alpha \in [0,\pi)$, $f, g \in C_0^\infty((a,\infty))$, $F \in C(\mathbb{R})$, *and* $\lambda_1, \lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$. *Then,*

$$\big(f, F(H_{+,\alpha})E_{H_{+,\alpha}}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)} = \big(\widehat{f}_{+,\alpha}, M_F M_{\chi_{(\lambda_1,\lambda_2]}} \widehat{g}_{+,\alpha}\big)_{L^2(\mathbb{R};d\rho_{+,\alpha})}, \quad (3.2.32)$$

where we introduced the notation

$$\widehat{h}_{+,\alpha}(\lambda) = \int_a^\infty dx\, \phi_\alpha(\lambda,x)h(x), \quad \lambda \in \mathbb{R},\ h \in C_0^\infty((a,\infty)), \quad (3.2.33)$$

and M_G *denotes the maximally defined operator of multiplication by the* $d\rho_{+,\alpha}$*-measurable function* G *in the Hilbert space* $L^2(\mathbb{R}; d\rho_{+,\alpha})$,

$$\begin{aligned}
&(M_G\widehat{h})(\lambda) = G(\lambda)\widehat{h}(\lambda) \ \text{ for a.e. } \lambda \in \mathbb{R},\\
&\widehat{h} \in \operatorname{dom}(M_G) = \big\{\widehat{k} \in L^2(\mathbb{R}; d\rho_{+,\alpha}) \,\big|\, G\widehat{k} \in L^2(\mathbb{R}; d\rho_{+,\alpha})\big\}.
\end{aligned} \quad (3.2.34)$$

Here $d\rho_{+,\alpha}$ *is the measure in the Herglotz representation of the Weyl–Titchmarsh function* $m_{+,\alpha}$ *(cf. (3.2.27)).*

Proof. The point of departure for deriving (3.2.32) is Stone's formula (3.2.29) applied to $T = H_{+,\alpha}$,

$$\begin{aligned}
&\big(f, F(H_{+,\alpha})E_{H_{+,\alpha}}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)} \\
&\quad = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, F(\lambda)\big[\big(f,(H_{+,\alpha}-(\lambda+i\varepsilon)I)^{-1}g\big)_{L^2([a,\infty);dx)} \\
&\qquad\qquad - \big(f,(H_{+,\alpha}-(\lambda-i\varepsilon)I)^{-1}g\big)_{L^2([a,\infty);dx)}\big].
\end{aligned} \tag{3.2.35}$$

Insertion of (3.2.18) and (3.2.19) into (3.2.35) then yields the following:

$$\begin{aligned}
&\big(f, F(H_{+,\alpha})E_{H_{+,\alpha}}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)} = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, F(\lambda) \\
&\quad\times\bigg\{\int_a^\infty dx\,\bigg[\overline{f(x)}\psi_{+,\alpha}(\lambda+i\varepsilon,x)\int_a^x dx'\,\phi_\alpha(\lambda+i\varepsilon,x')g(x') \\
&\qquad + \overline{f(x)}\phi_\alpha(\lambda+i\varepsilon,x)\int_x^\infty dx'\,\psi_{+,\alpha}(\lambda+i\varepsilon,x')g(x')\bigg] \\
&\qquad - \bigg[\overline{f(x)}\psi_{+,\alpha}(\lambda-i\varepsilon,x)\int_a^x dx'\,\phi_\alpha(\lambda-i\varepsilon,x')g(x') \\
&\qquad + \overline{f(x)}\phi_\alpha(\lambda-i\varepsilon,x)\int_x^\infty dx'\,\psi_{+,\alpha}(\lambda-i\varepsilon,x')g(x')\bigg]\bigg\}.
\end{aligned} \tag{3.2.36}$$

Freely interchanging the dx and dx' integrals with the limits and the $d\lambda$ integral (since all integration domains are finite and all integrands are continuous), and inserting expression (3.2.10) for $\psi_{+,\alpha}(z,x)$ into (3.2.36), one obtains

$$\begin{aligned}
&\big(f, F(H_{+,\alpha})E_{H_{+,\alpha}}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)} = \int_a^\infty dx\,\overline{f(x)}\bigg\{\int_a^x dx'\,g(x') \\
&\quad\times\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, F(\lambda)\Big[\big[\theta_\alpha(\lambda,x)+m_{+,\alpha}(\lambda+i\varepsilon)\phi_\alpha(\lambda,x)\big]\phi_\alpha(\lambda,x') \\
&\qquad - \big[\theta_\alpha(\lambda,x)+m_{+,\alpha}(\lambda-i\varepsilon)\phi_\alpha(\lambda,x)\big]\phi_\alpha(\lambda,x')\Big] \\
&\quad+\int_x^\infty dx'\,g(x')\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, F(\lambda) \\
&\qquad\times\Big[\phi_\alpha(\lambda,x)\big[\theta_\alpha(\lambda,x')+m_{+,\alpha}(\lambda+i\varepsilon)\phi_\alpha(\lambda,x')\big]
\end{aligned} \tag{3.2.37}$$

$$- \phi_\alpha(\lambda,x)\big[\theta_\alpha(\lambda,x') + m_{+,\alpha}(\lambda - i\varepsilon)\phi_\alpha(\lambda,x')\big]\Big]\Bigg\}.$$

Here we employed the fact that for fixed $x \in [a,\infty)$, $\theta_\alpha(z,x)$ and $\phi_\alpha(z,x)$ are entire with respect to z, that $\theta_\alpha(\lambda,x)$ and $\phi_\alpha(\lambda,x)$ are real-valued for $\lambda \in \mathbb{R}$, that $\theta_\alpha(z,\cdot), \phi_\alpha(z,\cdot) \in AC([a,c])$ for all $c > a$, and hence that

$$\begin{aligned}
\theta_\alpha(\lambda \pm i\varepsilon, x) &\underset{\varepsilon\downarrow 0}{=} \theta_\alpha(\lambda,x) \pm i\varepsilon(d/dz)\theta_\alpha(z,x)|_{z=\lambda} + O(\varepsilon^2), \\
\phi_\alpha(\lambda \pm i\varepsilon, x) &\underset{\varepsilon\downarrow 0}{=} \phi_\alpha(\lambda,x) \pm i\varepsilon(d/dz)\phi_\alpha(z,x)|_{z=\lambda} + O(\varepsilon^2)
\end{aligned} \tag{3.2.38}$$

with $O(\varepsilon^2)$ being uniform with respect to (λ,x) as long as λ and x vary in compact subsets of $\mathbb{R} \times [a,\infty)$. Moreover, we used that

$$\begin{aligned}
&\varepsilon|m_{+,\alpha}(\lambda + i\varepsilon)| \le C(\lambda_1,\lambda_2,\varepsilon_0) \ \text{ for } \ \lambda \in [\lambda_1,\lambda_2], \ 0 < \varepsilon \le \varepsilon_0, \\
&\varepsilon|\mathrm{Re}(m_{+,\alpha}(\lambda + i\varepsilon))| \underset{\varepsilon\downarrow 0}{=} o(1), \quad \lambda \in \mathbb{R}.
\end{aligned} \tag{3.2.39}$$

In particular, utilizing (3.2.38) and (3.2.39), $\phi_\alpha(\lambda \pm i\varepsilon, x)$ and $\theta_\alpha(\lambda \pm i\varepsilon, x)$ have been replaced by $\phi_\alpha(\lambda,x)$ and $\theta_\alpha(\lambda,x)$ under the $d\lambda$ integrals in (3.2.37). Cancelling appropriate terms in (3.2.37), simplifying the remaining terms, and using (3.2.16) then yield

$$\begin{aligned}
\big(f, F(H_{+,\alpha})E_{H_{+,\alpha}}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)} &= \int_a^\infty dx\, \overline{f(x)} \int_a^\infty dx'\, g(x') \\
\times \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0} \frac{1}{\pi}\int_{\lambda_1+\delta}^{\lambda_2+\delta} & d\lambda\, F(\lambda)\phi_\alpha(\lambda,x)\phi_\alpha(\lambda,x')\mathrm{Im}(m_{+,\alpha}(\lambda + i\varepsilon)).
\end{aligned} \tag{3.2.40}$$

Using the fact that by (B.4)

$$\int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda) = \rho_{+,\alpha}((\lambda_1,\lambda_2]) = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, \mathrm{Im}(m_{+,\alpha}(\lambda + i\varepsilon)), \tag{3.2.41}$$

and hence that

$$\int_{\mathbb{R}} d\rho_{+,\alpha}(\lambda)\, h(\lambda) = \lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\mathbb{R}} d\lambda\, \mathrm{Im}(m_{+,\alpha}(\lambda + i\varepsilon))\, h(\lambda), \quad h \in C_0(\mathbb{R}), \tag{3.2.42}$$

$$\int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)\, k(\lambda) = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, \mathrm{Im}(m_{+,\alpha}(\lambda+i\varepsilon))\, k(\lambda), \quad k\in C(\mathbb{R}), \tag{3.2.43}$$

(with $C_0(\mathbb{R})$ the space of continuous compactly supported functions on $\mathbb{R}$) one concludes

$$\begin{aligned}
&\big(f, F(H_{+,\alpha})E_{H_{+,\alpha}}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)} \\
&\quad = \int_a^\infty dx\, \overline{f(x)} \int_a^\infty dx'\, g(x') \int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda) F(\lambda)\phi_\alpha(\lambda,x)\phi_\alpha(\lambda,x') \\
&\quad = \int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda) F(\lambda)\, \overline{\widehat{f}_{+,\alpha}(\lambda)}\, \widehat{g}_{+,\alpha}(\lambda),
\end{aligned} \tag{3.2.44}$$

using (3.2.33) and interchanging the dx, dx' and $d\rho_{+,\alpha}$ integrals once more. $\square$

Remark 3.2.7. Theorem 3.2.6 is of course well-known. We presented a detailed proof since this proof will serve as the model for generalizations to strongly singular potentials and hence pave the way into somewhat unchartered territory in Section 3.3. In this context it is worthwhile to examine the principal ingredients entering the proof of Theorem 3.2.6: Let $\lambda_j \in \mathbb{R}$, $j = 0,1,2$, $\lambda_1 < \lambda_2$, and $\varepsilon_0 > 0$. Then the following items played a crucial role in the proof of Theorem 3.2.6:

(i) For all $x \in [a,\infty)$, $\theta_\alpha(z,x)$ and $\phi_\alpha(z,x)$ are entire with respect to z and real-valued for $z \in \mathbb{R}$.

(ii) $m_{+,\alpha}$ is analytic on $\mathbb{C}\backslash\mathbb{R}$.

(iii) $\overline{m_{+,\alpha}(z)} = m_{+,\alpha}(\overline{z}), \quad z \in \mathbb{C}_+$.

(iv) $\varepsilon|m_{+,\alpha}(\lambda+i\varepsilon)| \leq C, \quad \lambda \in [\lambda_1,\lambda_2],\ 0<\varepsilon\leq\varepsilon_0.$ (3.2.45)

(v) $\varepsilon|\mathrm{Re}(m_{+,\alpha}(\lambda+i\varepsilon))| \underset{\varepsilon\downarrow 0}{=} o(1), \quad \lambda \in \mathbb{R}.$

$$(vi)\quad \rho_{+,\alpha}(\lambda) - \rho_{+,\alpha}(\lambda_0) = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_0+\delta}^{\lambda+\delta} d\mu\, \mathrm{Im}(m_{+,\alpha}(\mu+i\varepsilon)).$$

defines a nondecreasing function $\rho_{+,\alpha}$ and hence a measure on $\mathbb{R}$.

Of course, properties (ii)–(vi) are satisfied by any Herglotz function. However, as we will see in Sections 3.3 and 3.4, properties (ii)–(vi) (possibly restricting z to a sufficiently small neighborhood of $\mathbb{R}$) are also crucial in connection with a class of strongly singular potentials at $x = a$, where the analog of the coefficient $m_{+,\alpha}$ will necessarily turn out to be a non-Herglotz function. In particular, one can (and we will in Section 3.3) use an analog of (3.2.20) to prove items (ii)–(vi) in (3.2.45) (for $|\mathrm{Im}(z)|$ sufficiently small) without ever invoking the Herglotz property of $m_{+,\alpha}$, by just using the fact that the left-hand side of (3.2.20) is a Herglotz function whether or not the potential V is strongly singular at the endpoint a. Thus, the mere existence of the family of spectral projections $\{E_{H_{+,\alpha}}(\lambda)\}_{\lambda\in\mathbb{R}}$ of the self-adjoint operator $H_{+,\alpha}$ implies properties of the type (ii)–(vi).

Remark 3.2.8. The effortless derivation of the link between the family of spectral projections $E_{H_{+,\alpha}}(\cdot)$ and the spectral function $\rho_{+,\alpha}(\cdot)$ of $H_{+,\alpha}$ in Theorem 3.2.6 applies equally well to half-line Dirac-type operators and Hamiltonian systems (see the extensive literature cited, e.g., in [31]) and to half-lattice Jacobi- (cf. [18]) and CMV operators (i.e., semi-infinite five-diagonal unitary matrices which are related to orthogonal polynomials on the unit circle in the manner that half-lattice tri-diagonal (Jacobi) matrices are related to orthogonal polynomials on the real line as discussed in detail in [172]; see Chapter 1 for an application of Theorem 3.2.6 to CMV operators). After circulating a first draft of this manuscript, it was kindly pointed out to us by Don Hinton that the idea of linking the family of spectral projections and the spectral function using Stone's formula as the starting point can already be found in a paper by Hinton and Schneider [95] published in 1998.

Actually, one can improve on Theorem 3.2.6 and remove the compact support restrictions on f and g in the usual way. To this end one considers the map

$$\widetilde{U}_{+,\alpha}\colon \begin{cases} C_0^\infty((a,\infty)) \to L^2(\mathbb{R}; d\rho_{+,\alpha}) \\ \qquad\qquad h \mapsto \widehat{h}_{+,\alpha}(\cdot) = \int_a^\infty dx\, \phi_\alpha(\cdot,x)h(x). \end{cases} \tag{3.2.46}$$

Taking $f = g$, $F = 1$, $\lambda_1 \downarrow -\infty$, and $\lambda_2 \uparrow \infty$ in (3.2.32) then shows that $\widetilde{U}_{+,\alpha}$ is a densely defined isometry in $L^2([a,\infty); dx)$, which extends by continuity to an isometry on $L^2([a,\infty); dx)$. The latter is denoted by $U_{+,\alpha}$ and given by

$$U_{+,\alpha}\colon \begin{cases} L^2([a,\infty); dx) \to L^2(\mathbb{R}; d\rho_{+,\alpha}) \\ \qquad\qquad h \mapsto \widehat{h}_{+,\alpha}(\cdot) = \text{l.i.m.}_{b\uparrow\infty} \int_a^b dx\, \phi_\alpha(\cdot,x)h(x), \end{cases} \tag{3.2.47}$$

where l.i.m. refers to the $L^2(\mathbb{R}; d\rho_{+,\alpha})$-limit.

The calculation in (3.2.44) also yields

$$(E_{H_{+,\alpha}}((\lambda_1,\lambda_2])g)(x) = \int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)\, \phi_\alpha(\lambda,x)\widehat{g}_{+,\alpha}(\lambda), \quad g \in C_0^\infty((a,\infty)) \tag{3.2.48}$$

and subsequently, (3.2.48) extends to all $g \in L^2([a,\infty); dx)$ by continuity. Moreover, taking $\lambda_1 \downarrow -\infty$ and $\lambda_2 \uparrow \infty$ in (3.2.48) using

$$\text{s-lim}_{\lambda\downarrow-\infty} E_{H_{+,\alpha}}(\lambda) = 0, \quad \text{s-lim}_{\lambda\uparrow\infty} E_{H_{+,\alpha}}(\lambda) = I_{L^2([a,\infty);dx)}, \tag{3.2.49}$$

where

$$E_{H_{+,\alpha}}(\lambda) = E_{H_{+,\alpha}}((-\infty,\lambda]), \tag{3.2.50}$$

then yields

$$g(\cdot) = \text{l.i.m.}_{\mu_1\downarrow -\infty, \mu_2\uparrow\infty} \int_{\mu_1}^{\mu_2} d\rho_{+,\alpha}(\lambda)\, \phi_\alpha(\lambda,\cdot)\widehat{g}_{+,\alpha}(\lambda), \quad g \in L^2([a,\infty);dx), \tag{3.2.51}$$

where l.i.m. refers to the $L^2([a,\infty);dx)$-limit.

In addition, one can show that the map $U_{+,\alpha}$ in (3.2.47) is onto and hence that $U_{+,\alpha}$ is unitary (i.e., $U_{+,\alpha}$ and $U_{+,\alpha}^{-1}$ are isometric isomorphisms between $L^2([a,\infty);dx)$ and $L^2(\mathbb{R};d\rho_{+,\alpha})$) with

$$U_{+,\alpha}^{-1}\colon \begin{cases} L^2(\mathbb{R};d\rho_{+,\alpha}) \to L^2([a,\infty);dx) \\ \qquad\qquad \widehat{h} \mapsto \text{l.i.m.}_{\mu_1\downarrow -\infty, \mu_2\uparrow\infty} \int_{\mu_1}^{\mu_2} d\rho_{+,\alpha}(\lambda)\, \phi_\alpha(\lambda,\cdot)\widehat{h}(\lambda). \end{cases} \tag{3.2.52}$$

Indeed, consider an arbitrary function $f \in L^2(\mathbb{R};d\rho_{+,\alpha})$ such that

$$\big(f, U_{+,\alpha}h\big)_{L^2(\mathbb{R};d\rho_{+,\alpha})} = 0 \text{ for all } h \in L^2([a,\infty);dx). \tag{3.2.53}$$

Then, (3.2.53) holds for $h = E_{H_{+,\alpha}}((\lambda_1,\lambda_2])g$, $\lambda_1,\lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$, $g \in C_0^\infty([a,\infty))$. Utilizing (3.2.48) one rewrites (3.2.53) as,

$$\begin{aligned} 0 &= \big(f, U_{+,\alpha}E_{H_{+,\alpha}}((\lambda_1,\lambda_2])g\big)_{L^2(\mathbb{R};d\rho_{+,\alpha})} = \big(f, U_{+,\alpha}U_{+,\alpha}^{-1}\chi_{(\lambda_1,\lambda_2]}U_{+,\alpha}g\big)_{L^2(\mathbb{R};d\rho_{+,\alpha})} \\ &= \int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)\, \overline{f(\lambda)} \int_{[a,\infty)} dx\, \phi_\alpha(\lambda,x)g(x) \\ &= \int_{[a,\infty)} dx\, g(x) \int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)\, \phi_\alpha(\lambda,x)\overline{f(\lambda)}. \end{aligned} \tag{3.2.54}$$

Since $C_0^\infty([a,\infty))$ is dense in $L^2([a,\infty);dx)$ one concludes that

$$\int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)\, \phi_\alpha(\lambda,x)\overline{f(\lambda)} = 0 \text{ for a.e. } x \in [a,\infty). \tag{3.2.55}$$

Differentiating (3.2.55) with respect to x leads to

$$\int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)\phi_\alpha'(\lambda,x)\overline{f(\lambda)} = 0 \text{ for a.e. } x \in [a,\infty). \tag{3.2.56}$$

Using the dominated convergence theorem and the fact that $f \in L^2(\mathbb{R}; d\rho_{+,\alpha}) \subseteq L^1((\lambda_1, \lambda_2]; d\rho_{+,\alpha})$ and that $\phi_\alpha(\lambda, x), \phi'_\alpha(\lambda, x)$ are continuous in $(\lambda, x) \in \mathbb{R} \times [a, \infty)$, one concludes

$$\begin{aligned} 0 &= \int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)\, \phi_\alpha(\lambda, a)\overline{f(\lambda)} = -\sin(\alpha) \int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)\, \overline{f(\lambda)}, \\ 0 &= \int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)\, \phi'_\alpha(\lambda, a)\overline{f(\lambda)} = \cos(\alpha) \int_{(\lambda_1,\lambda_2]} d\rho_{+,\alpha}(\lambda)\, \overline{f(\lambda)}. \end{aligned} \tag{3.2.57}$$

Since the interval $(\lambda_1, \lambda_2]$ was chosen arbitrary, (3.2.57) implies

$$f(\lambda) = 0 \;\; d\rho_{+,\alpha}\text{-a.e.}, \tag{3.2.58}$$

and hence $U_{+,\alpha}$ is onto.

We sum up these considerations in a variant of the spectral theorem for (functions of) $H_{+,\alpha}$.

Theorem 3.2.9. *Let $\alpha \in [0, \pi)$ and $F \in C(\mathbb{R})$. Then,*

$$U_{+,\alpha} F(H_{+,\alpha}) U_{+,\alpha}^{-1} = M_F \tag{3.2.59}$$

in $L^2(\mathbb{R}; d\rho_{+,\alpha})$ (cf. (3.2.34)). Moreover,

$$\sigma(F(H_{+,\alpha})) = \text{ess.ran}_{d\rho_{+,\alpha}}(F), \tag{3.2.60}$$

$$\sigma(H_{+,\alpha}) = \operatorname{supp}(d\rho_{+,\alpha}), \tag{3.2.61}$$

and the spectrum of $H_{+,\alpha}$ is simple.

Here the essential range of F with respect to a measure $d\mu$ is defined by

$$\text{ess.ran}_{d\mu}(F) = \{z \in \mathbb{C} \,|\, \text{for all } \varepsilon > 0, \mu(\{\lambda \in \mathbb{R} \,|\, |F(\lambda) - z| < \varepsilon\}) > 0\}. \tag{3.2.62}$$

We conclude the half-line case by recalling the following elementary example of the Fourier-sine transform.

Example 3.2.10. *Let $\alpha = 0$ and $V(x) = 0$ for a.e. $x \in (0,\infty)$. Then,*

$$\begin{aligned}
&\phi_0(\lambda, x) = \frac{\sin(\lambda^{1/2}x)}{\lambda^{1/2}}, \quad \lambda > 0, \ x \in (0,\infty), \\
&m_{+,0}(z) = iz^{1/2}, \quad z \in \mathbb{C}\backslash[0,\infty), \\
&d\rho_{+,0}(\lambda) = \pi^{-1}\chi_{[0,\infty)}(\lambda)\lambda^{1/2}d\lambda, \quad \lambda \in \mathbb{R},
\end{aligned} \tag{3.2.63}$$

and hence,

$$\begin{aligned}
&\widehat{h}(\lambda) = \text{l.i.m.}_{y\uparrow\infty} \int_0^y dx\, \frac{\sin(\lambda^{1/2}x)}{\lambda^{1/2}} h(x), \quad h \in L^2([0,\infty); dx), \\
&h(x) = \text{l.i.m.}_{\mu\uparrow\infty} \frac{1}{\pi} \int_0^\mu \lambda^{1/2} d\lambda\, \frac{\sin(\lambda^{1/2}x)}{\lambda^{1/2}}\, \widehat{h}(\lambda), \quad \widehat{h} \in L^2([0,\infty); \pi^{-1}\lambda^{1/2}d\lambda).
\end{aligned} \tag{3.2.64}$$

Introducing the change of variables

$$p = \lambda^{1/2} > 0, \quad \widehat{H}(p) = \left(\frac{2\lambda}{\pi}\right)^{1/2} \widehat{h}(\lambda), \tag{3.2.65}$$

the pair of equations in (3.2.64) *takes on the usual symmetric form of the Fourier-sine transform,*

$$\begin{aligned}
\widehat{H}(p) &= \text{l.i.m.}_{y\uparrow\infty} \left(\frac{2}{\pi}\right)^{1/2} \int_0^y dx\, \sin(px) h(x), \quad h \in L^2([0,\infty); dx), \\
h(x) &= \text{l.i.m.}_{q\uparrow\infty} \left(\frac{2}{\pi}\right)^{1/2} \int_0^q dp\, \sin(px) \widehat{H}(p), \quad \widehat{H} \in L^2([0,\infty); dp).
\end{aligned} \tag{3.2.66}$$

Next, we turn to the case of the entire real line and make the following basic assumption.

Hypothesis 3.2.11. (i) Assume that

$$V \in L^1_{\text{loc}}(\mathbb{R}; dx), \quad V \text{ real-valued.} \tag{3.2.67}$$

(ii) Introducing the differential expression τ given by

$$\tau = -\frac{d^2}{dx^2} + V(x), \quad x \in \mathbb{R}, \tag{3.2.68}$$

we assume τ to be in the limit point case at $+\infty$ and at $-\infty$.

Associated with the differential expression τ one introduces the self-adjoint Schrödinger operator H in $L^2(\mathbb{R}; dx)$ by

$$\begin{aligned} &Hf = \tau f, \\ &f \in \operatorname{dom}(H) = \{g \in L^2(\mathbb{R}; dx) \,|\, g, g' \in AC_{\text{loc}}(\mathbb{R});\ \tau g \in L^2(\mathbb{R}; dx)\}. \end{aligned} \tag{3.2.69}$$

Here $AC_{\text{loc}}(\mathbb{R})$ denotes the class of locally absolutely continuous functions on $\mathbb{R}$.

As in the half-line context we introduce the usual fundamental system of solutions $\phi_\alpha(z, \cdot, x_0)$ and $\theta_\alpha(z, \cdot, x_0)$, $z \in \mathbb{C}$, of

$$(\tau\psi)(z, x) = z\psi(z, x), \quad x \in \mathbb{R} \tag{3.2.70}$$

with respect to a fixed reference point $x_0 \in \mathbb{R}$, satisfying the initial conditions at the point $x = x_0$,

$$\begin{aligned} &\phi_\alpha(z, x_0, x_0) = -\theta'_\alpha(z, x_0, x_0) = -\sin(\alpha), \\ &\phi'_\alpha(z, x_0, x_0) = \theta_\alpha(z, x_0, x_0) = \cos(\alpha), \quad \alpha \in [0, \pi). \end{aligned} \tag{3.2.71}$$

Again we note that for any fixed $x, x_0 \in \mathbb{R}$, $\phi_\alpha(z, x, x_0)$ and $\theta_\alpha(z, x, x_0)$ are entire with respect to z and that

$$W(\theta_\alpha(z, \cdot, x_0), \phi_\alpha(z, \cdot, x_0))(x) = 1, \quad z \in \mathbb{C}. \tag{3.2.72}$$

Particularly important solutions of (3.2.70) are the *Weyl–Titchmarsh solutions* $\psi_{\pm,\alpha}(z, \cdot, x_0)$, $z \in \mathbb{C}\backslash\mathbb{R}$, uniquely characterized by

$$\begin{aligned} &\psi_{\pm,\alpha}(z, \cdot, x_0) \in L^2([x_0, \pm\infty); dx), \\ &\sin(\alpha)\psi'_{\pm,\alpha}(z, x_0, x_0) + \cos(\alpha)\psi_{\pm,\alpha}(z, x_0, x_0) = 1, \quad z \in \mathbb{C}\backslash\mathbb{R}. \end{aligned} \tag{3.2.73}$$

The crucial condition in (3.2.73) is again the L^2-property which uniquely determines $\psi_{\pm,\alpha}(z,\cdot,x_0)$ up to constant multiples by the limit point hypothesis of τ at $\pm\infty$. In particular, for $\alpha,\beta\in[0,\pi)$,

$$\psi_{\pm,\alpha}(z,\cdot,x_0)=C_\pm(z,\alpha,\beta,x_0)\psi_{\pm,\beta}(z,\cdot,x_0)$$
$$\text{for some coefficients } C_\pm(z,\alpha,\beta,x_0)\in\mathbb{C}. \tag{3.2.74}$$

The normalization in (3.2.73) shows that $\psi_{\pm,\alpha}(z,\cdot,x_0)$ are of the type

$$\psi_{\pm,\alpha}(z,x,x_0)=\theta_\alpha(z,x,x_0)+m_{\pm,\alpha}(z,x_0)\phi_\alpha(z,x,x_0), \quad z\in\mathbb{C}\backslash\mathbb{R},\ x\in\mathbb{R} \tag{3.2.75}$$

for some coefficients $m_{\pm,\alpha}(z,x_0)$, the *Weyl–Titchmarsh m-functions* associated with τ, α, and x_0.

Again we recall the fundamental identity

$$\int_{x_0}^{\pm\infty} dx\,\psi_{\pm,\alpha}(z_1,x,x_0)\psi_{\pm,\alpha}(z_2,x,x_0)=\frac{m_{\pm,\alpha}(z_1,x_0)-m_{\pm,\alpha}(z_2,x_0)}{z_1-z_2}, \tag{3.2.76}$$
$$z_1,z_2\in\mathbb{C}\backslash\mathbb{R},\ z_1\neq z_2,$$

and as before one concludes

$$\overline{m_{\pm,\alpha}(z,x_0)}=m_{\pm,\alpha}(\overline{z},x_0), \quad z\in\mathbb{C}\backslash\mathbb{R}. \tag{3.2.77}$$

Choosing $z_1=z$, $z_2=\overline{z}$ in (3.2.76), one infers

$$\int_{x_0}^{\pm\infty} dx\,|\psi_{\pm,\alpha}(z,x,x_0)|^2=\frac{\mathrm{Im}(m_{\pm,\alpha}(z,x_0))}{\mathrm{Im}(z)}, \quad z\in\mathbb{C}\backslash\mathbb{R}. \tag{3.2.78}$$

Since $m_{\pm,\alpha}(\cdot,x_0)$ are analytic on $\mathbb{C}\backslash\mathbb{R}$, $\pm m_{\pm,\alpha}(\cdot,x_0)$ are Herglotz functions.

The Green's function $G(z,x,x')$ of H then reads

$$G(z,x,x')=\frac{1}{W(\psi_{+,\alpha}(z,\cdot,x_0),\psi_{-,\alpha}(z,\cdot,x_0))}$$

$$\times \begin{cases} \psi_{-,\alpha}(z,x,x_0)\psi_{+,\alpha}(z,x',x_0), & x \le x', \\ \psi_{-,\alpha}(z,x',x_0)\psi_{+,\alpha}(z,x,x_0), & x' \le x, \end{cases} \quad z \in \mathbb{C}\backslash\mathbb{R} \tag{3.2.79}$$

with

$$W(\psi_{+,\alpha}(z,\cdot,x_0),\psi_{-,\alpha}(z,\cdot,x_0)) = m_{-,\alpha}(z,x_0) - m_{+,\alpha}(z,x_0), \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{3.2.80}$$

Thus,

$$((H - zI)^{-1}f)(x) = \int_{\mathbb{R}} dx'\, G(z,x,x')f(x'), \quad z \in \mathbb{C}\backslash\mathbb{R},\ x \in \mathbb{R},\ f \in L^2(\mathbb{R};dx). \tag{3.2.81}$$

Given $m_{\pm}(z,x_0)$, we also introduce the 2×2 matrix-valued Weyl–Titchmarsh function

$$M_\alpha(z,x_0) = \begin{pmatrix} \frac{1}{m_{-,\alpha}(z,x_0)-m_{+,\alpha}(z,x_0)} & \frac{1}{2}\frac{m_{-,\alpha}(z,x_0)+m_{+,\alpha}(z,x_0)}{m_{-,\alpha}(z,x_0)-m_{+,\alpha}(z,x_0)} \\ \frac{1}{2}\frac{m_{-,\alpha}(z,x_0)+m_{+,\alpha}(z,x_0)}{m_{-,\alpha}(z,x_0)-m_{+,\alpha}(z,x_0)} & \frac{m_{-,\alpha}(z,x_0)m_{+,\alpha}(z,x_0)}{m_{-,\alpha}(z,x_0)-m_{+,\alpha}(z,x_0)} \end{pmatrix}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{3.2.82}$$

$M_\alpha(z,x_0)$ is a Herglotz matrix with representation

$$\begin{aligned} &M_\alpha(z,x_0) = C_\alpha(x_0) + \int_{\mathbb{R}} d\Omega_\alpha(\lambda,x_0)\left[\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\right], \quad z \in \mathbb{C}\backslash\mathbb{R}, \\ &C_\alpha(x_0) = C_\alpha(x_0)^*, \quad \int_{\mathbb{R}} \frac{\|d\Omega_\alpha(\lambda,x_0)\|}{1+\lambda^2} < \infty. \end{aligned} \tag{3.2.83}$$

The Stieltjes inversion formula for the 2×2 nonnegative matrix-valued measure $d\Omega_\alpha(\cdot,x_0)$ then reads

$$\Omega_\alpha((\lambda_1,\lambda_2],x_0) = \pi^{-1}\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, \mathrm{Im}(M_\alpha(\lambda + i\varepsilon,x_0)), \quad \lambda_1,\lambda_2 \in \mathbb{R},\ \lambda_1 < \lambda_2. \tag{3.2.84}$$

In particular, this implies that the entries $d\Omega_{\alpha,\ell,\ell'}$, $\ell,\ell' = 0,1$, of the matrix-valued measure $d\Omega_\alpha$ are real-valued scalar measures. Moreover, since the diagonal entries of M_α are Herglotz functions, the diagonal entries of the measure $d\Omega_\alpha$ are nonnegative measures. The off-diagonal entries of the measure $d\Omega_\alpha$ equal a complex measure which naturally admits a decomposition into a linear combination of differences of two nonnegative measures.

We note that in formulas (3.2.73)–(3.2.83) one can replace $z \in \mathbb{C}\backslash\mathbb{R}$ by $z \in \mathbb{C}\backslash\sigma(H)$.

Next, we relate the family of spectral projections, $\{E_H(\lambda)\}_{\lambda\in\mathbb{R}}$, of the self-adjoint operator H and the 2×2 matrix-valued increasing spectral function $\Omega_\alpha(\lambda, x_0)$, $\lambda \in \mathbb{R}$, which generates the matrix-valued measure in the Herglotz representation (3.2.83) of $M_\alpha(z, x_0)$.

We first note that for $F \in C(\mathbb{R})$,

$$\begin{aligned} &\big(f, F(H)g\big)_{L^2(\mathbb{R};dx)} = \int_{\mathbb{R}} d\big(f, E_H(\lambda)g\big)_{L^2(\mathbb{R};dx)}\, F(\lambda), \\ &f, g \in \operatorname{dom}(F(H)) = \bigg\{h \in L^2(\mathbb{R}; dx) \,\bigg|\, \int_{\mathbb{R}} d\big\|E_H(\lambda)h\big\|^2_{L^2(\mathbb{R};dx)}\, |F(\lambda)|^2 < \infty\bigg\}. \end{aligned} \tag{3.2.85}$$

Given a 2×2 matrix-valued nonnegative measure $d\Omega = \big(d\Omega_{\ell,\ell'}\big)_{\ell,\ell'=0,1}$ on $\mathbb{R}$ with

$$d\Omega^{\mathrm{tr}} = d\Omega_{0,0} + d\Omega_{1,1} \tag{3.2.86}$$

its trace measure, the density matrix

$$\left(\frac{d\Omega_{\ell,\ell'}}{d\Omega^{\mathrm{tr}}}\right)_{\ell,\ell'=0,1} \tag{3.2.87}$$

is locally integrable on $\mathbb{R}$ with respect to $d\Omega^{\mathrm{tr}}$. One then introduces the vector-valued Hilbert space $L^2(\mathbb{R}; d\Omega)$ in the following manner. Consider ordered pairs $f = (f_0, f_1)^\top$ of $d\Omega^{\mathrm{tr}}$-measurable functions such that

$$\sum_{\ell,\ell'=0}^{1} \overline{f_\ell(\cdot)}\, \frac{d\Omega_{\ell,\ell'}(\cdot)}{d\Omega^{\mathrm{tr}}(\cdot)}\, f_{\ell'}(\cdot) \tag{3.2.88}$$

is $d\Omega^{\mathrm{tr}}$-integrable on $\mathbb{R}$ and define $L^2(\mathbb{R}; d\Omega)$ as the set of equivalence classes modulo $d\Omega$-null functions. Here $g = (g_0, g_1)^\top \in L^2(\mathbb{R}; d\Omega)$ is defined to be a $d\Omega$-null function if

$$\int_{\mathbb{R}} d\Omega^{\mathrm{tr}}(\lambda) \sum_{\ell,\ell'=0}^{1} \overline{g_\ell(\lambda)}\, \frac{d\Omega_{\ell,\ell'}(\lambda)}{d\Omega^{\mathrm{tr}}(\lambda)}\, g_{\ell'}(\lambda) = 0. \tag{3.2.89}$$

This space is complete with respect to the norm induced by the scalar product

$$(f,g)_{L^2(\mathbb{R};d\Omega)} = \int_{\mathbb{R}} d\Omega^{\mathrm{tr}}(\lambda) \sum_{\ell,\ell'=0}^{1} \overline{f_\ell(\lambda)}\, \frac{d\Omega_{\ell,\ell'}(\lambda)}{d\Omega^{\mathrm{tr}}(\lambda)}\, g_{\ell'}(\lambda), \quad f,g \in L^2(\mathbb{R}; d\Omega). \tag{3.2.90}$$

For notational simplicity, expressions of the type (3.2.90) will usually be abbreviated by

$$(f,g)_{L^2(\mathbb{R};d\Omega)} = \int_{\mathbb{R}} \overline{f(\lambda)^\top}\, d\Omega(\lambda)\, g(\lambda), \quad f,g \in L^2(\mathbb{R}; d\Omega). \tag{3.2.91}$$

(In this context we refer to [43, p. 1345–1346] for some peculiarities in connection with matrix-valued nonnegative measures.)

Theorem 3.2.12. *Let $\alpha \in [0,\pi)$, $f,g \in C_0^\infty(\mathbb{R})$, $F \in C(\mathbb{R})$, $x_0 \in \mathbb{R}$, and $\lambda_1, \lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$. Then,*

$$\begin{aligned} \big(f, F(H)E_H((\lambda_1,\lambda_2])g\big)_{L^2(\mathbb{R};dx)} &= \big(\widehat{f}_\alpha(\cdot,x_0), M_F M_{\chi_{(\lambda_1,\lambda_2]}} \widehat{g}_\alpha(\cdot,x_0)\big)_{L^2(\mathbb{R};d\Omega_\alpha(\cdot,x_0))} \\ &= \int_{(\lambda_1,\lambda_2]} \overline{\widehat{f}_\alpha(\lambda,x_0)^\top}\, d\Omega_\alpha(\lambda,x_0)\, \widehat{g}_\alpha(\lambda,x_0) F(\lambda), \end{aligned} \tag{3.2.92}$$

where we introduced the notation

$$\begin{aligned} &\widehat{h}_{\alpha,0}(\lambda,x_0) = \int_{\mathbb{R}} dx\, \theta_\alpha(\lambda,x,x_0) h(x), \quad \widehat{h}_{\alpha,1}(\lambda,x_0) = \int_{\mathbb{R}} dx\, \phi_\alpha(\lambda,x,x_0) h(x), \\ &\widehat{h}_\alpha(\lambda,x_0) = \big(\widehat{h}_{\alpha,0}(\lambda,x_0), \widehat{h}_{\alpha,1}(\lambda,x_0)\big)^\top, \quad \lambda \in \mathbb{R},\ h \in C_0^\infty(\mathbb{R}), \end{aligned} \tag{3.2.93}$$

and M_G *denotes the maximally defined operator of multiplication by the* $d\Omega_\alpha^{\rm tr}$*-measurable function* G *in the Hilbert space* $L^2(\mathbb{R}; d\Omega_\alpha(\cdot, x_0))$,

$$\begin{aligned}
&(M_G\widehat{h})(\lambda) = G(\lambda)\widehat{h}(\lambda) = \big(G(\lambda)\widehat{h}_0(\lambda), G(\lambda)\widehat{h}_1(\lambda)\big)^\top \ \text{ for a.e. } \lambda \in \mathbb{R}, \\
&\widehat{h} \in \operatorname{dom}(M_G) = \big\{\widehat{k} \in L^2(\mathbb{R}; d\Omega_\alpha(\cdot, x_0)) \,|\, G\widehat{k} \in L^2(\mathbb{R}; d\Omega_\alpha(\cdot, x_0))\big\}.
\end{aligned} \tag{3.2.94}$$

Proof. The point of departure for deriving (3.2.92) is again Stone's formula (3.2.29) applied to $T = H$,

$$\begin{aligned}
&\big(f, F(H)E_H((\lambda_1, \lambda_2])g\big)_{L^2(\mathbb{R};dx)} \\
&\quad = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0} \frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, F(\lambda)\big[\big(f, (H-(\lambda+i\varepsilon)I)^{-1}g\big)_{L^2(\mathbb{R};dx)} \\
&\qquad\qquad - \big(f, (H-(\lambda-i\varepsilon)I)^{-1}g\big)_{L^2(\mathbb{R};dx)}\big].
\end{aligned} \tag{3.2.95}$$

Insertion of (3.2.79) and (3.2.81) into (3.2.95) then yields the following:

$$\begin{aligned}
&\big(f, F(H)E_H((\lambda_1, \lambda_2])g\big)_{L^2(\mathbb{R};dx)} = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0} \frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, F(\lambda) \\
&\quad \times \bigg\{ \int_{\mathbb{R}} dx\, \frac{1}{W(\lambda+i\varepsilon)}\bigg[\overline{f(x)}\psi_{+,\alpha}(\lambda+i\varepsilon, x, x_0)\int_{-\infty}^{x} dx'\, \psi_{-,\alpha}(\lambda+i\varepsilon, x', x_0)g(x') \\
&\qquad + \overline{f(x)}\psi_{-,\alpha}(\lambda+i\varepsilon, x, x_0)\int_{x}^{\infty} dx'\, \psi_{+,\alpha}(\lambda+i\varepsilon, x', x_0)g(x')\bigg] \\
&\qquad - \frac{1}{W(\lambda-i\varepsilon)}\bigg[\overline{f(x)}\psi_{+,\alpha}(\lambda-i\varepsilon, x, x_0)\int_{-\infty}^{x} dx'\, \psi_{-,\alpha}(\lambda-i\varepsilon, x', x_0)g(x') \\
&\qquad + \overline{f(x)}\psi_{-,\alpha}(\lambda-i\varepsilon, x, x_0)\int_{x}^{\infty} dx'\, \psi_{+,\alpha}(\lambda-i\varepsilon, x', x_0)g(x')\bigg]\bigg\},
\end{aligned} \tag{3.2.96}$$

where we used the abbreviation

$$W(z) = W(\psi_{+,\alpha}(z, \cdot, x_0)), \psi_{-,\alpha}(z, \cdot, x_0)), \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{3.2.97}$$

Freely interchanging the dx and dx' integrals with the limits and the $d\lambda$ integral (since all integration domains are finite and all integrands are continuous), and inserting the expressions (3.2.75) for $\psi_{\pm,\alpha}(z,x,x_0)$ into (3.2.96), one obtains

$$
\begin{aligned}
&\big(f, F(H)E_H((\lambda_1,\lambda_2])g\big)_{L^2(\mathbb{R};dx)} = \int_{\mathbb{R}} dx\, \overline{f(x)} \bigg\{ \int_{-\infty}^{x} dx'\, g(x') \\
&\quad \times \lim_{\delta\downarrow 0} \lim_{\varepsilon\downarrow 0} \frac{1}{2\pi i} \int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, F(\lambda) \Big[\big[\theta_\alpha(\lambda,x,x_0) + m_{+,\alpha}(\lambda+i\varepsilon,x_0)\phi_\alpha(\lambda,x,x_0)\big] \\
&\qquad\qquad \times \big[\theta_\alpha(\lambda,x',x_0) + m_{-,\alpha}(\lambda+i\varepsilon,x_0)\phi_\alpha(\lambda,x',x_0)\big] W(\lambda+i\varepsilon)^{-1} \\
&\qquad\quad - \big[\theta_\alpha(\lambda,x,x_0) + m_{+,\alpha}(\lambda-i\varepsilon,x_0)\phi_\alpha(\lambda,x,x_0)\big] \\
&\qquad\qquad \times \big[\theta_\alpha(\lambda,x',x_0) + m_{-,\alpha}(\lambda-i\varepsilon,x_0)\phi_\alpha(\lambda,x',x_0)\big] W(\lambda-i\varepsilon)^{-1} \Big] \\
&\quad + \int_x^{\infty} dx'\, g(x') \lim_{\delta\downarrow 0} \lim_{\varepsilon\downarrow 0} \frac{1}{2\pi i} \int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, F(\lambda) \\
&\qquad\qquad \times \Big[\big[\theta_\alpha(\lambda,x,x_0) + m_{-,\alpha}(\lambda+i\varepsilon,x_0)\phi_\alpha(\lambda,x,x_0)\big] \\
&\qquad\qquad \times \big[\theta_\alpha(\lambda,x',x_0) + m_{+,\alpha}(\lambda+i\varepsilon,x_0)\phi_\alpha(\lambda,x',x_0)\big] W(\lambda+i\varepsilon)^{-1} \\
&\qquad\quad - \big[\theta_\alpha(\lambda,x,x_0) + m_{-,\alpha}(\lambda-i\varepsilon,x_0)\phi_\alpha(\lambda,x,x_0)\big] \\
&\qquad\qquad \times \big[\theta_\alpha(\lambda,x',x_0) + m_{+,\alpha}(\lambda-i\varepsilon,x_0)\phi_\alpha(\lambda,x',x_0)\big] W(\lambda-i\varepsilon)^{-1} \Big] \bigg\}.
\end{aligned} \tag{3.2.98}
$$

Here we employed the fact that for fixed $x \in \mathbb{R}$, $\theta_\alpha(z,x,x_0)$ and $\phi_\alpha(z,x,x_0)$ are entire with respect to z, that $\theta_\alpha(\lambda,x,x_0)$ and $\phi_\alpha(\lambda,x,x_0)$ are real-valued for $\lambda \in \mathbb{R}$, that $\phi_\alpha(z,\cdot,x_0), \theta_\alpha(z,\cdot,x_0) \in AC_{\text{loc}}(\mathbb{R})$, and hence that

$$
\begin{aligned}
\theta_\alpha(\lambda \pm i\varepsilon, x, x_0) &\underset{\varepsilon\downarrow 0}{=} \theta_\alpha(\lambda,x,x_0) \pm i\varepsilon (d/dz)\theta_\alpha(z,x,x_0)|_{z=\lambda} + O(\varepsilon^2), \\
\phi_\alpha(\lambda \pm i\varepsilon, x, x_0) &\underset{\varepsilon\downarrow 0}{=} \phi_\alpha(\lambda,x,x_0) \pm i\varepsilon (d/dz)\phi_\alpha(z,x,x_0)|_{z=\lambda} + O(\varepsilon^2)
\end{aligned} \tag{3.2.99}
$$

with $O(\varepsilon^2)$ being uniform with respect to (λ,x) as long as λ and x vary in compact subsets of $\mathbb{R}^2$. Moreover, we used that

$$
\begin{aligned}
&\varepsilon |M_{\alpha,\ell,\ell'}(\lambda+i\varepsilon,x_0)| \leq C(\lambda_1,\lambda_2,\varepsilon_0,x_0), \quad \lambda \in [\lambda_1,\lambda_2],\ 0<\varepsilon\leq\varepsilon_0,\ \ell,\ell'=0,1, \\
&\varepsilon |\mathrm{Re}(M_{\alpha,\ell,\ell'}(\lambda+i\varepsilon,x_0))| \underset{\varepsilon\downarrow 0}{=} o(1), \quad \lambda\in\mathbb{R},\ \ell,\ell'=0,1,
\end{aligned} \tag{3.2.100}
$$

which follows from the properties of Herglotz functions since $M_{\alpha,\ell,\ell}$, $\ell = 0,1$, are Herglotz and $M_{\alpha,0,1} = M_{\alpha,1,0}$ have Herglotz-type representations by decomposing the associated complex measure $d\Omega_{\alpha,0,1}$ into $d\Omega_{\alpha,0,1} = d(\omega_1 - \omega_2) + id(\omega_3 - \omega_4)$, with $d\omega_k$, $k = 1,\dots,4$, nonnegative measures. In particular, utilizing (3.2.77), (3.2.99), (3.2.100), and the elementary fact (cf. (3.2.80))

$$\operatorname{Im}\bigg[\frac{m_{\pm,\alpha}(\lambda+i\varepsilon,x_0)}{W(\lambda+i\varepsilon)}\bigg] = \frac{1}{2}\operatorname{Im}\bigg[\frac{m_{-,\alpha}(\lambda+i\varepsilon,x_0)+m_{+,\alpha}(\lambda+i\varepsilon,x_0)}{W(\lambda+i\varepsilon)}\bigg], \quad \lambda\in\mathbb{R},\ \varepsilon>0, \tag{3.2.101}$$

$\phi_\alpha(\lambda\pm i\varepsilon,x,x_0)$ and $\theta_\alpha(\lambda\pm i\varepsilon,x,x_0)$ under the $d\lambda$ integrals in (3.2.98) have immediately been replaced by $\phi_\alpha(\lambda,x,x_0)$ and $\theta_\alpha(\lambda,x,x_0)$. Collecting appropriate terms in (3.2.98) then yields

$$\begin{aligned}
&\big(f,F(H)E_H((\lambda_1,\lambda_2])g\big)_{L^2(\mathbb{R};dx)} \\
&\quad = \int_{\mathbb{R}} dx\,\overline{f(x)}\int_{\mathbb{R}} dx'\,g(x')\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\,F(\lambda) \\
&\qquad\times\bigg\{\theta_\alpha(\lambda,x,x_0)\theta_\alpha(\lambda,x',x_0)\operatorname{Im}\bigg[\frac{1}{m_{-,\alpha}(\lambda+i\varepsilon,x_0)-m_{+,\alpha}(\lambda+i\varepsilon,x_0)}\bigg] \\
&\qquad\quad + [\phi_\alpha(\lambda,x,x_0)\theta_\alpha(\lambda,x',x_0)+\theta_\alpha(\lambda,x,x_0)\phi_\alpha(\lambda,x',x_0)] \\
&\qquad\qquad\times\frac{1}{2}\operatorname{Im}\bigg[\frac{m_{-,\alpha}(\lambda+i\varepsilon,x_0)+m_{+,\alpha}(\lambda+i\varepsilon,x_0)}{m_{-,\alpha}(\lambda+i\varepsilon,x_0)-m_{+,\alpha}(\lambda+i\varepsilon,x_0)}\bigg] \\
&\qquad\quad + \phi_\alpha(\lambda,x,x_0)\phi_\alpha(\lambda,x',x_0)\operatorname{Im}\bigg[\frac{m_{-,\alpha}(\lambda+i\varepsilon,x_0)m_{+,\alpha}(\lambda+i\varepsilon,x_0)}{m_{-,\alpha}(\lambda+i\varepsilon,x_0)-m_{+,\alpha}(\lambda+i\varepsilon,x_0)}\bigg]\bigg\}.
\end{aligned} \tag{3.2.102}$$

Using the fact that by (3.2.84) ($\ell,\ell'=0,1$)

$$\begin{aligned}
&\int_{(\lambda_1,\lambda_2]} d\Omega_{\alpha,\ell,\ell'}(\lambda,x_0) = \Omega_{\alpha,\ell,\ell'}((\lambda_1,\lambda_2],x_0) \\
&\quad = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\,\operatorname{Im}(M_{\alpha,\ell,\ell'}(\lambda+i\varepsilon,x_0)),
\end{aligned} \tag{3.2.103}$$

and hence that

$$\int_{\mathbb{R}} d\Omega_{\alpha,\ell,\ell'}(\lambda,x_0)\,h(\lambda) = \lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\mathbb{R}} d\lambda\,\mathrm{Im}(M_{\alpha,\ell,\ell'}(\lambda+i\varepsilon,x_0))\,h(\lambda), \quad h\in C_0(\mathbb{R}), \tag{3.2.104}$$

$$\int_{(\lambda_1,\lambda_2]} d\Omega_{\alpha,\ell,\ell'}(\lambda,x_0)\,k(\lambda) = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\,\mathrm{Im}(M_{\alpha,\ell,\ell'}(\lambda+i\varepsilon,x_0))\,k(\lambda), \quad k\in C(\mathbb{R}), \tag{3.2.105}$$

one concludes

$$\begin{aligned}
\big(f, F(H)E_H((\lambda_1,\lambda_2])g\big)_{L^2(\mathbb{R};dx)} &= \int_{\mathbb{R}} dx\,\overline{f(x)}\int_{\mathbb{R}} dx'\,g(x')\int_{(\lambda_1,\lambda_2]} F(\lambda) \\
&\quad\times\Big\{\theta_\alpha(\lambda,x,x_0)\theta_\alpha(\lambda,x',x_0)d\Omega_{\alpha,0,0}(\lambda,x_0) \\
&\qquad + [\phi_\alpha(\lambda,x,x_0)\theta_\alpha(\lambda,x',x_0)+\theta_\alpha(\lambda,x,x_0)\phi_\alpha(\lambda,x',x_0)]d\Omega_{\alpha,0,1}(\lambda,x_0) \\
&\qquad + \phi_\alpha(\lambda,x,x_0)\phi_\alpha(\lambda,x',x_0)d\Omega_{\alpha,1,1}(\lambda,x_0)\Big\} \\
&= \int_{(\lambda_1,\lambda_2]} \overline{\widehat{f}_\alpha(\lambda,x_0)^\top}\,d\Omega_\alpha(\lambda,x_0)\,\widehat{g}_\alpha(\lambda,x_0)F(\lambda),
\end{aligned} \tag{3.2.106}$$

using (3.2.93), $d\Omega_{\alpha,0,1}(\cdot,x_0) = d\Omega_{\alpha,1,0}(\cdot,x_0)$, and interchanging the dx, dx' and $d\Omega_{\alpha,\ell,\ell'}(\cdot,x_0)$, $\ell,\ell'=0,1$, integrals once more. $\square$

Remark 3.2.13. Again we emphasize that the idea of a straightforward derivation of the link between the family of spectral projections $E_H(\cdot)$ and the 2×2 matrix-valued spectral function $\Omega_\alpha(\cdot)$ of H in Theorem 3.2.12 can already be found in [95] as pointed out in Remark 3.2.8. It applies equally well to Dirac-type operators and Hamiltonian systems on $\mathbb{R}$ (see the extensive literature cited, e.g., in [31]) and to Jacobi and CMV operators on $\mathbb{Z}$ (cf. Chapter 1 and [18]).

As in the half-line case before, one can improve on Theorem 3.2.12 and remove the compact support restrictions on f and g in the usual way. To this end one considers the map

$$\widetilde{U}_\alpha(x_0)\colon \begin{cases} C_0^\infty(\mathbb{R}) \to L^2(\mathbb{R}; d\Omega_\alpha(\cdot, x_0)) \\ \qquad\qquad h \mapsto \widehat{h}_\alpha(\cdot, x_0) = \big(\widehat{h}_{\alpha,0}(\lambda, x_0), \widehat{h}_{\alpha,1}(\lambda, x_0)\big)^\top, \end{cases} \tag{3.2.107}$$
$$\widehat{h}_{\alpha,0}(\lambda, x_0) = \int_{\mathbb{R}} dx\, \theta_\alpha(\lambda, x, x_0) h(x), \quad \widehat{h}_{\alpha,1}(\lambda, x_0) = \int_{\mathbb{R}} dx\, \phi_\alpha(\lambda, x, x_0) h(x).$$

Taking $f = g$, $F = 1$, $\lambda_1 \downarrow -\infty$, and $\lambda_2 \uparrow \infty$ in (3.2.92) then shows that $\widetilde{U}_\alpha(x_0)$ is a densely defined isometry in $L^2(\mathbb{R}; dx)$, which extends by continuity to an isometry on $L^2(\mathbb{R}; dx)$. The latter is denoted by $U_\alpha(x_0)$ and given by

$$U_\alpha(x_0)\colon \begin{cases} L^2(\mathbb{R}; dx) \to L^2(\mathbb{R}; d\Omega_\alpha(\cdot, x_0)) \\ \qquad\qquad h \mapsto \widehat{h}_\alpha(\cdot, x_0) = \big(\widehat{h}_{\alpha,0}(\cdot, x_0), \widehat{h}_{\alpha,1}(\cdot, x_0)\big)^\top, \end{cases} \tag{3.2.108}$$
$$\widehat{h}_\alpha(\cdot, x_0) = \begin{pmatrix} \widehat{h}_{\alpha,0}(\cdot, x_0) \\ \widehat{h}_{\alpha,1}(\cdot, x_0) \end{pmatrix} = \text{l.i.m.}_{a\downarrow -\infty, b\uparrow\infty} \begin{pmatrix} \int_a^b dx\, \theta_\alpha(\cdot, x, x_0) h(x) \\ \int_a^b dx\, \phi_\alpha(\cdot, x, x_0) h(x) \end{pmatrix},$$

where l.i.m. refers to the $L^2(\mathbb{R}; d\Omega_\alpha(\cdot, x_0))$-limit.

The calculation in (3.2.106) also yields

$$\begin{aligned} (E_H((\lambda_1, \lambda_2])g)(x) &= \int_{(\lambda_1,\lambda_2]} (\theta_\alpha(\lambda, x, x_0), \phi_\alpha(\lambda, x, x_0))\, d\Omega_\alpha(\lambda, x_0)\, \widehat{g}_\alpha(\lambda) \\ &= \int_{(\lambda_1,\lambda_2]} \Big\{ d\Omega_{\alpha,0,0}(\lambda, x_0)\, \theta_\alpha(\lambda, x, x_0) \widehat{g}_{\alpha,0}(\lambda, x_0) \\ &\quad + d\Omega_{\alpha,0,1}(\lambda, x_0)\, [\theta_\alpha(\lambda, x, x_0) \widehat{g}_{\alpha,1}(\lambda, x_0) + \phi_\alpha(\lambda, x, x_0) \widehat{g}_{\alpha,0}(\lambda, x_0)] \\ &\quad + d\Omega_{\alpha,1,1}(\lambda, x_0)\, \phi_\alpha(\lambda, x, x_0) \widehat{g}_{\alpha,1}(\lambda, x_0) \Big\}, \quad g \in C_0^\infty(\mathbb{R}) \end{aligned} \tag{3.2.109}$$

and subsequently, (3.2.109) extends to all $g \in L^2(\mathbb{R}; dx)$ by continuity. Moreover, taking $\lambda_1 \downarrow -\infty$ and $\lambda_2 \uparrow \infty$ in (3.2.109) and using

$$\text{s-lim}_{\lambda\downarrow -\infty} E_H(\lambda) = 0, \quad \text{s-lim}_{\lambda\uparrow\infty} E_H(\lambda) = I_{L^2(\mathbb{R}; dx)}, \tag{3.2.110}$$

where

$$E_H(\lambda) = E_H((-\infty, \lambda]), \quad \lambda \in \mathbb{R}, \tag{3.2.111}$$

then yield

$$
\begin{aligned}
g(\cdot) &= \text{l.i.m.}_{\mu_1\downarrow-\infty,\mu_2\uparrow\infty} \int_{(\mu_1,\mu_2]} (\theta_\alpha(\lambda,\cdot,x_0),\phi_\alpha(\lambda,\cdot,x_0))\, d\Omega_\alpha(\lambda,x_0)\, \widehat{g}_\alpha(\lambda) \\
&= \text{l.i.m.}_{\mu_1\downarrow-\infty,\mu_2\uparrow\infty} \int_{\mu_1}^{\mu_2} \Big\{ d\Omega_{\alpha,0,0}(\lambda,x_0)\, \theta_\alpha(\lambda,\cdot,x_0)\widehat{g}_{\alpha,0}(\lambda,x_0) \\
&\qquad + d\Omega_{\alpha,0,1}(\lambda,x_0)\, [\theta_\alpha(\lambda,\cdot,x_0)\widehat{g}_{\alpha,1}(\lambda,x_0) + \phi_\alpha(\lambda,\cdot,x_0)\widehat{g}_{\alpha,0}(\lambda,x_0)] \\
&\qquad + d\Omega_{\alpha,1,1}(\lambda,x_0)\, \phi_\alpha(\lambda,\cdot,x_0)\widehat{g}_{\alpha,1}(\lambda,x_0) \Big\}, \quad g \in L^2(\mathbb{R};dx),
\end{aligned} \tag{3.2.112}
$$

where l.i.m. refers to the $L^2(\mathbb{R};dx)$-limit. In addition, one can show that the map $U_\alpha(x_0)$ in (3.2.108) is onto and hence that $U_\alpha(x_0)$ is unitary with

$$
U_\alpha(x_0)^{-1} \colon \begin{cases} L^2(\mathbb{R};d\Omega_\alpha(\cdot,x_0)) \to L^2(\mathbb{R};dx) \\ \qquad\qquad \widehat{h}_\alpha(\cdot,x_0) \mapsto h, \end{cases} \tag{3.2.113}
$$

$$
h(\cdot) = \text{l.i.m.}_{\mu_1\downarrow-\infty,\mu_2\uparrow\infty} \int_{\mu_1}^{\mu_2} (\theta_\alpha(\lambda,\cdot,x_0),\phi_\alpha(\lambda,\cdot,x_0))\, d\Omega_\alpha(\lambda,x_0)\, \widehat{h}_\alpha(\lambda,x_0).
$$

Indeed, consider an arbitrary element $f = (f_0,\ f_1)^\top \in L^2(\mathbb{R};d\Omega_\alpha(\cdot,x_0))$ such that

$$
\big(f, U_\alpha(x_0)h\big)_{L^2(\mathbb{R};d\Omega_\alpha(\cdot,x_0))} = 0 \text{ for all } h \in L^2(\mathbb{R};dx). \tag{3.2.114}
$$

Then, (3.2.114) holds for $h = E_{H_\alpha}((\lambda_1,\lambda_2])g$, $\lambda_1,\lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$, $g \in C_0^\infty(\mathbb{R})$. Utilizing (3.2.109) one rewrites (3.2.114) as,

$$
0 = \big(f, U_\alpha(x_0)E_{H_\alpha}((\lambda_1,\lambda_2])g\big)_{L^2(\mathbb{R};d\Omega_\alpha(\cdot,x_0))} \tag{3.2.115}
$$

$$
= \big(f, U_\alpha(x_0)U_\alpha(x_0)^{-1}\chi_{(\lambda_1,\lambda_2]}U_\alpha(x_0)g\big)_{L^2(\mathbb{R};d\Omega_\alpha(\cdot,x_0))}
$$

$$
= \int_{(\lambda_1,\lambda_2]} \overline{f(\lambda)^\top}\, d\Omega_\alpha(\lambda,x_0) \int_{\mathbb{R}} dx\, (\theta_\alpha(\lambda,x,x_0),\phi_\alpha(\lambda,x,x_0))^\top g(x) \tag{3.2.116}
$$

$$
= \int_{\mathbb{R}} dx\, g(x) \int_{(\lambda_1,\lambda_2]} \overline{f(\lambda)^\top}\, d\Omega_\alpha(\lambda,x_0)(\theta_\alpha(\lambda,x,x_0),\phi_\alpha(\lambda,x,x_0))^\top.
$$

Since $C_0^\infty(\mathbb{R})$ is dense in $L^2(\mathbb{R};dx)$ one concludes that

$$
\int_{(\lambda_1,\lambda_2]} \overline{f(\lambda)^\top} d\Omega_\alpha(\lambda,x_0)(\theta_\alpha(\lambda,x,x_0),\phi_\alpha(\lambda,x,x_0))^\top = 0 \text{ for a.e. } x \in \mathbb{R}. \tag{3.2.117}
$$

Differentiating (3.2.117) with respect to x leads to

$$\int_{(\lambda_1,\lambda_2]} \overline{f(\lambda)^\top} d\Omega_\alpha(\lambda, x_0)(\theta'_\alpha(\lambda, x, x_0), \phi'_\alpha(\lambda, x, x_0))^\top = 0 \text{ for a.e. } x \in \mathbb{R}. \tag{3.2.118}$$

Using the dominated convergence theorem and the fact that

$$f \in L^2(\mathbb{R}; d\Omega_\alpha(\cdot, x_0)) \subseteq L^1((\lambda_1, \lambda_2]; d\Omega_\alpha(\cdot, x_0)) \tag{3.2.119}$$

and that $\theta_\alpha(\lambda, x), \theta'_\alpha(\lambda, x), \phi_\alpha(\lambda, x), \phi'_\alpha(\lambda, x)$ are continuous with respect to $(\lambda, x) \in \mathbb{R}^2$, one concludes

$$\begin{aligned}
&\int_{(\lambda_1,\lambda_2]} \overline{f(\lambda)^\top} d\Omega_\alpha(\lambda, x_0)(\theta_\alpha(\lambda, x_0, x_0), \phi_\alpha(\lambda, x_0, x_0))^\top \\
&\quad = \int_{(\lambda_1,\lambda_2]} \overline{f(\lambda)^\top} d\Omega_\alpha(\lambda, x_0)(\cos(\alpha), -\sin(\alpha))^\top = 0, \\
&\int_{(\lambda_1,\lambda_2]} \overline{f(\lambda)^\top} d\Omega_\alpha(\lambda, x_0)(\theta'_\alpha(\lambda, x_0, x_0), \phi'_\alpha(\lambda, x_0, x_0))^\top \\
&\quad = \int_{(\lambda_1,\lambda_2]} \overline{f(\lambda)^\top} d\Omega_\alpha(\lambda, x_0)(\sin(\alpha), \cos(\alpha))^\top = 0.
\end{aligned} \tag{3.2.120}$$

Since the interval $(\lambda_1, \lambda_2]$ was chosen arbitrary, (3.2.120) implies

$$f(\lambda) = 0 \;\; d\Omega_\alpha(\cdot, x_0)\text{-a.e.}, \tag{3.2.121}$$

and hence $U_\alpha(x_0)$ is onto.

We sum up these considerations in a variant of the spectral theorem for (functions of) H.

Theorem 3.2.14. *Let $F \in C(\mathbb{R})$ and $x_0 \in \mathbb{R}$. Then,*

$$U_\alpha(x_0)F(H)U_\alpha(x_0)^{-1} = M_F \tag{3.2.122}$$

in $L^2(\mathbb{R}; d\Omega_\alpha(\cdot, x_0))$ (cf. (3.2.94)). Moreover,

$$\sigma(H) = \operatorname{supp}(d\Omega_\alpha(\cdot, x_0)) = \operatorname{supp}(d\Omega^{\mathrm{tr}}_\alpha(\cdot, x_0)). \tag{3.2.123}$$

Here $d\Omega_\alpha^{\rm tr}(\cdot,x_0) = d\Omega_{\alpha,0,0}(\cdot,x_0) + d\Omega_{\alpha,1,1}(\cdot,x_0)$ *denotes the trace measure of* $d\Omega_\alpha(\cdot,x_0)$.

We conclude the case of the entire line with an elementary example.

Example 3.2.15. *Let* $\alpha = 0$, $x_0 = 0$ *and* $V(x) = 0$ *for a.e.* $x \in \mathbb{R}$. *Then,*

$$\begin{aligned}
&\phi_0(\lambda,x,0) = \frac{\sin(\lambda^{1/2}x)}{\lambda^{1/2}}, \quad \theta_0(\lambda,x,0) = \cos(\lambda^{1/2}x), \quad \lambda > 0,\ x \in \mathbb{R},\\
&m_{\pm,0}(z,0) = \pm i z^{1/2}, \quad z \in \mathbb{C}\backslash[0,\infty), \qquad\qquad (3.2.124)\\
&d\Omega_0(\lambda,0) = \frac{1}{2\pi}\chi_{(0,\infty)}(\lambda)\begin{pmatrix} \lambda^{-1/2} & 0 \\ 0 & \lambda^{1/2}\end{pmatrix} d\lambda, \quad \lambda \in \mathbb{R},
\end{aligned}$$

and hence,

$$\begin{aligned}
&\widehat h(\lambda) = \begin{pmatrix} \widehat h_0(\lambda,0) \\ \widehat h_1(\lambda,0)\end{pmatrix} = \text{l.i.m.}_{a\downarrow-\infty,b\uparrow\infty}\begin{pmatrix} \int_a^b dx\, \cos(\lambda^{1/2}x)h(x) \\ \int_a^b dx\,\lambda^{-1/2}\sin(\lambda^{1/2}x)h(x)\end{pmatrix},\\
&\qquad\qquad h \in L^2(\mathbb{R};dx),\\
&h(x) = \text{l.i.m.}_{\mu\uparrow\infty}\frac{1}{2\pi}\int_0^\mu \lambda^{1/2}d\lambda\left[\frac{\cos(\lambda^{1/2}x)}{\lambda}\widehat h_0(\lambda) + \frac{\sin(\lambda^{1/2}x)}{\lambda^{1/2}}\,\widehat h_1(\lambda)\right], \qquad (3.2.125)\\
&\qquad\qquad \widehat h \in L^2([0,\infty);d\Omega_0(\cdot,0)).
\end{aligned}$$

Introducing the change of variables

$$p = \lambda^{1/2} > 0, \quad \widehat H(p) = \begin{pmatrix} \widehat H_0(p) \\ \widehat H_1(p)\end{pmatrix} = \frac{1}{\pi^{1/2}}\begin{pmatrix} \widehat h_0(\lambda) \\ \lambda^{1/2}\widehat h_1(\lambda)\end{pmatrix}, \qquad (3.2.126)$$

the pair of equations in (3.2.125) *take on the symmetric form,*

$$\begin{aligned}
&\widehat H(p) = \text{l.i.m.}_{a\downarrow-\infty,b\uparrow\infty}\frac{1}{\pi^{1/2}}\begin{pmatrix} \int_a^b dx\, \cos(px)h(x) \\ \int_a^b dx\, \sin(px)h(x)\end{pmatrix}, \quad h \in L^2(\mathbb{R};dx),\\
&h(x) = \text{l.i.m.}_{\mu\uparrow\infty}\frac{1}{\pi^{1/2}}\int_0^\mu dp\,\big[\cos(px)\widehat H_0(p) + \sin(px)\,\widehat H_1(p)\big], \qquad (3.2.127)\\
&\qquad\qquad \widehat H_\ell \in L^2([0,\infty);dp),\ \ell = 0,1.
\end{aligned}$$

One verifies that the pair of equations in (3.2.127) *is equivalent to the usual Fourier transform*

$$\begin{aligned} \widetilde{h}(q) &= \text{l.i.m.}_{y\uparrow\infty} \frac{1}{(2\pi)^{1/2}} \int_{-y}^{y} dx\, e^{iqx} h(x), \quad h \in L^2(\mathbb{R}; dx), \\ h(x) &= \text{l.i.m.}_{\mu\uparrow\infty} \frac{1}{(2\pi)^{1/2}} \int_{-\mu}^{\mu} dq\, e^{-iqx} \widetilde{h}(q), \quad \widetilde{h} \in L^2(\mathbb{R}; dq). \end{aligned} \tag{3.2.128}$$

3.3 The Case of Strongly Singular Potentials

In this section we extend our discussion to a class of strongly singular potentials V on the half-line (a,∞) with the singularity of V being concentrated at the endpoint a. We will present and contrast two approaches to this problem: One in which the reference point x_0 coincides with the singular endpoint a leading to a (scalar) spectral function, and one in which x_0 lies in the interior of the half-line (a,∞) and hence is a regular point for the half-line Schrödinger differential expression. The latter case naturally leads to a 2×2 matrix-valued spectral function which will be shown to be essentially equivalent to the scalar spectral function obtained from the former approach. While Herglotz functions still lie at the heart of the matter of spectral functions (resp., matrices), the direct analog of half-line Weyl–Titchmarsh coefficients will cease to be Herglotz functions in the first approach where the reference point x_0 coincides with the endpoint a.

Hypothesis 3.3.1. (i) Let $a \in \mathbb{R}$ and assume that

$$V \in L^1_{\text{loc}}((a,\infty); dx), \quad V \text{ real-valued.} \tag{3.3.1}$$

(ii) Introducing the differential expression τ_+ given by

$$\tau_+ = -\frac{d^2}{dx^2} + V(x), \quad x \in (a, \infty), \tag{3.3.2}$$

we assume τ_+ to be in the limit point case at a and at $+\infty$.

(iii) Assume there exists an analytic Weyl–Titchmarsh solution $\widetilde{\phi}(z, \cdot)$ of

$$(\tau_+\psi)(z, x) = z\psi(z, x), \quad x \in (a, \infty), \tag{3.3.3}$$

for z in an open neighborhood $\mathcal{O}$ of $\mathbb{R}$ (containing $\mathbb{R}$) in the following sense:

(α) For all $x \in (a, \infty)$, $\widetilde{\phi}(z, x)$ is analytic with respect to $z \in \mathcal{O}$.

(β) $\widetilde{\phi}(z, x)$, $x \in \mathbb{R}$, is real-valued for $z \in \mathbb{R}$.

(γ) $\widetilde{\phi}(z, \cdot)$ satisfies an L^2-condition near the end point a

$$\int_a^b dx \, \big|\widetilde{\phi}(z, x)\big|^2 < \infty \ \text{ for all } b \in (a, \infty) \tag{3.3.4}$$

for all $z \in \mathbb{C}\backslash\mathbb{R}$ with $|\mathrm{Im}(z)|$ sufficiently small.

Without loss of generality we assumed in Hypothesis 3.3.1 (iii) that the analytic Weyl–Titchmarsh solution satisfies the L^2-condition near the left end point a. One can replace this by the analogous L^2-condition at ∞.

A class of examples of strongly singular potentials satisfying Hypothesis 3.3.1 will be discussed in Examples 3.3.10 and 3.3.13 at the end of this section.

While we focus on strongly singular potentials with τ_+ in the limit point case at both endpoints a and ∞, the case of strongly singular potentials with τ_+ in the limit circle case at both endpoints has been studied by Fulton [53].

Associated with the differential expression τ_+ one introduces the self-adjoint Schrödinger operator H_+ in $L^2([a,\infty);dx)$ by

$$H_+ f = \tau_+ f, \tag{3.3.5}$$
$$f \in \operatorname{dom}(H_+) = \{g \in L^2([a,\infty);dx) \,|\, g, g' \in AC_{\mathrm{loc}}((a,\infty));\ \tau_+ g \in L^2([a,\infty);dx)\}.$$

Next, we introduce the usual fundamental system of solutions $\phi(z,\cdot,x_0)$ and $\theta(z,\cdot,x_0)$, $z \in \mathbb{C}$, of (3.3.3) satisfying the initial conditions at the fixed reference point $x_0 \in (a,\infty)$,

$$\phi(z,x_0,x_0) = \theta'(z,x_0,x_0) = 0, \quad \phi'(z,x_0,x_0) = \theta(z,x_0,x_0) = 1. \tag{3.3.6}$$

Thus, for any fixed $x \in (a,\infty)$, the solutions $\phi(z,x,x_0)$ and $\theta(z,x,x_0)$ are entire with respect to z and

$$W(\theta(z,\cdot,x_0), \phi(z,\cdot,x_0))(x) = 1, \quad z \in \mathbb{C}. \tag{3.3.7}$$

We note, that Hypothesis 3.3.1 *(iii)* implies that for fixed $x \in (a,\infty)$, $\widetilde{\phi}'(z,x)$ is also analytic with respect to $z \in \mathcal{O}$. This follows from differentiating the identity

$$\widetilde{\phi}(z,x) = \widetilde{\phi}'(z,x_0)\phi(z,x,x_0) + \widetilde{\phi}(z,x_0)\theta(z,x,x_0), \quad x, x_0 \in (a,\infty) \tag{3.3.8}$$

for $z \in \mathcal{O}$.

Next, we also introduce the *Weyl–Titchmarsh solutions* $\psi_\pm(z,\cdot,x_0)$, $x_0 \in (a,\infty)$, $z \in \mathbb{C}\backslash\mathbb{R}$ of (3.3.3). Since by Hypothesis 3.3.1 *(ii)*, τ_+ is assumed to be in the limit point case at a and at ∞, the Weyl–Titchmarsh solutions are uniquely characterized (up to constant multiples) by

$$\psi_-(z,\cdot,x_0) \in L^2([a,x_0];dx), \quad \psi_+(z,\cdot,x_0) \in L^2([x_0,\infty);dx), \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{3.3.9}$$

We fix the normalization of $\psi_\pm(z,\cdot,x_0)$ by requiring $\psi_\pm(z,x_0,x_0) = 1$ and hence $\psi_\pm(z,\cdot,x_0)$ have the following structure,

$$\psi_\pm(z,x,x_0) = \theta(z,x,x_0) + m_\pm(z,x_0)\phi(z,x,x_0), \quad x,x_0 \in (a,\infty),\ z \in \mathbb{C}\backslash\mathbb{R}, \tag{3.3.10}$$

where the coefficients $m_\pm(z,x_0)$ are given by

$$m_\pm(z,x) = \frac{\psi'_\pm(z,x,x_0)}{\psi_\pm(z,x,x_0)}, \quad x,x_0 \in (a,\infty),\ z \in \mathbb{C}\backslash\mathbb{R}, \tag{3.3.11}$$

and are Herglotz and anti-Herglotz functions, respectively.

Lemma 3.3.2. *Assume Hypothesis 3.3.1 (i) and (ii). Then Hypothesis 3.3.1 (iii) is equivalent to the assumption that for any fixed $x \in (a,\infty)$, $m_-(z,x)$ is meromorphic with respect to $z \in \mathbb{C}$.*

Proof. In the following we fix $x \in (a,\infty)$. First, assume Hypothesis 3.3.1. By Hypothesis 3.3.1 (*ii*), the Weyl–Titchmarsh solutions are unique up to constant multiples and one concludes that $\psi_-(z,\cdot,x_0) = c(z,x_0)\widetilde{\phi}(z,\cdot)$. Hence by (3.3.11),

$$m_-(z,x) = \frac{\widetilde{\phi}'(z,x)}{\widetilde{\phi}(z,x)}, \quad x \in (a,\infty),\ z \in \mathbb{C}\backslash\mathbb{R}. \tag{3.3.12}$$

Since by Hypothesis 3.3.1 (*iii*), $\widetilde{\phi}(z,x)$ and $\widetilde{\phi}'(z,x)$ are analytic with respect to $z \in \mathcal{O}$ (cf. the paragraph preceding (3.3.8)), one concludes that $m_-(z,x)$ is meromorphic in $z \in \mathcal{O}$ and since m_- is analytic in $\mathbb{C}\backslash\mathbb{R}$, m_- is meromorphic on $\mathbb{C}$.

Conversely, if $m_-(z,x)$ is meromorphic with respect to $z \in \mathbb{C}$, then it has the following structure,

$$m_-(z,x) = \frac{\eta_1(z,x)}{\eta_2(z,x)}, \tag{3.3.13}$$

where $\eta_1(z,x)$ and $\eta_2(z,x)$ can be chosen to be entire such that they do not have common zeros. Moreover, since the zeros of $\eta_j(\cdot,x)$, $j=1,2$, are necessarily all real, the Weierstrass factorization theorem (cf., e.g., Corollary 2 of Theorem II.10.1 in [129, p. 284–285]) shows that $\eta_1(z,x)$ and $\eta_2(z,x)$ can be chosen to be real for $z\in\mathbb{R}$. Thus, for $x_0\in(a,\infty)$,

$$\widetilde{\phi}(z,\cdot)=\eta_2(z,x_0)\psi_-(z,\cdot,x_0)=\eta_2(z,x_0)\theta(z,\cdot,x_0)+\eta_1(z,x_0)\phi(z,\cdot,x_0) \tag{3.3.14}$$

is entire in z, and moreover, it is a Weyl–Titchmarsh solution of (3.3.3) that satisfies Hypothesis 3.3.1 (*iii*). □

Lemma 3.3.3. *Assume Hypothesis 3.3.1 (iii). Then, there is an open neighborhood $\mathcal{O}'$ of $\mathbb{R}$ (containing $\mathbb{R}$), $\mathcal{O}'\subseteq\mathcal{O}$, and a solution $\widetilde{\theta}(z,\cdot)$ of (3.3.3), which, for each $x\in(a,\infty)$, is analytic with respect to $z\in\mathcal{O}'$, real-valued for $z\in\mathbb{R}$, such that,*

$$W(\widetilde{\theta}(z,\cdot),\widetilde{\phi}(z,\cdot))(x)=1,\quad z\in\mathcal{O}'. \tag{3.3.15}$$

Proof. Let $x_0\in(a,\infty)$ and consider the following solution of (3.3.3),

$$\widetilde{\theta}(z,x)=\frac{\widetilde{\phi}'(z,x_0)}{\widetilde{\phi}(z,x_0)^2+\widetilde{\phi}'(z,x_0)^2}\theta(z,x,x_0)-\frac{\widetilde{\phi}(z,x_0)}{\widetilde{\phi}(z,x_0)^2+\widetilde{\phi}'(z,x_0)^2}\phi(z,x,x_0),$$
$$x\in(a,\infty) \tag{3.3.16}$$

for z in a sufficiently small neighborhood of $\mathbb{R}$. Since for $x,x_0\in(a,\infty)$, $\widetilde{\phi}(z,x)$, $\theta(z,x,x_0)$, and $\phi(z,x,x_0)$ are analytic with respect to $z\in\mathcal{O}$, real-valued for $z\in\mathbb{R}$, and $\widetilde{\phi}(z,x_0)$, $\widetilde{\phi}'(z,x_0)$ are not both zero for all z in a sufficiently small neighborhood of $\mathbb{R}$, $\widetilde{\theta}(z,x)$ in (3.3.16) is analytic with respect to $z\in\mathcal{O}'$, $\mathcal{O}'\subseteq\mathcal{O}$, for fixed $x\in(a,\infty)$ and real-valued for $z\in\mathbb{R}$. Moreover, $\widetilde{\theta}(z,x)$ satisfies (3.3.15) since for $z\in\mathcal{O}'$,

$$W(\widetilde{\theta}(z,\cdot),\widetilde{\phi}(z,\cdot))(x)=W(\widetilde{\theta}(z,\cdot),\widetilde{\phi}(z,\cdot))(x_0) \tag{3.3.17}$$

$$= \frac{\widetilde{\phi}'(z,x_0)}{\widetilde{\phi}(z,x_0)^2 + \widetilde{\phi}'(z,x_0)^2}\widetilde{\phi}'(z,x_0) + \frac{\widetilde{\phi}(z,x_0)}{\widetilde{\phi}(z,x_0)^2 + \widetilde{\phi}'(z,x_0)^2}\widetilde{\phi}(z,x_0) = 1. \tag{3.3.18}$$

$\square$

Having a system of two linearly independent solutions $\widetilde{\phi}(z,x)$ and $\widetilde{\theta}(z,x)$ we introduce a function $\widetilde{m}_+(z)$ such that the following solution of (3.3.3)

$$\widetilde{\psi}_+(z,x) = \widetilde{\theta}(z,x) + \widetilde{m}_+(z)\widetilde{\phi}(z,x), \quad x \in (a,\infty), \tag{3.3.19}$$

satisfies

$$\widetilde{\psi}_+(z,\cdot) \in L^2([b,\infty);dx) \text{ for all } b \in (a,\infty), \tag{3.3.20}$$

for $z \in \mathcal{O}'\backslash\mathbb{R}$. By Hypothesis 3.3.1 (ii), the solution $\widetilde{\psi}_+(z,\cdot)$ is proportional to $\psi_+(z,\cdot,x_0)$. Hence, using (3.3.11) and (3.3.12), one computes,

$$m_+(z,x) = \frac{\widetilde{\theta}'(z,x) + \widetilde{m}_+(z)\widetilde{\phi}'(z,x)}{\widetilde{\theta}(z,x) + \widetilde{m}_+(z)\widetilde{\phi}(z,x)}, \tag{3.3.21}$$

$$\widetilde{m}_+(z) = \frac{\widetilde{\theta}(z,x)m_+(z,x) - \widetilde{\theta}'(z,x)}{\widetilde{\phi}'(z,x) - \widetilde{\phi}(z,x)m_+(z,x)} = \frac{W(\widetilde{\theta}(z,\cdot),\psi_+(z,\cdot,x_0))}{W(\psi_+(z,\cdot,x_0),\widetilde{\phi}(z,\cdot))} \tag{3.3.22}$$

$$= \frac{\widetilde{\theta}(z,x)}{\widetilde{\phi}(z,x)}\frac{m_+(z,x)}{m_-(z,x) - m_+(z,x)} - \frac{\widetilde{\theta}'(z,x)}{\widetilde{\phi}(z,x)}\frac{1}{m_-(z,x) - m_+(z,x)}. \tag{3.3.23}$$

By (3.3.22), $\widetilde{m}_+$ is independent of $x \in (a,\infty)$.

Having in mind the fact that $m_\pm(\cdot,x)$ are Herglotz and anti-Herglotz functions, that $\widetilde{\phi}(z,x) \neq 0$ for $z \in \mathbb{C}\backslash\mathbb{R}$, $|\mathrm{Im}(z)|$ sufficiently small, and that $\widetilde{\theta}(z,x)$ and $\widetilde{\theta}'(z,x)$ are analytic with respect to $z \in \mathcal{O}'$, one concludes from (3.3.23) that $\widetilde{m}_+$ is analytic in $\mathcal{O}'\backslash\mathbb{R}$. In contrast to m_+, the function $\widetilde{m}_+$, in general, is not a Herglotz function. Nevertheless, $\widetilde{m}_+$ shares some properties with Herglotz functions which are crucial for the proof of our main result, Theorem 3.3.5. Before we derive these properties we mention that by using Hypothesis 3.3.1 (*iii*), (3.3.15), and (3.3.20), a computation of the Green's function $G_+(z,x,x')$ of H_+ yields

$$G_+(z,x,x') = \begin{cases} \widetilde{\phi}(z,x)\widetilde{\psi}_+(z,x'), & a < x \le x', \\ \widetilde{\phi}(z,x')\widetilde{\psi}_+(z,x), & a < x' \le x \end{cases} \tag{3.3.24}$$

and thus,

$$\begin{gathered} ((H_+ - zI)^{-1}f)(x) = \int_a^\infty dx'\, G_+(z,x,x')f(x'), \\ x \in (a,\infty), \quad f \in L^2([a,\infty);dx) \end{gathered} \tag{3.3.25}$$

for $z \in \mathcal{O}'\backslash\mathbb{R}$.

The basic properties of $\widetilde{m}_+$ then read as follows:

Lemma 3.3.4. *Assume Hypothesis 3.3.1. Then the function $\widetilde{m}_+(\cdot)$ introduced in* (3.3.19) *satisfies the following properties:*

(*i*) $\widetilde{m}_+(z) = \overline{\widetilde{m}_+(\overline{z})}, \quad z \in \mathbb{C}_+,\ |\mathrm{Im}(z)|$ *sufficiently small.*

(*ii*) $\varepsilon|\widetilde{m}_+(\lambda + i\varepsilon)| \le C(\lambda_1,\lambda_2,\varepsilon_0)$ *for* $\lambda \in [\lambda_1,\lambda_2],\ 0 < \varepsilon \le \varepsilon_0$.

(*iii*) $\varepsilon|\mathrm{Re}(\widetilde{m}_+(\lambda + i\varepsilon))| \underset{\varepsilon\to 0}{=} o(1)$ *for* $\lambda \in [\lambda_1,\lambda_2],\ 0 < \varepsilon \le \varepsilon_0$.

(*iv*) $-i\varepsilon \lim_{\varepsilon\downarrow 0} \widetilde{m}_+(\lambda + i\varepsilon) = \varepsilon \lim_{\varepsilon\downarrow 0} \mathrm{Im}(\widetilde{m}_+(\lambda + i\varepsilon))$ *exists for all* $\lambda \in \mathbb{R}$ *and is nonnegative.*

(*v*) $\widetilde{m}_+(\lambda + i0) = \lim_{\varepsilon\downarrow 0} \widetilde{m}_+(\lambda + i\varepsilon)$ *exists for a.e.* $\lambda \in [\lambda_1,\lambda_2]$ *and* $\mathrm{Im}(\widetilde{m}_+(\lambda + i0)) \ge 0$ *for a.e.* $\lambda \in [\lambda_1,\lambda_2]$.

Here $0 < \varepsilon_0 = \varepsilon(\lambda_1, \lambda_2)$ *is assumed to be sufficiently small. Moreover, one can introduce a nonnegative measure* $d\widetilde{\rho}_+$ *associated with* $\widetilde{m}_+$ *in a manner similar to the Herglotz situation* (B.4) *by*

$$\int_{(\lambda_1,\lambda_2]} d\widetilde{\rho}_+(\lambda) = \widetilde{\rho}_+((\lambda_1,\lambda_2]) = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, \mathrm{Im}(\widetilde{m}_+(\lambda+i\varepsilon)). \tag{3.3.26}$$

Proof. Since $\widetilde{\phi}(\lambda,x)$ and $\widetilde{\theta}(\lambda,x)$ are real-valued for $(\lambda,x)\in\mathbb{R}\times(a,\infty)$, and analytic for $\lambda\in\mathcal{O}'$ for fixed $x\in(a,\infty)$, an application of the Schwarz reflection principle yields

$$\widetilde{\phi}(z,x) = \overline{\widetilde{\phi}(\overline{z},x)}, \quad \widetilde{\theta}(z,x) = \overline{\widetilde{\theta}(\overline{z},x)}, \quad x\in(a,\infty),\ z\in\mathcal{O}'. \tag{3.3.27}$$

Thus, picking real numbers c and d such that $a\le c<d<\infty$, (3.3.24) and (3.3.25) imply for the analog of (3.2.20) in the present context of H_+,

$$\begin{aligned}
&\int_{\sigma(H_+)} \frac{d\big\|E_{H_+}(\lambda)\chi_{[c,d]}\big\|^2_{L^2([a,\infty);dx)}}{\lambda-z} = \big(\chi_{[c,d]},(H_+-zI)^{-1}\chi_{[c,d]}\big)_{L^2([a,\infty);dx)}\\
&\quad = \int_c^d dx\int_c^x dx'\,\widetilde{\theta}(z,x)\widetilde{\phi}(z,x') + \int_c^d dx\int_x^d dx'\,\widetilde{\phi}(z,x)\widetilde{\theta}(z,x')\\
&\qquad + \widetilde{m}_+(z)\bigg[\int_c^d dx\,\widetilde{\phi}(z,x)\bigg]^2, \quad z\in\mathbb{C}\backslash\sigma(H_+).
\end{aligned} \tag{3.3.28}$$

Choosing $c(z_0), d(z_0)\in[a,\infty)$ such that

$$\int_{c(z_0)}^{d(z_0)} dx\,\widetilde{\phi}(z,x)\neq 0 \tag{3.3.29}$$

for z in an open neighborhood $\mathcal{N}(z_0)$ of $z_0\in\mathbb{C}\backslash\sigma(H_+)$ with $\mathrm{Im}(z_0)$ sufficiently small (cf. the proof of Lemma 3.2.3), items (i)–(v) follow from (3.3.27) and (3.3.28) since the left-hand side in (3.3.28),

$$\int_{\sigma(H_+)} \frac{d\big\|E_{H_+}(\lambda)\chi_{[c,d]}\big\|^2_{L^2([a,\infty);dx)}}{\lambda-z}, \quad z\in\mathbb{C}\backslash\sigma(H_+), \tag{3.3.30}$$

is a Herglotz function and $\widetilde{\phi}(z,x)$, $\widetilde{\theta}(z,x)$ are analytic with respect to $z \in \mathcal{O}'$, where $\mathcal{O}' \subseteq \mathcal{O}$ is an open neighborhood of $\mathbb{R}$. In addition, $\widetilde{\phi}(z,x)$ and $\widetilde{\theta}(z,x)$ are real-valued for $(z,x) \in \mathbb{R} \times (a,\infty)$. Next, we pick $\lambda_1, \lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$, such that for some $c_0, d_0 \in [a,\infty)$,

$$\int_{c_0}^{d_0} dx\, \widetilde{\phi}(z,x) \neq 0 \tag{3.3.31}$$

for all z in a complex neighborhood of the interval (λ_1, λ_2). Then (3.3.28) applied to $z = \lambda + i\varepsilon$, for real-valued λ in a neighborhood of (λ_1, λ_2), $0 < \varepsilon \leq \varepsilon_0$, implies that $\widetilde{\rho}_+$ defined in (3.3.26) satisfies

$$\begin{aligned}
\widetilde{\rho}_+((\lambda_1,\lambda_2]) &= \lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, \operatorname{Im}(\widetilde{m}_+(\lambda + i\varepsilon)) \\
&= \lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, \operatorname{Im}\bigg\{ \int_{\sigma(H_+)} \frac{d\big\|E_{H_+}(\lambda')\chi_{[c_0,d_0]}\big\|^2_{L^2([a,\infty);dx)}}{\lambda' - \lambda - i\varepsilon} \\
&\quad \times \bigg[\bigg(\int_{c_0}^{d_0} dx\, \widetilde{\phi}(\lambda,x)\bigg)^2 + 2i\varepsilon\bigg(\int_{c_0}^{d_0} dx\, (d/dz)\widetilde{\phi}(z,x)|_{z=\lambda}\bigg) + O(\varepsilon^2)\bigg]^{-1} \\
&\quad + O(\varepsilon)\bigg\} \\
&= \int_{(\lambda_1,\lambda_2]} d\big\|E_{H_+}(\lambda)\chi_{[c_0,d_0]}\big\|^2_{L^2([a,\infty);dx)} \bigg[\int_{c_0}^{d_0} dx\, \widetilde{\phi}(\lambda,x)\bigg]^{-2},
\end{aligned} \tag{3.3.32}$$

using item (ii), item (iii), the dominated convergence theorem, and the analog of (3.2.50) applied to the present context. Hence, $\widetilde{\rho}_+$ generates the nonnegative measure $d\widetilde{\rho}_+$. $\square$

Next, we relate the family of spectral projections, $\{E_{H_+}(\lambda)\}_{\lambda \in \mathbb{R}}$, of the self-adjoint operator H_+ and the spectral function $\widetilde{\rho}_+(\lambda)$, $\lambda \in \mathbb{R}$, defined in (3.3.26).

We first note that for $F \in C(\mathbb{R})$,

$$\big(f, F(H_+)g\big)_{L^2([a,\infty);dx)} = \int_{\mathbb{R}} d\big(f, E_{H_+}(\lambda)g\big)_{L^2([a,\infty);dx)}\, F(\lambda), \tag{3.3.33}$$

$$
\begin{aligned}
&f, g \in \operatorname{dom}(F(H_+)) \\
&\quad = \left\{ h \in L^2([a,\infty); dx) \,\middle|\, \int_{\mathbb{R}} d\big\|E_{H_+}(\lambda)h\big\|^2_{L^2([a,\infty);dx)} \, |F(\lambda)|^2 < \infty \right\}.
\end{aligned}
$$

Theorem 3.3.5. *Let $f, g \in C_0^\infty((a,\infty))$, $F \in C(\mathbb{R})$, and $\lambda_1, \lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$. Then,*

$$
\big(f, F(H_+)E_{H_+}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)} = \big(\widehat{f}_+, M_F M_{\chi_{(\lambda_1,\lambda_2]}} \widehat{g}_+\big)_{L^2(\mathbb{R};d\widetilde{\rho}_+)}, \tag{3.3.34}
$$

where we introduced the notation

$$
\widehat{h}_+(\lambda) = \int_a^\infty dx\, \widetilde{\phi}(\lambda,x)h(x), \quad \lambda \in \mathbb{R},\ h \in C_0^\infty((a,\infty)), \tag{3.3.35}
$$

and M_G denotes again the maximally defined operator of multiplication by the $d\widetilde{\rho}_+$-measurable function G in the Hilbert space $L^2(\mathbb{R}; d\widetilde{\rho}_+)$,

$$
\begin{aligned}
&(M_G\widehat{h})(\lambda) = G(\lambda)\widehat{h}(\lambda) \ \text{ for a.e. } \lambda \in \mathbb{R}, \\
&\widehat{h} \in \operatorname{dom}(M_G) = \big\{\widehat{k} \in L^2(\mathbb{R}; d\widetilde{\rho}_+) \,\big|\, G\widehat{k} \in L^2(\mathbb{R}; d\widetilde{\rho}_+)\big\}.
\end{aligned} \tag{3.3.36}
$$

Proof. The point of departure for deriving (3.3.34) is again Stone's formula (3.2.29) applied to $T = H_+$,

$$
\begin{aligned}
&\big(f, F(H_+)E_{H_+}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)} \\
&\quad = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0} \frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, F(\lambda)\big[\big(f, (H_+ - (\lambda+i\varepsilon)I)^{-1}g\big)_{L^2([a,\infty);dx)} \\
&\qquad\qquad - \big(f, (H_+ - (\lambda-i\varepsilon)I)^{-1}g\big)_{L^2([a,\infty);dx)}\big].
\end{aligned} \tag{3.3.37}
$$

Insertion of (3.3.24) and (3.3.25) into (3.3.37) then yields the following:

$$
\begin{aligned}
\big(f, F(H_+)E_{H_+}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)} &= \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0} \frac{1}{2\pi i}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, F(\lambda) \\
\times \bigg\{ \int_a^\infty dx \bigg[&\overline{f(x)}\widetilde{\psi}_+(\lambda+i\varepsilon,x)\int_a^x dx'\,\widetilde{\phi}(\lambda+i\varepsilon,x')g(x') \\
&+ \overline{f(x)}\widetilde{\phi}(\lambda+i\varepsilon,x)\int_x^\infty dx'\,\widetilde{\psi}_+(\lambda+i\varepsilon,x')g(x')\bigg]
\end{aligned}
$$

$$
\begin{aligned}
&- \bigg[\overline{f(x)}\widetilde{\psi}_+(\lambda - i\varepsilon, x) \int_a^x dx' \, \widetilde{\phi}(\lambda - i\varepsilon, x') g(x') \\
&\quad + \overline{f(x)}\widetilde{\phi}(\lambda - i\varepsilon, x) \int_x^\infty dx' \, \widetilde{\psi}_+(\lambda - i\varepsilon, x') g(x')\bigg]\bigg\}.
\end{aligned} \tag{3.3.38}
$$

Freely interchanging the dx and dx' integrals with the limits and the $d\lambda$ integral (since all integration domains are finite and all integrands are continuous), and inserting expression (3.3.19) for $\widetilde{\psi}_+(z, x)$ into (3.3.38), one obtains

$$
\begin{aligned}
&\big(f, F(H_+)E_{H_+}((\lambda_1, \lambda_2])g\big)_{L^2([a,\infty);dx)} = \int_a^\infty dx \, \overline{f(x)} \bigg\{ \int_a^x dx' \, g(x') \\
&\quad \times \lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} \frac{1}{2\pi i} \int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda \, F(\lambda) \Big[\big[\widetilde{\theta}(\lambda, x) + \widetilde{m}_+(\lambda + i\varepsilon)\widetilde{\phi}(\lambda, x)\big]\widetilde{\phi}(\lambda, x') \\
&\qquad - \big[\widetilde{\theta}(\lambda, x) + \widetilde{m}_+(\lambda - i\varepsilon)\widetilde{\phi}(\lambda, x)\big]\widetilde{\phi}(\lambda, x')\Big] \\
&\quad + \int_x^\infty dx' \, g(x') \lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} \frac{1}{2\pi i} \int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda \, F(\lambda) \\
&\qquad \times \Big[\widetilde{\phi}(\lambda, x)\big[\widetilde{\theta}(\lambda, x') + \widetilde{m}_+(\lambda + i\varepsilon)\widetilde{\phi}(\lambda, x')\big] \\
&\qquad - \widetilde{\phi}(\lambda, x)\big[\widetilde{\theta}(\lambda, x') + \widetilde{m}_+(\lambda - i\varepsilon)\widetilde{\phi}(\lambda, x')\big]\Big]\bigg\}.
\end{aligned} \tag{3.3.39}
$$

Here we employed the fact that for fixed $x \in (a, \infty)$, $\widetilde{\phi}(z, x)$, $\widetilde{\theta}(z, x)$ are analytic with respect to $z \in \mathcal{O}$ and real-valued for $z \in \mathbb{R}$, the fact that $\widetilde{\phi}(z, \cdot), \widetilde{\theta}(z, \cdot) \in AC_{\text{loc}}((a, \infty))$, and hence that

$$
\begin{aligned}
\widetilde{\phi}(\lambda \pm i\varepsilon, x) &\underset{\varepsilon \downarrow 0}{=} \widetilde{\phi}(\lambda, x) \pm i\varepsilon (d/dz)\widetilde{\phi}(z, x)|_{z=\lambda} + O(\varepsilon^2), \\
\widetilde{\theta}(\lambda \pm i\varepsilon, x) &\underset{\varepsilon \downarrow 0}{=} \widetilde{\theta}(\lambda, x) \pm i\varepsilon (d/dz)\widetilde{\theta}(z, x)|_{z=\lambda} + O(\varepsilon^2),
\end{aligned} \tag{3.3.40}
$$

with $O(\varepsilon^2)$ being uniform with respect to (λ, x) as long as λ and x vary in compact subsets of $\mathbb{R} \times (a, \infty)$. (Here real-valuedness of $\widetilde{\phi}(z, x)$ and $\widetilde{\theta}(z, x)$ for $z \in \mathbb{R}$, $x \in (a, \infty)$ yields a purely imaginary $O(\varepsilon)$-term in (3.3.40).) Moreover, we used items *(ii)* and *(iii)* of Lemma 3.3.4 to replace $\widetilde{\phi}(\lambda \pm i\varepsilon, x)$ and $\widetilde{\theta}(\lambda \pm i\varepsilon, x)$ by $\widetilde{\phi}(\lambda, x)$ and $\widetilde{\theta}(\lambda, x)$ under the $d\lambda$ integrals in (3.3.39). Cancelling appropriate terms in (3.3.39), simplifying the remaining terms, and using item (i) of Lemma 3.3.4 then yield

$$\begin{aligned}\big(f, F(H_+)E_{H_+}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)} &= \int_a^\infty dx\,\overline{f(x)}\int_a^\infty dx'\,g(x')\\ \times \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, F(\lambda)\widetilde{\phi}(\lambda,x)\widetilde{\phi}(\lambda,x')\mathrm{Im}(\widetilde{m}_+(\lambda+i\varepsilon)).\end{aligned} \tag{3.3.41}$$

Using (3.3.26),

$$\int_{\mathbb{R}} d\widetilde{\rho}_+(\lambda)\,h(\lambda) = \lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\mathbb{R}} d\lambda\,\mathrm{Im}(\widetilde{m}_+(\lambda+i\varepsilon))\,h(\lambda), \quad h\in C_0(\mathbb{R}), \tag{3.3.42}$$

$$\int_{(\lambda_1,\lambda_2]} d\widetilde{\rho}_+(\lambda)\,k(\lambda) = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\,\mathrm{Im}(\widetilde{m}_+(\lambda+i\varepsilon))\,k(\lambda), \quad k\in C(\mathbb{R}), \tag{3.3.43}$$

and hence

$$\begin{aligned}&\big(f, F(H_+)E_{H_+}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)}\\ &\quad= \int_a^\infty dx\,\overline{f(x)}\int_a^\infty dx'\,g(x')\int_{(\lambda_1,\lambda_2]} d\widetilde{\rho}_+(\lambda)F(\lambda)\widetilde{\phi}(\lambda,x)\widetilde{\phi}(\lambda,x')\\ &\quad= \int_{(\lambda_1,\lambda_2]} d\widetilde{\rho}_+(\lambda)F(\lambda)\,\overline{\widehat{f}_+(\lambda)}\,\widehat{g}_+(\lambda),\end{aligned} \tag{3.3.44}$$

using (3.3.35) and interchanging the dx, dx' and $d\widetilde{\rho}_+$ integrals once more. □

Again one can improve on Theorem 3.3.5 and remove the compact support restrictions on f and g in the usual way. To this end we consider the map

$$\widetilde{U}_+ \colon \begin{cases} C_0^\infty((a,\infty)) \to L^2(\mathbb{R}; d\widetilde{\rho}_+) \\ \qquad h \mapsto \widehat{h}_+(\cdot) = \int_a^\infty dx\,\widetilde{\phi}(\cdot,x)h(x). \end{cases} \tag{3.3.45}$$

Taking $f=g$, $F=1$, $\lambda_1\downarrow -\infty$, and $\lambda_2\uparrow\infty$ in (3.3.34) then shows that $\widetilde{U}_+$ is a densely defined isometry in $L^2([a,\infty);dx)$, which extends by continuity to an isometry on $L^2([a,\infty);dx)$. The latter is denoted by U_+ and given by

$$U_+ \colon \begin{cases} L^2([a,\infty);dx) \to L^2(\mathbb{R}; d\widetilde{\rho}_+) \\ \qquad h \mapsto \widehat{h}_+(\cdot) = \mathrm{l.i.m.}_{b\uparrow\infty}\int_a^b dx\,\widetilde{\phi}(\cdot,x)h(x), \end{cases} \tag{3.3.46}$$

where l.i.m. refers to the $L^2(\mathbb{R}; d\widetilde{\rho}_+)$-limit.

The calculation in (3.3.44) also yields

$$(E_{H_+}((\lambda_1, \lambda_2])g)(\cdot) = \int_{(\lambda_1,\lambda_2]} d\widetilde{\rho}_+(\lambda)\, \widetilde{\phi}(\lambda, \cdot)\widehat{g}_+(\lambda), \quad g \in C_0^\infty((a, \infty)) \tag{3.3.47}$$

and subsequently, (3.3.47) extends to all $g \in L^2([a, \infty); dx)$ by continuity. Moreover, taking $\lambda_1 \downarrow -\infty$ and $\lambda_2 \uparrow \infty$ in (3.3.47) and using

$$\text{s-lim}_{\lambda\downarrow-\infty} E_{H_+}(\lambda) = 0, \quad \text{s-lim}_{\lambda\uparrow\infty} E_{H_+}(\lambda) = I_{L^2([a,\infty);dx)}, \tag{3.3.48}$$

where

$$E_{H_+}(\lambda) = E_{H_+}((-\infty, \lambda]), \tag{3.3.49}$$

then yield

$$g(\cdot) = \text{l.i.m.}_{\mu_1\downarrow-\infty,\mu_2\uparrow\infty} \int_{\mu_1}^{\mu_2} d\widetilde{\rho}_+(\lambda)\, \widetilde{\phi}(\lambda, \cdot)\widehat{g}_+(\lambda), \quad g \in L^2([a, \infty); dx), \tag{3.3.50}$$

where l.i.m. refers to the $L^2([a, \infty); dx)$-limit.

In addition, one can show that the map U_+ in (3.3.46) is onto and hence that U_+ is unitary (i.e., U_+ and U_+^{-1} are isometric isomorphisms between $L^2([a, \infty); dx)$ and $L^2(\mathbb{R}; d\widetilde{\rho}_+)$) with

$$U_+^{-1} \colon \begin{cases} L^2(\mathbb{R}; d\widetilde{\rho}_+) \to L^2([a, \infty); dx) \\ \qquad\qquad \widehat{h} \mapsto \text{l.i.m.}_{\mu_1\downarrow-\infty,\mu_2\uparrow\infty} \int_{\mu_1}^{\mu_2} d\widetilde{\rho}_+(\lambda)\, \widetilde{\phi}(\lambda, \cdot)\widehat{h}(\lambda). \end{cases} \tag{3.3.51}$$

Indeed, consider an arbitrary function $f \in L^2(\mathbb{R}; d\widetilde{\rho}_+)$ such that

$$\big(f, U_+h\big)_{L^2(\mathbb{R};d\rho_{+,\alpha})} = 0 \text{ for all } h \in L^2([a, \infty); dx). \tag{3.3.52}$$

Then, (3.3.52) holds for $h = E_{H_+}((\lambda_1, \lambda_2])g$, $\lambda_1, \lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$, $g \in C_0^\infty((a, \infty))$. Utilizing (3.3.47) one rewrites (3.3.52) as,

$$0 = \big(f, U_+E_{H_+}((\lambda_1, \lambda_2])g\big)_{L^2(\mathbb{R};d\widetilde{\rho}_+)} = \big(f, U_+U_+^{-1}\chi_{(\lambda_1,\lambda_2]}U_+g\big)_{L^2(\mathbb{R};d\widetilde{\rho}_+)}$$

$$= \int_{(\lambda_1,\lambda_2]} d\widetilde{\rho}_+(\lambda)\, \overline{f(\lambda)} \int_{(a,\infty)} dx\, \widetilde{\phi}(\lambda,x) g(x) \tag{3.3.53}$$
$$= \int_{(a,\infty)} dx\, g(x) \int_{(\lambda_1,\lambda_2]} d\widetilde{\rho}_+(\lambda)\, \widetilde{\phi}(\lambda,x)\overline{f(\lambda)}.$$

Since $C_0^\infty((a,\infty))$ is dense in $L^2([a,\infty);dx)$ one concludes that

$$\int_{(\lambda_1,\lambda_2]} d\widetilde{\rho}_+(\lambda)\, \widetilde{\phi}(\lambda,x)\overline{f(\lambda)} = 0 \text{ for a.e. } x \in (a,\infty). \tag{3.3.54}$$

Differentiating (3.3.54) with respect to x leads to

$$\int_{(\lambda_1,\lambda_2]} d\widetilde{\rho}_+(\lambda)\, \widetilde{\phi}'(\lambda,x)\overline{f(\lambda)} = 0 \text{ for a.e. } x \in (a,\infty). \tag{3.3.55}$$

Using the dominated convergence theorem and the fact that $f \in L^2(\mathbb{R};d\widetilde{\rho}_+) \subseteq L^1((\lambda_1,\lambda_2];d\widetilde{\rho}_+)$ and that $\widetilde{\phi}(\lambda,x), \widetilde{\phi}'(\lambda,x)$ are continuous in $(\lambda,x) \in \mathbb{R}\times(a,\infty)$, one obtains (3.3.54) and (3.3.55) for all $x \in (a,\infty)$, in particular, for some fixed $x_0 \in (a,\infty)$. Since the interval $(\lambda_1,\lambda_2]$ was chosen arbitrary (3.3.54) and (3.3.55) imply

$$\widetilde{\phi}(\lambda,x_0)\overline{f(\lambda)} = \widetilde{\phi}'(\lambda,x_0)\overline{f(\lambda)} = 0 \;\; d\widetilde{\rho}_+\text{-a.e.} \tag{3.3.56}$$

Finally, the fact that $\widetilde{\phi}(\lambda,x_0)$ and $\widetilde{\phi}'(\lambda,x_0)$ are not both zero for $\lambda \in \mathbb{R}$ implies

$$f(\lambda) = 0 \;\; d\widetilde{\rho}_+\text{-a.e.}, \tag{3.3.57}$$

and hence U_+ is onto.

We sum up these considerations in a variant of the spectral theorem for (functions of) H_+.

Theorem 3.3.6. *Let $F \in C(\mathbb{R})$, Then,*

$$U_+ F(H_+) U_+^{-1} = M_F \tag{3.3.58}$$

in $L^2(\mathbb{R}; d\widetilde{\rho}_+)$ *(cf.* (3.3.36)*). Moreover,*

$$\sigma(F(H_+)) = \text{ess.ran}_{d\widetilde{\rho}_+}(F), \tag{3.3.59}$$

$$\sigma(H_+) = \text{supp}\,(d\widetilde{\rho}_+), \tag{3.3.60}$$

and the spectrum of H_+ *is simple.*

Simplicity of the spectrum of H_+ is consistent with the observation that

$$\begin{aligned}
&\det\left(\mathrm{Im}(M(\lambda+i0,x_0))\right) \\
&\quad = \det\left(\begin{pmatrix} \frac{\mathrm{Im}(m_+(\lambda+i0,x_0))}{|m_-(\lambda+i0,x_0)-m_+(\lambda+i0,x_0)|^2} & \frac{m_-(\lambda+i0,x_0)\mathrm{Im}(m_+(\lambda+i0,x_0))}{|m_-(\lambda+i0,x_0)-m_+(\lambda+i0,x_0)|^2} \\ \frac{m_-(\lambda+i0,x_0)\mathrm{Im}(m_+(\lambda+i0,x_0))}{|m_-(\lambda+i0,x_0)-m_+(\lambda+i0,x_0)|^2} & \frac{|m_-(\lambda+i0,x_0)|^2\mathrm{Im}(m_+(\lambda+i0,x_0))}{|m_-(\lambda+i0,x_0)-m_+(\lambda+i0,x_0)|^2} \end{pmatrix}\right) \\
&\quad = 0 \ \text{ for a.e. } \lambda \in \mathbb{R}
\end{aligned} \tag{3.3.61}$$

since by Lemma 3.3.2, $m_-(z,x_0)$ is meromorphic and real-valued for $z \in \mathbb{R}$. In this context we also refer to [84], [85], [105], [106], where necessary and sufficient conditions for simplicity of the spectrum in terms of properties of $m_\pm(\cdot,x_0)$ can be found.

Next, we consider the alternative way of deriving the (matrix-valued) spectral function corresponding to a reference point $x_0 \in (a,\infty)$ and subsequently compare the two approaches.

As in the half-line context in Section 3.2 we introduce the usual fundamental system of solutions $\phi(z,\cdot,x_0)$ and $\theta(z,\cdot,x_0)$, $z \in \mathbb{C}$, of

$$(\tau_+\psi)(z,x) = z\psi(z,x), \quad x \in (a,\infty) \tag{3.3.62}$$

with respect to a fixed reference point $x_0 \in (a,\infty)$, satisfying the initial conditions at the point $x = x_0$,

$$\phi(z,x_0,x_0) = \theta'(z,x_0,x_0) = 0, \quad \phi'(z,x_0,x_0) = \theta(z,x_0,x_0) = 1. \tag{3.3.63}$$

Again we note that for any fixed $x, x_0 \in (a, \infty)$, $\phi(z, x, x_0)$ and $\theta(z, x, x_0)$ are entire with respect to z and that

$$W(\theta(z, \cdot, x_0), \phi(z, \cdot, x_0))(x) = 1, \quad z \in \mathbb{C}. \tag{3.3.64}$$

The *Weyl–Titchmarsh solutions* $\psi_{\pm,\alpha}(z, \cdot, x_0)$, $z \in \mathbb{C}\backslash\mathbb{R}$, of (3.3.62) are uniquely characterized by

$$\begin{aligned}
&\psi_-(z, \cdot, x_0) \in L^2([a, x_0]; dx),\ \psi_+(z, \cdot, x_0) \in L^2([x_0, \infty); dx),\ z \in \mathbb{C}\backslash\mathbb{R}, \\
&\psi_\pm(z, x_0, x_0) = 1.
\end{aligned} \tag{3.3.65}$$

The normalization in (3.3.65) shows that $\psi_\pm(z, \cdot, x_0)$ are of the type

$$\psi_\pm(z, x, x_0) = \theta(z, x, x_0) + m_\pm(z, x_0)\phi(z, x, x_0), \quad z \in \mathbb{C}\backslash\mathbb{R},\ x \in \mathbb{R} \tag{3.3.66}$$

for some coefficients $m_\pm(z, x_0)$, the half-line *Weyl–Titchmarsh m-functions* associated with τ_+ and x_0. Again we recall the fundamental identity

$$\int_a^{x_0} dx\, \psi_-(z_1, x, x_0)\psi_-(z_2, x, x_0) = -\frac{m_-(z_1, x_0) - m_-(z_2, x_0)}{z_1 - z_2}, \tag{3.3.67}$$

$$\int_{x_0}^{\infty} dx\, \psi_+(z_1, x, x_0)\psi_+(z_2, x, x_0) = \frac{m_+(z_1, x_0) - m_+(z_2, x_0)}{z_1 - z_2}, \tag{3.3.68}$$

$$z_1, z_2 \in \mathbb{C}\backslash\mathbb{R},\ z_1 \neq z_2,$$

and as before one concludes

$$\overline{m_\pm(z, x_0)} = m_\pm(\overline{z}, x_0), \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{3.3.69}$$

Choosing $z_1 = z$, $z_2 = \overline{z}$ in (3.3.67), (3.3.68) one infers

$$\begin{aligned}
\int_a^{x_0} dx\, |\psi_-(z, x, x_0)|^2 &= -\frac{\operatorname{Im}(m_-(z, x_0))}{\operatorname{Im}(z)}, \\
\int_{x_0}^{\infty} dx\, |\psi_+(z, x, x_0)|^2 &= \frac{\operatorname{Im}(m_+(z, x_0))}{\operatorname{Im}(z)}, \quad z \in \mathbb{C}\backslash\mathbb{R}.
\end{aligned} \tag{3.3.70}$$

Since $m_\pm(\cdot, x_0)$ are analytic on $\mathbb{C}\backslash\mathbb{R}$, $\pm m_\pm(\cdot, x_0)$ are Herglotz functions.

The Green's function $G_+(z, x, x')$ of H_+ then admits the alternative representation (cf. also (3.3.24), (3.3.25))

$$G_+(z,x,x') = \frac{1}{W(\psi_+(z,\cdot,x_0),\psi_-(z,\cdot,x_0))}\begin{cases}\psi_-(z,x,x_0)\psi_+(z,x',x_0), & x \le x',\\ \psi_-(z,x',x_0)\psi_+(z,x,x_0), & x' \le x,\end{cases}$$
$$z \in \mathbb{C}\backslash\mathbb{R} \qquad (3.3.71)$$

with

$$W(\psi_+(z,\cdot,x_0),\psi_-(z,\cdot,x_0)) = m_-(z,x_0) - m_+(z,x_0), \quad z \in \mathbb{C}\backslash\mathbb{R}. \qquad (3.3.72)$$

Thus,

$$\begin{gathered}((H_+ - zI)^{-1}f)(x) = \int_a^\infty dx'\, G_+(z,x,x')f(x'),\\ z \in \mathbb{C}\backslash\mathbb{R},\ x \in [a,\infty),\ f \in L^2([a,\infty);dx).\end{gathered} \qquad (3.3.73)$$

Given $m_\pm(z, x_0)$, we also introduce the 2×2 matrix-valued Weyl–Titchmarsh function

$$M(z,x_0) = \begin{pmatrix} \frac{1}{m_-(z,x_0)-m_+(z,x_0)} & \frac{1}{2}\frac{m_-(z,x_0)+m_+(z,x_0)}{m_-(z,x_0)-m_+(z,x_0)} \\ \frac{1}{2}\frac{m_-(z,x_0)+m_+(z,x_0)}{m_-(z,x_0)-m_+(z,x_0)} & \frac{m_-(z,x_0)m_+(z,x_0)}{m_-(z,x_0)-m_+(z,x_0)} \end{pmatrix}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \qquad (3.3.74)$$

$M(z, x_0)$ is a Herglotz matrix with representation

$$\begin{aligned} &M(z,x_0) = C(x_0) + \int_{\mathbb{R}} d\Omega(\lambda,x_0)\left[\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\right], \quad z \in \mathbb{C}\backslash\mathbb{R},\\ &C(x_0) = C(x_0)^*, \quad \int_{\mathbb{R}} \frac{\|d\Omega(\lambda,x_0)\|}{1+\lambda^2} < \infty, \end{aligned} \qquad (3.3.75)$$

where

$$\Omega((\lambda_1,\lambda_2],x_0) = \frac{1}{\pi}\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, \mathrm{Im}(M(\lambda+i\varepsilon,x_0)), \quad \lambda_1,\lambda_2 \in \mathbb{R},\ \lambda_1 < \lambda_2. \qquad (3.3.76)$$

Again one can of course replace $z \in \mathbb{C}\backslash\mathbb{R}$ by $z \in \mathbb{C}\backslash\sigma(H_+)$ in formulas (3.3.65)–(3.3.75).

Next, we relate once more the family of spectral projections, $\{E_{H_+}(\lambda)\}_{\lambda\in\mathbb{R}}$, of the self-adjoint operator H_+ and the 2×2 matrix-valued nondecreasing spectral function $\Omega(\lambda, x_0)$, $\lambda \in \mathbb{R}$, which generates the matrix-valued measure in the Herglotz representation (3.3.75) of $M(z, x_0)$.

Theorem 3.3.7. *Let $f, g \in C_0^\infty((a,\infty))$, $F \in C(\mathbb{R})$, $x_0 \in (a,\infty)$, and $\lambda_1, \lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$. Then,*

$$\begin{aligned}
&\big(f, F(H_+)E_{H_+}((\lambda_1,\lambda_2])g\big)_{L^2([a,\infty);dx)} = \big(\widehat{f}(\cdot,x_0), M_F M_{\chi_{(\lambda_1,\lambda_2]}}\widehat{g}(\cdot,x_0)\big)_{L^2(\mathbb{R};d\Omega(\cdot,x_0))} \\
&\quad = \int_{(\lambda_1,\lambda_2]} \overline{\widehat{f}(\lambda,x_0)^\top}\, d\Omega(\lambda,x_0)\, \widehat{g}(\lambda,x_0) F(\lambda),
\end{aligned} \tag{3.3.77}$$

where we introduced the notation

$$\begin{aligned}
&\widehat{h}_0(\lambda,x_0) = \int_a^\infty dx\, \theta(\lambda,x,x_0)h(x), \quad \widehat{h}_1(\lambda,x_0) = \int_a^\infty dx\, \phi(\lambda,x,x_0)h(x), \\
&\widehat{h}(\lambda,x_0) = (\widehat{h}_0(\lambda,x_0), \widehat{h}_1(\lambda,x_0))^\top, \quad \lambda\in\mathbb{R},\ h \in C_0^\infty((a,\infty)),
\end{aligned} \tag{3.3.78}$$

and M_G denotes the maximally defined operator of multiplication by the $d\Omega^{\rm tr}(\cdot,x_0)$-measurable function G in the Hilbert space $L^2(\mathbb{R}; d\Omega(\cdot,x_0))$,

$$\begin{aligned}
&(M_G\widehat{h})(\lambda) = G(\lambda)\widehat{h}(\lambda) = \big(G(\lambda)\widehat{h}_0(\lambda), G(\lambda)\widehat{h}_1(\lambda)\big)^\top \text{ for a.e. } \lambda\in\mathbb{R}, \\
&\widehat{h} \in \operatorname{dom}(M_G) = \big\{\widehat{k} \in L^2(\mathbb{R}; d\Omega(\cdot,x_0)) \,\big|\, G\widehat{k} \in L^2(\mathbb{R}; d\Omega(\cdot,x_0))\big\}.
\end{aligned} \tag{3.3.79}$$

We omit the proof of Theorem 3.3.7 since it parallels that of Theorem 3.2.12.

Repeating the proof of Theorem 3.2.14 one also obtains the following result.

Theorem 3.3.8. *Let $F \in C(\mathbb{R})$, $x_0 \in (a,\infty)$,*

$$U(x_0)\colon \begin{cases} L^2([a,\infty);dx) \to L^2(\mathbb{R}; d\Omega(\cdot,x_0)) \\ \qquad\qquad h \mapsto \widehat{h}(\cdot,x_0) = \big(\widehat{h}_0(\cdot,x_0), \widehat{h}_1(\cdot,x_0)\big)^\top, \end{cases} \tag{3.3.80}$$

$$\widehat{h}(\cdot, x_0) = \begin{pmatrix} \widehat{h}_0(\cdot, x_0) \\ \widehat{h}_1(\cdot, x_0) \end{pmatrix} = \text{l.i.m.}_{b\downarrow a, c\uparrow\infty} \begin{pmatrix} \int_b^c dx\, \theta(\cdot, x, x_0) h(x) \\ \int_b^c dx\, \phi(\cdot, x, x_0) h(x) \end{pmatrix},$$

where l.i.m. *refers to the* $L^2(\mathbb{R}; d\Omega(\cdot, x_0))$*-limit and*

$$U(x_0)^{-1} \colon \begin{cases} L^2(\mathbb{R}; d\Omega(\cdot, x_0)) \to L^2([a,\infty); dx) \\ \qquad\qquad \widehat{h} \mapsto h, \end{cases} \tag{3.3.81}$$

$$h(\cdot) = \text{l.i.m.}_{\mu_1\downarrow -\infty, \mu_2\uparrow\infty} \int_{\mu_1}^{\mu_2} (\theta(\lambda, \cdot, x_0), \phi(\lambda, \cdot, x_0))\, d\Omega(\lambda, x_0)\, \widehat{h}(\lambda, x_0),$$

where l.i.m. *refers to the* $L^2([a,\infty); dx)$*-limit. Then,*

$$U(x_0) F(H_+) U(x_0)^{-1} = M_F \tag{3.3.82}$$

in $L^2(\mathbb{R}; d\Omega(\cdot, x_0))$ (*cf.* (3.3.79)). *Moreover,*

$$\sigma(H_+) = \operatorname{supp}(d\Omega(\cdot, x_0)) = \operatorname{supp}(d\Omega^{\text{tr}}(\cdot, x_0)). \tag{3.3.83}$$

Corollary 3.3.9. *The expansions in* (3.3.35) *and* (3.3.80) *are related by,*

$$\widehat{h}_+(\lambda) = \widetilde{\phi}(\lambda, x_0) \widehat{h}_0(\lambda, x_0) + \widetilde{\phi}'(\lambda, x_0) \widehat{h}_1(\lambda, x_0), \quad \lambda \in \sigma(H_+). \tag{3.3.84}$$

The measures $d\widetilde{\rho}_+$ *and* $d\Omega(\cdot, x_0)$ *are related by,*

$$d\widetilde{\rho}_+(\lambda) = \frac{\widetilde{\theta}(\lambda, x_0)}{\widetilde{\phi}(\lambda, x_0)} d\Omega_{0,1}(\lambda, x_0) - \frac{\widetilde{\theta}'(\lambda, x_0)}{\widetilde{\phi}(\lambda, x_0)} d\Omega_{0,0}(\lambda, x_0) \tag{3.3.85}$$

$$= \frac{\widetilde{\phi}'(\lambda, x_0)}{\widetilde{\phi}(\lambda, x_0)} \frac{1}{\widetilde{\phi}(\lambda, x_0)^2 + \widetilde{\phi}'(\lambda, x_0)^2} d\Omega_{0,1}(\lambda, x_0) + \frac{1}{\widetilde{\phi}(\lambda, x_0)^2 + \widetilde{\phi}'(\lambda, x_0)^2} d\Omega_{0,0}(\lambda, x_0), \quad \lambda \in \sigma(H_+). \tag{3.3.86}$$

Proof. (3.3.84) follows from (3.3.8), (3.3.35), and (3.3.78). (3.3.85) and (3.3.86) follow from (3.3.6), (3.3.16), (3.3.23), (3.3.26), (3.3.74), and (3.3.76). □

Finally, we illustrate the applicability of our approach to strongly singular potentials by verifying Hypothesis 3.3.1 under very general circumstances.

We start with a simple example first.

Example 3.3.10. *The class of potentials V of the form*

$$V(x) = \frac{\gamma^2 - 1/4}{x^2} + \widetilde{V}(x), \quad \gamma \in [1,\infty),\ x \in (0,\infty), \tag{3.3.87}$$

where $\widetilde{V}$ is a real-valued measurable function on $[0,\infty)$ such that

$$\widetilde{V} \in L^1([0,b]; x\,dx) \text{ for all } b > 0, \tag{3.3.88}$$

assuming that $\tau_+ = -d^2/dx^2 + [\gamma^2 - (1/4)]x^{-2} + \widetilde{V}(x)$ is in the limit point case at ∞, satisfies Hypothesis 3.3.1.

To verify that the potential V in (3.3.87) indeed satisfies Hypothesis 3.3.1 we first state the following result. As kindly pointed out to us by Don Hinton, this is a special case of his Theorem 1 in [94]. For convenience of the reader we include the following elementary and short proof we found independently (and which differs from the proof in [94]).

Lemma 3.3.11. ([94].) Let $b \in (0,\infty)$. Then the differential expression τ_+ given by

$$\tau_+ = -\frac{d^2}{dx^2} + \frac{\gamma^2 - (1/4)}{x^2} + \widetilde{V}(x), \quad x \in (0,b),\ \gamma \in [1,\infty), \tag{3.3.89}$$

with $\widetilde{V}$ a real-valued and measurable function on $[0,b]$ satisfying

$$\widetilde{V} \in L^1([0,b]; x\,dx), \tag{3.3.90}$$

is in the limit point case at $x = 0$.

Proof. Consider a solution θ of

$$\begin{aligned}&(\tau_+\theta)(x) = 0, \quad x \in (0,b),\\ &\theta(x_0) = x_0^{1/2-\gamma},\ \theta'(x_0) = (1/2-\gamma)x_0^{-1/2-\gamma} \quad \text{for some } x_0 \in (0,b).\end{aligned} \tag{3.3.91}$$

By the "variation of constants" formula, θ satisfies

$$\theta(x) = x^{1/2-\gamma} + \frac{1}{2\gamma}\int_{x_0}^{x} dt\big[x^{1/2+\gamma}t^{1/2-\gamma} - x^{1/2-\gamma}t^{1/2+\gamma}\big]\widetilde{V}(t)\theta(t). \tag{3.3.92}$$

Introducing

$$\begin{aligned}&\theta_0(x) = x^{1/2-\gamma},\\ &\theta_k(x) = \frac{1}{2\gamma}\int_{x_0}^{x} dt\big[x^{1/2+\gamma}t^{1/2-\gamma} - x^{1/2-\gamma}t^{1/2+\gamma}\big]\widetilde{V}(t)\theta_{k-1}(t), \quad k \in \mathbb{N},\end{aligned} \tag{3.3.93}$$

and estimating θ_k by

$$|\theta_k(x)| \le x^{1/2-\gamma}\frac{1}{k!}\left(\frac{1}{2\gamma}\int_0^{x_0} dt\, t\big|\widetilde{V}(t)\big|\right)^k, \quad x \in (0,x_0),\ k \ge 0, \tag{3.3.94}$$

then imply

$$\theta(x) = \sum_{k=0}^{\infty}\theta_k(x), \tag{3.3.95}$$

where the sum converges absolutely and uniformly on any compact subset of $(0,x_0)$.

In addition,

$$|\theta(x)| \le \sum_{k=0}^{\infty}|\theta_k(x)| \le x^{1/2-\gamma}\exp\left(\frac{1}{2\gamma}\int_0^{x_0} dt\, t\big|\widetilde{V}(t)\big|\right), \quad x \in (0,x_0). \tag{3.3.96}$$

Since $\widetilde{V} \in L^1([0,b]; x\,dx)$, there exists $x_0 \in (0,b)$ such that

$$\frac{1}{2\gamma}\int_0^{x_0} dt\, t\big|\widetilde{V}(t)\big| \le \ln(3/2), \tag{3.3.97}$$

and hence by (3.3.93), (3.3.95), (3.3.96), and (3.3.97),

$$\theta(x) \geq 2\theta_0 - \sum_{k=0}^{\infty} \big|\theta_k(x)\big| \geq x^{1/2-\gamma}\Big(2 - e^{\ln(3/2)}\Big) \geq \frac{1}{2} x^{1/2-\gamma}, \quad x \in (0, x_0). \tag{3.3.98}$$

Thus, $\theta \notin L^2((0, x_0); dx)$ and hence τ_+ is in the limit point case at $x = 0$. $\square$

Moreover, by the "variation of constants" formula, the Weyl–Titchmarsh solution $\widetilde{\phi}(z, \cdot)$ of

$$- \psi''(z, x) + V(x)\psi(z, x) = z\psi(z, x), \quad x \in (0, \infty), \tag{3.3.99}$$

$$\psi(z, \cdot) \in L^2((0, b); dx) \text{ for some } b \in (0, \infty),\ z \in \mathbb{C} \tag{3.3.100}$$

satisfies the Volterra integral equation

$$\widetilde{\phi}(z, x) = x^{1/2+\gamma} + \frac{1}{2\gamma}\int_0^x dt\, \big[x^{1/2+\gamma}t^{1/2-\gamma} - t^{1/2+\gamma}x^{1/2-\gamma}\big] U(z, t)\widetilde{\phi}(z, t), \tag{3.3.101}$$

where

$$U(z, x) = \widetilde{V}(x) - z. \tag{3.3.102}$$

To verify this claim one iterates (3.3.101) to obtain a solution $\widetilde{\phi}(z, x)$ of (3.3.99) in the form

$$\widetilde{\phi}(z, x) = \sum_{k=0}^{\infty} \widetilde{\phi}_k(z, x), \quad z \in \mathbb{C},\ x \in (0, \infty), \tag{3.3.103}$$

where

$$\widetilde{\phi}_0(z, x) = x^{1/2+\gamma},$$
$$\widetilde{\phi}_k(z, x) = \frac{1}{2\gamma}\int_0^x dx' \big[x^{1/2+\gamma}(x')^{1/2-\gamma} - (x')^{1/2+\gamma}x^{1/2-\gamma}\big] U(z, x')\widetilde{\phi}_{k-1}(z, x'),$$

$$k \in \mathbb{N},\ z \in \mathbb{C},\ x \in (0,\infty). \qquad (3.3.104)$$

Since $\widetilde{\phi}_k(z,x)$, $k \in \mathbb{N}$, is continuous in $(z,x) \in \mathbb{C} \times (0,\infty)$, entire with respect to z for all fixed $x \in (0,\infty)$, and since

$$|\widetilde{\phi}_k(z,x)| \leq \frac{x^{1/2+\gamma}}{k!} \left(\frac{1}{\gamma}\int_0^x dx' x' |U(z,x')|\right)^k, \quad (z,x) \in K, \qquad (3.3.105)$$

where K is any compact subs et of $\mathbb{C} \times (0,\infty)$, the series in (3.3.103) converges absolutely and uniformly on K, and hence $\widetilde{\phi}(z,x)$ is continuous in $(z,x) \in \mathbb{C} \times (0,\infty)$ and entire in z for all fixed $x \in (0,\infty)$. Moreover, it follows from (3.3.103) and (3.3.105) that

$$|\widetilde{\phi}(z,x)| \leq x^{1/2+\gamma} \exp\left(\frac{1}{\gamma}\int_0^x dx' x' |U(z,x')|\right), \quad (z,x) \in K, \qquad (3.3.106)$$

and hence, $\widetilde{\phi}(z,\cdot)$ satisfies (3.3.100). Summarizing these considerations, $\widetilde{\phi}(z,\cdot)$ satisfies Hypotheses 3.3.1 (iii) (α)–(γ).

While this represents just an elementary example, we now turn to a vast class of singular potentials.

We first state the following auxiliary result.

Lemma 3.3.12. *Let* $b \in (0,\infty)$ *and* $f, f' \in AC_{\mathrm{loc}}((0,b))$, f *real-valued, and* $f(x) \neq 0$ *for all* $x \in (0,b)$.

(i) *Introduce*

$$\eta_\pm(x) = 2^{-1/2} f(x) \exp\left(\pm \int_x^{x_0} dx'\, f(x')^{-2}\right), \quad x, x_0 \in (0,b). \qquad (3.3.107)$$

Then $\eta_\pm$ *represent a fundamental system of solutions of*

$$-\psi''(x) + \left[\frac{f''(x)}{f(x)} + \frac{1}{f(x)^4}\right]\psi(x) = 0, \quad x \in (0,b) \qquad (3.3.108)$$

and

$$W(\eta_+,\eta_-)(x)=1. \tag{3.3.109}$$

(ii) In addition, assume $f\in L^2([0,b'];dx)$ for some $b'\in(0,b)$ and $\widetilde V\in L^1([0,c];f^2dx)$ for all $c\in(0,b)$. Then there exists an entire Weyl–Titchmarsh solution $\widetilde\phi(z,\cdot)$ of

$$-\phi''(z,x)+\bigg[\frac{f''(x)}{f(x)}+\frac{1}{f(x)^4}+\widetilde V(x)\bigg]\phi(z,x)=z\phi(z,x),\quad z\in\mathbb{C},\ x\in(0,b) \tag{3.3.110}$$

in the following sense:

(α) *For all $x\in(0,b)$, $\widetilde\phi(\cdot,x)$ is entire.*

(β) *$\widetilde\phi(z,x)$, $x\in(0,b)$, is real-valued for $z\in\mathbb{R}$.*

(γ) *$\widetilde\phi(z,\cdot)$ satisfies the L^2-condition near the end point 0 and hence*

$$\widetilde\phi(z,\cdot)\in L^2([0,c];dx)\ \text{ for all } z\in\mathbb{C} \text{ and all } c\in(0,b). \tag{3.3.111}$$

Proof. Verifying item (i) is a straightforward computation. To verify item (ii), consider the Volterra integral equation

$$\widetilde\phi(z,x)=\eta_-(x)+\int_0^x dx'\,[\eta_+(x')\eta_-(x)-\eta_+(x)\eta_-(x')]\big[\widetilde V(x')-z\big]\widetilde\phi(z,x'),$$
$$z\in\mathbb{C},\ x\in(0,b). \tag{3.3.112}$$

Again, iterating (3.3.112) then yields

$$\widetilde\phi(z,x)=\sum_{k=0}^\infty\widetilde\phi_k(z,x),\quad \widetilde\phi_0(z,x)=\eta_-(x), \tag{3.3.113}$$
$$\widetilde\phi_k(z,x)=\int_0^x dx'\,[\eta_+(x')\eta_-(x)-\eta_+(x)\eta_-(x')]\big[\widetilde V(x')-z\big]\widetilde\phi_{k-1}(z,x'),\quad k\in\mathbb{N}. \tag{3.3.114}$$

The elementary estimate

$$\bigg|\frac{\eta_+(x)}{\eta_-(x)}\frac{\eta_-(x')}{\eta_+(x')}\bigg|\le\exp\bigg(-\int_{x'}^x dy\,f(y)^{-2}\bigg)\le 1,\quad 0\le x'\le x<b \tag{3.3.115}$$

then yields

$$\begin{aligned}\big|\widetilde{\phi}_1(z,x)\big| &\leq |\eta_-(x)| \int_0^x dx'\,|\eta_+(x')\eta_-(x')| \left|1 + \frac{\eta_+(x)}{\eta_-(x)}\frac{\eta_-(x')}{\eta_+(x')}\right| \big|\widetilde{V}(x') - z\big| \\ &\leq |\eta_-(x)| \int_0^x dx' f(x')^2 |\widetilde{V}(x') - z| \end{aligned} \tag{3.3.116}$$

and hence

$$\big|\widetilde{\phi}_k(z,x)\big| \leq |\eta_-(x)| \frac{1}{k!}\bigg(\int_0^x dx' f(x')^2 \big|\widetilde{V}(x) - z\big|\bigg)^k, \quad k \in \mathbb{N},\ z \in \mathbb{C},\ x \in (0,b). \tag{3.3.117}$$

Thus,

$$\big|\widetilde{\phi}(z,x)\big| \leq |\eta_-(x)| \exp\bigg(\int_0^x dx' f(x')^2 \big|\widetilde{V}(x) - z\big|\bigg), \quad k \in \mathbb{N},\ z \in \mathbb{C},\ x \in (0,b). \tag{3.3.118}$$

This proves items $(ii)\,(\alpha)$ and $(ii)\,(\beta)$. Since by hypothesis, $f \in L^2([0,b'];dx)$ for some $b' \in (0,b)$ and hence $\eta_- \in L^2([0,c];dx)$ for all $c \in (0,b)$, item $(ii)\,(\gamma)$ holds as well. $\square$

A general class of examples of strongly singular potentials satisfying Hypothesis 3.3.1 (iii) is then described in the following example.

Example 3.3.13. *Let $b \in (0,\infty)$. Then the class of potentials V such that*

$$V, V' \in AC_{\text{loc}}((0,b)),\ V \in L^1_{\text{loc}}((0,\infty);dx), \ \ V \text{ real-valued}, \tag{3.3.119}$$

$$V(x) > 0, \quad x \in (0,b), \tag{3.3.120}$$

$$V^{-1/2} \in L^1([0,b];dx), \tag{3.3.121}$$

$$V'V^{-5/4} \in L^2([0,b];dx), \tag{3.3.122}$$

$$\textit{either } V^{-3/2}V'' \in L^1([0,b];dx), \textit{ or else,} \tag{3.3.123}$$

$$V'' > 0 \textit{ a.e. on } (0,b) \textit{ and } \lim_{x\downarrow 0} V'(x)V(x)^{-3/2} \textit{ exists and is finite,} \tag{3.3.124}$$

satisfies Hypothesis 3.3.1 (iii) (α)–(γ) in the following sense: There exists an entire Weyl–Titchmarsh solution $\widetilde{\phi}(z,\cdot)$ *of*

$$-\psi''(z,x) + V(x)\psi(z,x) = z\psi(z,x), \quad z \in \mathbb{C},\ x \in (0,\infty) \tag{3.3.125}$$

satisfying the following conditions (α)–(β):

(α) *For all* $x \in (0,\infty)$, $\widetilde{\phi}(\cdot,x)$ *is entire.*

(β) $\widetilde{\phi}(z,x)$, $x \in (0,\infty)$, *is real-valued for* $z \in \mathbb{R}$.

(γ) $\widetilde{\phi}(z,\cdot)$ *satisfies the* L^2*-condition near the end point* 0 *and hence*

$$\widetilde{\phi}(z,\cdot) \in L^2([0,c];dx) \textit{ for all } z \in \mathbb{C} \textit{ and all } c \in (0,\infty). \tag{3.3.126}$$

Since V is strongly singular at most at $x = 0$, it suffices to discuss this example for $x \in (0,b)$ only. Moreover, for simplicity, we focus only on sufficient conditions for Hypotheses 3.3.1 (*iii*) (α)–(γ) to hold. The additional limit point assumptions on V at zero and at infinity can easily be supplied (cf. [43, Sects. XIII.6, XIII.9, XIII.10]). Moreover, we made no efforts to optimize the conditions on V. The point of the example is just to show the wide applicability of our approach based on Hypothesis 3.3.1.

In order to reduce Example 3.3.13 to Lemma 3.3.12, one can argue as follows: Introduce

$$f(x) = V(x)^{-1/4}, \tag{3.3.127}$$

$$\widetilde{V}(x) = -f''(x)/f(x). \tag{3.3.128}$$

Then $f, f' \in AC_{\mathrm{loc}}((0,b))$, $f \neq 0$ on $(0,b)$, and $f \in L^2([0,c];dx)$ for all $c \in (0,b)$. Moreover, since

$$f^2\widetilde{V} = -ff'' = -\frac{5}{16}\big[V^{-5/4}V'\big]^2 + \frac{1}{4}V^{-3/2}V'', \tag{3.3.129}$$

$\widetilde{V} \in L^1([0,c];f^2dx)$ for some $c \in (0,b)$. (This is clear from (3.3.122) if condition in (3.3.123) is assumed. In case (3.3.124) is assumed, a straightforward integration by parts, using (3.3.122), yields $\widetilde{V} \in L^1([0,c];f^2dx)$ for some $c \in (0,b)$.) Thus, Lemma 3.3.12 applies to

$$V = f^{-4} = [(f''/f) + f^{-4}] + \widetilde{V}. \tag{3.3.130}$$

Remark 3.3.14. We focused on the strongly singular case where τ_+ is in the limit point case at the singular endpoint $x = a$. The singular case, where V is not integrable at the endpoint a and τ_+ is in the limit circle case at a is similar to the regular case (associated with a Weyl–Titchmarsh coefficient having the Herglotz property) considered in Section 3.2. For pertinent references to this case see [53], [57].

3.4 An Illustrative Example

In this section we provide a detailed treatment of the following well-known singular potential example (which fits into Lemma 3.3.12 with $f(x) = (x/\gamma)^{1/2}$, $x > 0$, $\gamma \in [1,\infty)$, and $\widetilde{V} = 0$),

$$V(x,\gamma) = \frac{\gamma^2 - (1/4)}{x^2}, \quad x \in (0,\infty),\ \gamma \in [1,\infty) \tag{3.4.1}$$

with associated differential expression

$$\tau_+(\gamma) = -\frac{d^2}{dx^2} + V(x,\gamma), \quad x \in (0,\infty), \ \gamma \in [1,\infty). \tag{3.4.2}$$

Numerous references have been devoted to this example, we refer, for instance, to [40], [41], [43, p. 1532–1536], [48], [57], [58], [131], [135, p. 142–144], [137], [184, p. 87–90], and the literature therein. The corresponding maximally defined self-adjoint Schrödinger operator $H_+(\gamma)$ in $L^2([0,\infty);dx)$ is then defined by

$$\begin{aligned} &H_+(\gamma)f = \tau_+(\gamma)f, \\ &f \in \mathrm{dom}(H_+(\gamma)) = \{g \in L^2([0,\infty);dx) \,|\, g, g' \in AC_{\mathrm{loc}}((0,\infty)); \\ &\qquad\qquad\qquad\qquad\qquad \tau_+(\gamma)g \in L^2([0,\infty);dx)\}. \end{aligned} \tag{3.4.3}$$

The potential $V(\cdot,\gamma)$ in (3.4.1) is so strongly singular at the finite end point $x = 0$ that $H_+(\gamma)$ (in stark contrast to cases regular at $x = 0$, cf. (3.2.3)) is self-adjoint in $L^2([0,\infty);dx)$ without imposing any boundary condition at $x = 0$. Equivalently, the corresponding minimal Schrödinger operator $\widetilde{H}_+(\gamma)$, defined by

$$\begin{aligned} &\widetilde{H}_+(\gamma)f = \tau_+(\gamma)f, \\ &f \in \mathrm{dom}(\widetilde{H}_+(\gamma)) = \{g \in L^2([0,\infty);dx) \,|\, g, g' \in AC_{\mathrm{loc}}((0,\infty)); \\ &\qquad\qquad \mathrm{supp}\,(g) \subset (0,\infty) \text{ compact}; \tau_+(\gamma)g \in L^2([0,\infty);dx)\}, \end{aligned} \tag{3.4.4}$$

is essentially self-adjoint in $L^2([0,\infty);dx)$.

A fundamental system of solutions of

$$(\tau_+(\gamma)\psi)(z,x) = z\psi(z,x), \quad x \in (0,\infty) \tag{3.4.5}$$

is given by

$$x^{1/2}J_\gamma(z^{1/2}x),\ x^{1/2}Y_\gamma(z^{1/2}x), \quad z\in\mathbb{C}\backslash\{0\},\ x\in(0,\infty),\ \gamma\in[1,\infty) \tag{3.4.6}$$

with $J_\gamma(\cdot)$ and $Y_\gamma(\cdot)$ the usual Bessel functions of order γ (cf. [3, Ch. 9]). We first treat the case where

$$\gamma\in(1,\infty), \quad \gamma\notin\mathbb{N}, \tag{3.4.7}$$

in which case

$$x^{1/2}J_\gamma(z^{1/2}x),\ x^{1/2}J_{-\gamma}(z^{1/2}x), \quad z\in\mathbb{C}\backslash\{0\},\ x\in(0,\infty),\ \gamma\in(1,\infty)\backslash\mathbb{N} \tag{3.4.8}$$

is a fundamental system of solutions of (3.4.5). Since the system of solutions in (3.4.8) exhibits the branch cut $[0,\infty)$ with respect to z, we slightly change it into the following system,

$$\begin{aligned}&\phi(z,x,\gamma)=C^{-1}\pi[2\sin(\pi\gamma)]^{-1}z^{-\gamma/2}x^{1/2}J_\gamma(z^{1/2}x),\\&\theta(z,x,\gamma)=Cz^{\gamma/2}x^{1/2}J_{-\gamma}(z^{1/2}x), \quad z\in\mathbb{C},\ x\in(0,\infty),\ \gamma\in(1,\infty)\backslash\mathbb{N},\end{aligned} \tag{3.4.9}$$

which for each $x\in(0,\infty)$ represents entire functions with respect to z. Here $C\in\mathbb{R}\backslash\{0\}$ is a normalization constant to be discussed in Remark 3.4.4. One verifies that (cf. [3, p. 360])

$$W(\theta(z,\cdot,\gamma),\phi(z,\cdot,\gamma))=1, \quad z\in\mathbb{C},\ \gamma\in(1,\infty)\backslash\mathbb{N} \tag{3.4.10}$$

and that (cf. [3, p. 360])

$$\begin{aligned}z^{\mp\gamma/2}x^{1/2}J_{\pm\gamma}(z^{1/2}x)=2^{-\gamma}x^{(1/2)\pm\gamma}\sum_{k=0}^\infty\frac{(-zx^2/4)^k}{k!\Gamma(k+1\pm\gamma)},\\ z\in\mathbb{C},\ x\in(0,\infty),\ \gamma\in(1,\infty)\backslash\mathbb{N}.\end{aligned} \tag{3.4.11}$$

Hence the fundamental system $\phi(z,\cdot,\gamma), \theta(z,\cdot,\gamma)$ in (3.4.9) of solutions of (3.4.5) is entire with respect to z and real-valued for $z \in \mathbb{R}$.

The corresponding solution of (3.4.5), square integrable in a neighborhood of infinity, is given by

$$x^{1/2}H_\gamma^{(1)}(z^{1/2}x) = \frac{i}{\sin(\pi\gamma)} x^{1/2}\big[e^{-i\pi\gamma}J_\gamma(z^{1/2}x) - J_{-\gamma}(z^{1/2}x)\big],$$
$$z \in \mathbb{C}\backslash[0,\infty),\ x \in (0,\infty),\ \gamma \in (1,\infty)\backslash\mathbb{N} \tag{3.4.12}$$

with $H_\gamma^{(1)}(\cdot)$ the usual Hankel function of order γ (cf. [3, Ch. 9]). In order to be compatible with our modified system ϕ, θ of solutions of (3.4.5), we replace it by

$$\begin{aligned}\psi_+(z,x,\gamma) &= Cz^{\gamma/2}x^{1/2}J_{-\gamma}(z^{1/2}x) - C^2e^{-i\pi\gamma}z^\gamma C^{-1}z^{-\gamma/2}x^{1/2}J_\gamma(z^{1/2}x) \\ &= \theta(z,x,\gamma) + m_+(z,\gamma)\phi(z,x,\gamma), \\ &\quad z \in \mathbb{C}\backslash[0,\infty),\ x \in (0,\infty),\ \gamma \in (1,\infty)\backslash\mathbb{N},\end{aligned} \tag{3.4.13}$$

where

$$m_+(z,\gamma) = -C^2(2/\pi)\sin(\pi\gamma)e^{-i\pi\gamma}z^\gamma, \quad z \in \mathbb{C}\backslash[0,\infty),\ \gamma \in (1,\infty)\backslash\mathbb{N} \tag{3.4.14}$$

and

$$\overline{m_+(z,\gamma)} = m_+(\overline{z},\gamma), \quad z \in \mathbb{C}\backslash[0,\infty). \tag{3.4.15}$$

Next, we consider the case,

$$\gamma = n \in \mathbb{N}, \tag{3.4.16}$$

in which

$$x^{1/2}J_n(z^{1/2}x),\ x^{1/2}Y_n(z^{1/2}x), \quad z \in \mathbb{C}\backslash\{0\},\ x \in (0,\infty),\ n \in \mathbb{N}, \tag{3.4.17}$$

is a fundamental system of solutions of (3.4.5). As before, we slightly change it into the following system,

$$\begin{aligned}
&\phi(z,x,n) = C^{-1}(\pi/2)z^{-n/2}x^{1/2}J_n(z^{1/2}x),\\
&\theta(z,x,n) = Cz^{n/2}x^{1/2}\big[-Y_n(z^{1/2}x) + \pi^{-1}\ln(z)J_n(z^{1/2}x)\big],\\
&\qquad\qquad z\in\mathbb{C},\ x\in(0,\infty),\ n\in\mathbb{N}.
\end{aligned}\tag{3.4.18}$$

Here $C\in\mathbb{R}\backslash\{0\}$ is a normalization constant to be discussed in Remark 3.4.4. One verifies that (cf. [3, p. 360])

$$W(\theta(z,\cdot,n),\phi(z,\cdot,n))(x) = 1, \quad z\in\mathbb{C},\ n\in\mathbb{N}, \tag{3.4.19}$$

and that the fundamental system of solutions of (3.4.5), $\phi(z,\cdot,n),\theta(z,\cdot,n)$ in (3.4.18), is entire with respect to z and real-valued for $z\in\mathbb{R}$.

The corresponding solution of (3.4.5), square integrable in a neighborhood of infinity, is given by

$$\begin{aligned}
&x^{1/2}H_n^{(1)}(z^{1/2}x) = x^{1/2}\big[J_n(z^{1/2}x) + iY_n(z^{1/2}x)\big],\\
&\qquad z\in\mathbb{C}\backslash[0,\infty), x\in(0,\infty),\ n\in\mathbb{N}
\end{aligned}\tag{3.4.20}$$

with $H_n^{(1)}(\cdot)$ the usual Hankel function of order n (cf. [3, Ch. 9]). In order to be compatible with our modified system ϕ,θ of solutions of (3.4.5), we replace it by

$$\begin{aligned}
\psi_+(z,x,n) &= Cz^{n/2}x^{1/2}iH_n(z^{1/2}x) = Cz^{1/2}x^{1/2}\big[-Y_n(z^{1/2}x) + iJ_n(z^{1/2}x)\big]\\
&= \theta(z,x,n) + m_+(z,n)\phi(z,x,n),\\
&\quad z\in\mathbb{C}\backslash[0,\infty),\ x\in(0,\infty),\ n\in\mathbb{N},
\end{aligned}\tag{3.4.21}$$

where

$$m_+(z,n) = C^2(2/\pi)z^n\big[i-(1/\pi)\ln(z)\big], \quad z\in\mathbb{C}\backslash[0,\infty),\ n\in\mathbb{N} \tag{3.4.22}$$

and

$$\overline{m_+(z,n)} = m_+(\overline{z},n), \quad z \in \mathbb{C}\backslash[0,\infty). \tag{3.4.23}$$

Remark 3.4.1. (i) We emphasize that in stark contrast to the case of regular half-line Schrödinger operators in Section 3.2, $m_+(\cdot,\gamma)$ in (3.4.14) and (3.4.22) is not a Herglotz function for $\gamma \in [1,\infty)$.

(ii) In the paper by Everitt and Kalf [48] the Friedrichs extension and the associated Hankel eigenfunction transform are treated in detail for the case $\gamma \in [0,1)$ in (3.4.1). In this case the corresponding Weyl–Titchmarsh coefficient turns out to be a Herglotz function.

Since $\tau_+(\gamma)$ is in the limit point case at $x=0$ and at $x=\infty$, (3.4.5) has a unique solution (up to constant multiples) that is L^2 near 0 and L^2 near ∞. Indeed, that unique L^2-solution near 0 (up to normalization) is precisely $\phi(z,\cdot,\gamma)$; similarly, the unique L^2-solution near ∞ (up to normalization) is $\psi_+(z,\cdot,\gamma)$.

By (3.4.10) and (3.4.19), a computation of the Green's function $G_+(z,x,x',\gamma)$ of $H_+(\gamma)$ yields

$$G_+(z,x,x',\gamma) = \frac{i\pi}{2}\begin{cases} x^{1/2}J_\gamma(z^{1/2}x)x'^{1/2}H_\gamma^{(1)}(z^{1/2}x'), & 0<x\leq x', \\ x'^{1/2}J_\gamma(z^{1/2}x')x^{1/2}H_\gamma^{(1)}(z^{1/2}x), & 0<x'\leq x, \end{cases} \tag{3.4.24}$$

$$= \begin{cases} \phi(z,x,\gamma)\psi_+(z,x',\gamma), & 0<x\leq x', \\ \phi(z,x',\gamma)\psi_+(z,x,\gamma), & 0<x'\leq x, \end{cases} \tag{3.4.25}$$

$$z \in \mathbb{C}\backslash[0,\infty),\ \gamma \in [1,\infty).$$

Thus,

$$\begin{gathered} ((H_+(\gamma)-zI)^{-1}f)(x) = \int_0^\infty dx'\, G_+(z,x,x',\gamma)f(x'), \\ z \in \mathbb{C}\backslash[0,\infty),\ x\in(0,\infty),\ f\in L^2([0,\infty);dx),\ \gamma\in[1,\infty). \end{gathered} \tag{3.4.26}$$

Given $m_+(z,\gamma)$ in (3.4.14), we define the associated measure $\rho_+(\cdot,\gamma)$ by

$$\rho_+((\lambda_1,\lambda_2],\gamma) = \pi^{-1}\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda\, \mathrm{Im}(m_+(\lambda+i\varepsilon,\gamma)) \tag{3.4.27}$$

$$= C^2\frac{\lambda_2^{\gamma+1}-\lambda_1^{\gamma+1}}{\gamma+1}\frac{2}{\pi^2}\begin{cases}\sin^2(\pi\gamma), & \gamma\notin\mathbb{N},\\ 1, & \gamma\in\mathbb{N},\end{cases} \tag{3.4.28}$$

$$0\le\lambda_1<\lambda_2,\ \gamma\in[1,\infty),$$

generated by the function

$$\rho_+(\lambda,\gamma) = C^2\chi_{[0,\infty)}(\lambda)\frac{\lambda^{\gamma+1}}{\gamma+1}\frac{2}{\pi^2}\begin{cases}\sin^2(\pi\gamma), & \gamma\notin\mathbb{N},\\ 1, & \gamma\in\mathbb{N},\end{cases} \quad \lambda\in\mathbb{R},\ \gamma\in[1,\infty). \tag{3.4.29}$$

Even though $m_+(\cdot,\gamma)$ is not a Herglotz function for $\gamma\in[1,\infty)$, $d\rho_+(\cdot,\gamma)$ is defined as in (3.3.26), in analogy to the case of Herglotz functions discussed in Appendix B (cf. (B.4)).

Next, we introduce the family of spectral projections, $\{E_{H_+(\gamma)}(\lambda)\}_{\lambda\in\mathbb{R}}$, of the self-adjoint operator $H_+(\gamma)$ and note that for $F\in C(\mathbb{R})$,

$$\big(f, F(H_+(\gamma))g\big)_{L^2([0,\infty);dx)} = \int_{\mathbb{R}} d\big(f, E_{H_+(\gamma)}(\lambda)g\big)_{L^2([0,\infty);dx)}\, F(\lambda),$$

$$f,g\in\mathrm{dom}(F(H_+(\gamma))) \tag{3.4.30}$$

$$= \bigg\{h\in L^2([0,\infty);dx)\,\bigg|\, \int_{\mathbb{R}} d\big\|E_{H_+(\gamma)}(\lambda)h\big\|^2_{L^2([0,\infty);dx)}\,|F(\lambda)|^2<\infty\bigg\}.$$

The connection between $\{E_{H_+(\gamma)}(\lambda)\}_{\lambda\in\mathbb{R}}$ and $\rho_+(\lambda,\gamma)$, $\lambda\ge 0$, is described in the next result.

Lemma 3.4.2. *Let $\gamma\in[1,\infty)$, $f,g\in C_0^\infty((0,\infty))$, $F\in C(\mathbb{R})$, and $\lambda_1,\lambda_2\in[0,\infty)$, $\lambda_1<\lambda_2$. Then,*

$$\begin{aligned}&\big(f, F(H_+(\gamma))E_{H_+(\gamma)}((\lambda_1,\lambda_2])g\big)_{L^2([0,\infty);dx)}\\ &\quad= \big(\widehat{f}_+(\gamma), M_F M_{\chi_{(\lambda_1,\lambda_2]}}\widehat{g}_+(\gamma)\big)_{L^2(\mathbb{R};d\rho_+(\cdot,\gamma))},\end{aligned} \tag{3.4.31}$$

where

$$\widehat{h}_+(\gamma)(\lambda) = \int_0^\infty dx\, \phi(\lambda, x, \gamma) h(x), \quad \lambda \in [0, \infty),\ h \in C_0^\infty((0,\infty)) \tag{3.4.32}$$

and M_G denotes the operator of multiplication by the $d\rho_+(\cdot,\gamma)$-measurable function G in the Hilbert space $L^2(\mathbb{R}; d\rho_+(\cdot,\gamma))$.

The proof of Lemma 3.4.2 is a special case of that of Theorem 3.3.5 and hence omitted.

As in Section 3.3 one can remove the compact support restrictions on f and g in Lemma 3.4.2. To this end one considers the map

$$U_+(\gamma)\colon \begin{cases} L^2([0,\infty); dx) \to L^2(\mathbb{R}; d\rho_+(\cdot,\gamma)) \\ \qquad\qquad h \mapsto \widehat{h}_+(\cdot,\gamma) = \text{l.i.m.}_{b\uparrow\infty} \int_0^b dx\, \phi(\cdot, x, \gamma) h(x), \end{cases} \tag{3.4.33}$$

where l.i.m. refers to the $L^2(\mathbb{R}; d\rho_+(\cdot,\gamma))$-limit.

In addition, it is of course known (cf., e.g., [43, p. 1535]) that the Bessel transform $U_+(\gamma)$ in (3.4.33) is onto and hence that $U_+(\gamma)$ is unitary with

$$U_+(\gamma)^{-1}\colon \begin{cases} L^2(\mathbb{R}; d\rho_+(\cdot,\gamma)) \to L^2([0,\infty); dx) \\ \qquad\qquad \widehat{h} \mapsto \text{l.i.m.}_{\mu_1\downarrow-\infty,\mu_2\uparrow\infty} \int_{\mu_1}^{\mu_2} d\rho_+(\lambda,\gamma)\, \phi(\lambda,\cdot,\gamma)\widehat{h}(\lambda), \end{cases} \tag{3.4.34}$$

where l.i.m. refers to the $L^2([0,\infty); dx)$-limit.

Again we sum up these considerations in a variant of the spectral theorem for (functions of) $H_+(\gamma)$.

Theorem 3.4.3. *Let $\gamma \in [1,\infty)$, $F \in C(\mathbb{R})$. Then,*

$$U_+(\gamma) F(H_+(\gamma)) U_+(\gamma)^{-1} = M_F \tag{3.4.35}$$

in $L^2(\mathbb{R}; d\rho_+(\cdot,\gamma))$. *Moreover,*

$$\sigma(F(H_+(\gamma))) = \text{ess.ran}_{d\rho_+(\cdot,\gamma)}(F), \tag{3.4.36}$$

$$\sigma(H_+(\gamma)) = \text{supp}\,(d\rho_+(\cdot,\gamma)), \tag{3.4.37}$$

and the spectrum of $H_+(\gamma)$ *is simple.*

Next, we reconsider spectral theory for $H_+(\gamma)$ by choosing a reference point $x_0 \in (0,\infty)$ away from the singularity of $V(\cdot,\gamma)$ at $x=0$.

Consider a system $\phi(z,\cdot,x_0,\gamma)$, $\theta(z,\cdot,x_0,\gamma)$ of solutions of (3.4.5) with the following initial conditions at the reference point $x_0 \in (0,\infty)$,

$$\phi(z,x_0,x_0,\gamma) = \theta'(z,x_0,x_0,\gamma) = 0, \quad \phi'(z,x_0,x_0,\gamma) = \theta(z,x_0,x_0,\gamma) = 1.$$

Denote by $m_\pm(z,x_0,\gamma)$ two Weyl–Titchmarsh m-functions corresponding to the restriction of our problem to the intervals $(0,x_0]$ and $[x_0,\infty)$, respectively. Then the Weyl–Titchmarsh solutions $\psi_\pm(z,\cdot,x_0,\gamma)$ and the 2×2 matrix-valued Weyl–Titchmarsh M-function $M(z,x_0,\gamma)$ are given by

$$\psi_\pm(z,x,x_0,\gamma) = \theta(z,x,x_0,\gamma) + m_\pm(z,x_0,\gamma)\phi(z,x,x_0,\gamma), \tag{3.4.38}$$

$$M(z,x_0,\gamma) = \begin{pmatrix} \frac{1}{m_-(z,x_0,\gamma)-m_+(z,x_0,\gamma)} & \frac{1}{2}\frac{m_-(z,x_0,\gamma)+m_+(z,x_0,\gamma)}{m_-(z,x_0,\gamma)-m_+(z,x_0,\gamma)} \\ \frac{1}{2}\frac{m_-(z,x_0,\gamma)+m_+(z,x_0,\gamma)}{m_-(z,x_0,\gamma)-m_+(z,x_0,\gamma)} & \frac{m_-(z,x_0,\gamma)m_+(z,x_0,\gamma)}{m_-(z,x_0,\gamma)-m_+(z,x_0,\gamma)} \end{pmatrix}. \tag{3.4.39}$$

Since any L^2-solution near 0 and near ∞ (i.e., any Weyl–Titchmarsh solution) is necessarily proportional to $x^{1/2}J_\gamma(z^{1/2}x)$ and $x^{1/2}H_\gamma^{(1)}(z^{1/2}x)$, respectively, one explicitly computes for $m_\pm(z,x_0,\gamma)$,

$$m_-(z,x_0,\gamma) = \frac{1}{2x_0} + z^{1/2}\frac{J_\gamma'(z^{1/2}x_0)}{J_\gamma(z^{1/2}x_0)}, \tag{3.4.40}$$

$$m_+(z,x_0,\gamma) = \frac{1}{2x_0} + z^{1/2}\frac{H^{(1)\prime}_\gamma(z^{1/2}x_0)}{H^{(1)}_\gamma(z^{1/2}x_0)}, \tag{3.4.41}$$

and for $M(z,x_0,\gamma)$,

$$M_{0,0}(z,x_0,\gamma) = \frac{i\pi x_0}{2} J_\gamma(z^{1/2}x_0)H^{(1)}_\gamma(z^{1/2}x_0), \tag{3.4.42}$$

$$\begin{aligned} M_{0,1}(z,x_0,\gamma) = M_{1,0}(z,x_0,\gamma) = \frac{i\pi}{4}\bigg[& J_\gamma(z^{1/2}x_0)H^{(1)}_\gamma(z^{1/2}x_0) + x_0 z^{1/2} \\ & \times \Big(J_\gamma(z^{1/2}x_0)H^{(1)\prime}_\gamma(z^{1/2}x_0) + J'_\gamma(z^{1/2}x_0)H^{(1)}_\gamma(z^{1/2}x_0)\Big)\bigg], \end{aligned} \tag{3.4.43}$$

$$\begin{aligned} M_{1,1}(z,x_0,\gamma) = \frac{i\pi}{8x_0}\bigg[& J_\gamma(z^{1/2}x_0)H^{(1)}_\gamma(z^{1/2}x_0) + 2x_0 z^{1/2} \\ & \times \Big(J_\gamma(z^{1/2}x_0)H^{(1)\prime}_\gamma(z^{1/2}x_0) + J'_\gamma(z^{1/2}x_0)H^{(1)}_\gamma(z^{1/2}x_0)\Big) \\ & + 4x_0^2 z J'_\gamma(z^{1/2}x_0)H^{(1)\prime}_\gamma(z^{1/2}x_0)\bigg]. \end{aligned} \tag{3.4.44}$$

Using (3.4.12), (3.4.20), and the calculation above, one can also compute the 2×2 spectral measure $d\Omega(\cdot,x_0,\gamma)$ and its density $d\Omega(\cdot,x_0,\gamma)/d\lambda$,

$$\frac{d\Omega(\lambda,x_0,\gamma)}{d\lambda} = \frac{1}{\pi}\lim_{\varepsilon\downarrow 0}\operatorname{Im}(M(\lambda+i\varepsilon,x_0)), \quad \lambda\in\mathbb{R}, \tag{3.4.45}$$

$$\frac{d\Omega_{0,0}(\lambda,x_0,\gamma)}{d\lambda} = \begin{cases} \frac{x_0}{2}J_\gamma(\lambda^{1/2}x_0)^2, & \lambda>0,\\ 0, & \lambda\le 0,\end{cases} \tag{3.4.46}$$

$$\begin{aligned}\frac{d\Omega_{0,1}(\lambda,x_0,\gamma)}{d\lambda} &= \frac{d\Omega_{1,0}(\lambda,x_0)}{d\lambda} \\ &= \begin{cases} \frac{1}{4}\left[J_\gamma(\lambda^{1/2}x_0)^2 + 2x_0\lambda^{1/2}J_\gamma(\lambda^{1/2}x_0)J'_\gamma(\lambda^{1/2}x_0)\right], & \lambda>0,\\ 0, & \lambda\le 0,\end{cases}\end{aligned} \tag{3.4.47}$$

$$\frac{d\Omega_{1,1}(\lambda,x_0,\gamma)}{d\lambda} = \begin{cases} \frac{1}{8x_0}\left[J_\gamma(\lambda^{1/2}x_0) + 2x_0\lambda^{1/2}J'_\gamma(\lambda^{1/2}x_0)\right]^2, & \lambda>0,\\ 0, & \lambda\le 0.\end{cases} \tag{3.4.48}$$

Moreover, one verifies that,

$$\operatorname{rank}\left(\frac{d\Omega(\lambda,x_0,\gamma)}{d\lambda}\right) = \begin{cases} 1, & \lambda>0,\\ 0, & \lambda\le 0.\end{cases} \tag{3.4.49}$$

Finally, we will show that the results of Section 3.3 which let one obtain a scalar spectral measure $d\widetilde{\rho}_+(\lambda, \gamma)$ from the 2×2 spectral measure $d\Omega(\lambda, x_0, \gamma)$ lead to the measure equivalent to $d\rho_+(\lambda, \gamma)$ obtained in the first part of this section.

Let

$$\widetilde{\phi}(z, x, \gamma) = z^{-\gamma/2} x^{1/2} J_\gamma(z^{1/2} x) \tag{3.4.50}$$

be the Weyl–Titchmarsh solution satisfying Hypothesis 3.3.1 (iii). Inserting (3.4.46), (3.4.47), and (3.4.50) into (3.3.86) then yields

$$\frac{d\widetilde{\rho}_+(\lambda, \gamma)}{d\lambda} = \begin{cases} \frac{1}{2}\lambda^\gamma, & \lambda > 0, \\ 0, & \lambda \leq 0, \end{cases} \tag{3.4.51}$$

which, up to a constant multiple, is the same as $d\rho_+(\lambda, \gamma)/d\lambda$ in (3.4.29).

Of course the analogs of Theorem 3.3.7, Theorem 3.3.8, and Corollary 3.3.9 all hold in the present context of the potential (3.4.1); we omit the details.

Remark 3.4.4. We explicitly introduced the normalization constant $C \in \mathbb{R}\backslash\{0\}$ in (3.4.9) and (3.4.18) to determine its effect on (the analog of) the Weyl–Titchmarsh coefficient m_+ (cf. (3.4.14) and (3.4.22)) and the associated spectral function ρ_+ (cf. (3.4.29)). As C enters quadratically in m_+ and ρ_+, it clearly has an effect on their asymptotic behavior as $|z| \to \infty$, respectively, $|\lambda| \to \infty$. The same observation applies of course in the regular half-line case considered in the first half of Section 3.2. It just so happens that in this case the standard normalization of the fundamental system of solutions ϕ_α and θ_α of (3.2.4) in (3.2.5) represents a canonical choice and the normalization dependence can safely be ignored. In the strongly singular case in Sections 3.3 and 3.4 no such canonical choice of normalization exists. Of course, the actual spectral properties of the corresponding half-line Schrödinger operator are independent of such a choice of normalization.

Chapter 4

Non-self-adjoint operators, Infinite Determinants, and some Applications

4.1 Introduction

This chapter has been written in response to the increased demand of spectral theoretic aspects of non-self-adjoint operators in contemporary applied and mathematical physics. What we have in mind, in particular, concerns the following typical two scenarios: First, the construction of certain classes of solutions of a number of completely integrable hierarchies of evolution equations by means of the inverse scattering method, for instance, in the context of the focusing nonlinear Schrödinger equation in $(1 + 1)$-dimensions, naturally leads to non-self-adjoint Lax operators. Specifically, in the particular case of the focusing nonlinear Schrödinger equation the corresponding Lax operator is a non-self-adjoint one-dimensional Dirac-type operator. Second, linearizations of nonlinear partial differential equations around steady state and solitary-type solutions, frequently, lead to a linear non-self-adjoint spectral problem. In the latter context, the use of the so-called Evans function (an analog of the one-dimensional Jost function for Schrödinger operators) in the course of a linear stability analysis has become a cornerstone of this circle of ideas. As shown in [71], the Evans function equals a (modified) Fredholm determinant associated with an underlying Birman–Schwinger-type operator. This observation naturally leads to the second main theme of this chapter and a concrete application to non-self-adjoint operators, viz., a study of properly symmetrized (modified) perturbation determinants of non-self-adjoint Schrödinger operators in dimensions $n = 1, 2, 3$.

Next, we briefly summarize the content of each section. In Section 4.2, following the seminal work of Kato [108] (see also Konno and Kuroda [113] and Howland [96]), we consider a class of factorable non-self-adjoint perturbations, formally given by B^*A, of a given unperturbed non-self-adjoint operator H_0 in a Hilbert space $\mathcal{H}$ and introduce a densely defined, closed linear operator H in $\mathcal{H}$ which represents an extension of $H_0 + B^*A$. Closely following Konno and Kuroda [113], we subsequently derive a general Birman–Schwinger principle for H in Section 4.3. A variant of the essential spectrum of H and a local Weinstein–Aronszajn formula is discussed in Section 4.4. The corresponding global Weinstein–Aronszajn formula in terms of modified Fredholm determinants associated with the Birman–Schwinger kernel of H is the content of Section 4.5. Both, Sections 4.4 and 4.5 are modeled after an exemplary treatment of these topics by Howland [96] in the case where H_0 and H are self-adjoint. In Section 4.6 we turn to concrete applications to properly symmetrized (modified) perturbation determinants of non-self-adjoint Dirichlet- and Neumann-type Schrödinger operators in $L^2(\Omega; d^nx)$ with $\Omega = (0, \infty)$ in the case $n = 1$ and rather general open domains

$\Omega \subset \mathbb{R}^n$ with a compact boundary in dimensions $n = 2, 3$. The corresponding potentials V considered are of the form $V \in L^1((0,\infty); dx)$ for $n = 1$ and $V \in L^2(\Omega; d^n x)$ for $n = 2, 3$. Our principal result in this section concerns a reduction of the Fredholm determinant of the Birman–Schwinger kernel of H in $L^2(\Omega; d^n x)$ to a Fredholm determinant associated with operators in $L^2(\partial\Omega; d^{n-1}\sigma)$. The latter should be viewed as a proper multi-dimensional extension of the celebrated result by Jost and Pais [104] concerning the equality of the Jost function (a Wronski determinant) and the associated Fredholm determinant of the underlying Birman–Schwinger kernel. In Section 4.8 we briefly discuss an application to scattering theory in dimensions $n = 2, 3$ and re-derive a formula for the Krein spectral shift function (related to the logarithm of the determinant of the scattering matrix) in terms of modified Fredholm determinants of the underlying Birman–Schwinger kernel. We present an alternative derivation of this formula originally due to Cheney [29] for $n = 2$ and Newton [141] for $n = 3$ (in the latter case we obtain the result under weaker assumptions on the potential V than in [141]). Finally, Appendix C summarizes results on Dirichlet and Neumann Laplacians in $L^2(\Omega; d^n x)$ for a general class of open domains $\Omega \subseteq \mathbb{R}^n$, $n \geq 2$, with a compact boundary. We prove the equality of two natural definitions of Dirichlet and Neumann Laplacians for such domains and prove mapping properties between appropriate scales of Sobolev spaces. These results are crucial ingredients in our treatment of modified Fredholm determinants in Section 4.6, but they also appear to be of independent interest.

We will use the following notation in this chapter. Let $\mathcal{H}$ and $\mathcal{K}$ be separable complex Hilbert spaces, $(\cdot,\cdot)_{\mathcal{H}}$ and $(\cdot,\cdot)_{\mathcal{K}}$ the scalar products in $\mathcal{H}$ and $\mathcal{K}$ (linear in the second factor), and $I_{\mathcal{H}}$ and $I_{\mathcal{K}}$ the identity operators in $\mathcal{H}$ and $\mathcal{K}$, respectively. Next, let T be a closed linear operator from $\operatorname{dom}(T) \subseteq \mathcal{H}$ to $\operatorname{ran}(T) \subseteq \mathcal{K}$, with $\operatorname{dom}(T)$ and $\operatorname{ran}(T)$ denoting the domain and range of T. The closure of a closable operator S is denoted by $\overline{S}$. The kernel (null space) of T is denoted by $\ker(T)$. The spectrum and resolvent set of a closed linear operator in $\mathcal{H}$ will be denoted by $\sigma(\cdot)$ and $\rho(\cdot)$. The Banach spaces of bounded and compact linear operators in $\mathcal{H}$ are denoted by $\mathcal{B}(\mathcal{H})$ and $\mathcal{B}_\infty(\mathcal{H})$, respectively. Similarly, the Schatten–von Neumann (trace) ideals will subsequently be denoted by $\mathcal{B}_p(\mathcal{H})$, $p \in \mathbb{N}$. Analogous notation $\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)$, $\mathcal{B}_\infty(\mathcal{H}_1, \mathcal{H}_2)$, etc., will be used for bounded, compact, etc., operators between two Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$. In addition, $\operatorname{tr}(T)$ denotes the trace of a trace class operator $T \in \mathcal{B}_1(\mathcal{H})$ and $\det_p(I_{\mathcal{H}} + S)$ represents the (modified) Fredholm determinant associated with an operator $S \in \mathcal{B}_p(\mathcal{H})$, $p \in \mathbb{N}$ (for $p = 1$ we omit the subscript 1). Moreover, $\mathcal{X}_1 \hookrightarrow \mathcal{X}_2$ denotes the continuous embedding of the Banach space $\mathcal{X}_1$ into the Banach space $\mathcal{X}_2$.

Finally, in Sections 4.6 and 4.8 we will introduce various operators of multiplication, M_f, in $L^2(\Omega; d^n x)$ by elements $f \in L^1_{\mathrm{loc}}(\Omega; d^n x)$, where $\Omega \subseteq \mathbb{R}^n$ is open and nonempty.

4.2 Abstract Perturbation Theory

In this section, following Kato [108], Konno and Kuroda [113], and Howland [96], we consider a class of factorable non-self-adjoint perturbations of a given unperturbed non-self-adjoint operator. For reasons of completeness we will present proofs of many of the subsequent results even though most of them are only slight deviations from the original proofs in the self-adjoint context.

We start with our first set of hypotheses.

Hypothesis 4.2.1. (i) Suppose that $H_0\colon \operatorname{dom}(H_0) \to \mathcal{H}$, $\operatorname{dom}(H_0) \subseteq \mathcal{H}$ is a densely defined, closed, linear operator in $\mathcal{H}$ with nonempty resolvent set,

$$\rho(H_0) \neq \emptyset, \tag{4.2.1}$$

$A\colon \operatorname{dom}(A) \to \mathcal{K}$, $\operatorname{dom}(A) \subseteq \mathcal{H}$ a densely defined, closed, linear operator from $\mathcal{H}$ to $\mathcal{K}$, and $B\colon \operatorname{dom}(B) \to \mathcal{K}$, $\operatorname{dom}(B) \subseteq \mathcal{H}$ a densely defined, closed, linear operator from $\mathcal{H}$ to $\mathcal{K}$ such that

$$\operatorname{dom}(A) \supseteq \operatorname{dom}(H_0), \quad \operatorname{dom}(B) \supseteq \operatorname{dom}(H_0^*). \tag{4.2.2}$$

In the following we denote

$$R_0(z) = (H_0 - zI_{\mathcal{H}})^{-1}, \quad z \in \rho(H_0). \tag{4.2.3}$$

(ii) For some (and hence for all) $z \in \rho(H_0)$, the operator $-AR_0(z)B^*$, defined on $\operatorname{dom}(B^*)$, has a bounded extension in $\mathcal{K}$, denoted by $K(z)$,

$$K(z) = -\overline{AR_0(z)B^*} \in \mathcal{B}(\mathcal{K}). \tag{4.2.4}$$

(iii) $1 \in \rho(K(z_0))$ for some $z_0 \in \rho(H_0)$.

That $K(z_0) \in \mathcal{B}(\mathcal{K})$ for some $z_0 \in \rho(H_0)$ implies $K(z) \in \mathcal{B}(\mathcal{K})$ for all $z \in \rho(H_0)$ (as mentioned in Hypothesis 4.2.1 (ii)) is an immediate consequence of (4.2.2) and the resolvent equation for H_0.

We emphasize that in the case where H_0 is self-adjoint, the following results in Lemma 4.2.2, Theorem 4.2.3, and Remark 4.2.4 are due to Kato [108] (see also [96], [113]). The more general case we consider here requires only minor modifications. But for the convenience of the reader we will sketch most of the proofs.

Lemma 4.2.2. *Let $z, z_1, z_2 \in \rho(H_0)$. Then Hypothesis 4.2.1 implies the following facts:*

$$AR_0(z) \in \mathcal{B}(\mathcal{H}, \mathcal{K}), \quad \overline{R_0(z)B^*} = [B(H_0^* - \overline{z})^{-1}]^* \in \mathcal{B}(\mathcal{K}, \mathcal{H}), \tag{4.2.5}$$

$$\overline{R_0(z_1)B^*} - \overline{R_0(z_2)B^*} = (z_1 - z_2)R_0(z_1)\overline{R_0(z_2)B^*} \tag{4.2.6}$$

$$= (z_1 - z_2)R_0(z_2)\overline{R_0(z_1)B^*}, \tag{4.2.7}$$

$$K(z) = -A\overline{[R_0(z)B^*]}, \quad K(\overline{z})^* = -B\overline{[R_0(\overline{z})^*A^*]}, \tag{4.2.8}$$

$$\operatorname{ran}(\overline{R_0(z)B^*}) \subseteq \operatorname{dom}(A), \quad \operatorname{ran}(\overline{R_0(\overline{z})^*A^*}) \subseteq \operatorname{dom}(B), \tag{4.2.9}$$

$$K(z_1) - K(z_2) = (z_2 - z_1)AR_0(z_1)\overline{R_0(z_2)B^*} \tag{4.2.10}$$

$$= (z_2 - z_1)AR_0(z_2)\overline{R_0(z_1)B^*}. \tag{4.2.11}$$

Proof. Equations (4.2.5) follow from the relations in (4.2.2) and the Closed Graph Theorem. (4.2.6) and (4.2.7) follow from combining (4.2.5) and the resolvent equation for H_0^*. Next, let $f \in \operatorname{dom}(B^*)$, $g \in \operatorname{dom}(A^*)$, then

$$(\overline{R_0(z)B^*}f, A^*g)_{\mathcal{H}} = (R_0(z)B^*f, A^*g)_{\mathcal{H}} = (AR_0(z)B^*f, g)_{\mathcal{K}} = -(K(z)f, g)_{\mathcal{K}}. \tag{4.2.12}$$

By continuity this extends to all $f \in \mathcal{K}$. Thus, $-A\overline{[R_0(z)B^*]}f$ exists and equals $K(z)f$ for all $f \in \mathcal{K}$. This proves the first assertions in (4.2.8) and (4.2.9). The remaining assertions in (4.2.8) and (4.2.9) are of course proved analogously. Multiplying (4.2.6) and (4.2.7) by A from the left and taking into account the first relation in (4.2.8), then proves (4.2.10) and (4.2.11). $\square$

Next, following Kato [108], one introduces

$$
\begin{gathered}
R(z) = R_0(z) - \overline{R_0(z)B^*}[I_{\mathcal{K}} - K(z)]^{-1}AR_0(z), \\
z \in \{\zeta \in \rho(H_0) \,|\, 1 \in \rho(K(\zeta))\}.
\end{gathered} \tag{4.2.13}
$$

Theorem 4.2.3. *Assume Hypothesis 4.2.1 and let $z \in \{\zeta \in \rho(H_0) \,|\, 1 \in \rho(K(\zeta))\}$. Then, $R(z)$ defined in (4.2.13) defines a densely defined, closed, linear operator H in $\mathcal{H}$ by*

$$
R(z) = (H - zI_{\mathcal{H}})^{-1}. \tag{4.2.14}
$$

Moreover,

$$
AR(z), BR(z)^* \in \mathcal{B}(\mathcal{H}, \mathcal{K}) \tag{4.2.15}
$$

and

$$
R(z) = R_0(z) - \overline{R(z)B^*}AR_0(z) \tag{4.2.16}
$$

$$
= R_0(z) - \overline{R_0(z)B^*}AR(z). \tag{4.2.17}
$$

Finally, H is an extension of $(H_0 + B^*A)|_{\mathrm{dom}(H_0)\cap\mathrm{dom}(B^*A)}$ (the latter intersection domain may consist of $\{0\}$ only),

$$
H \supseteq (H_0 + B^*A)|_{\mathrm{dom}(H_0)\cap\mathrm{dom}(B^*A)}. \tag{4.2.18}
$$

Proof. Suppose $z \in \{\zeta \in \rho(H_0) \,|\, 1 \in \rho(K(\zeta))\}$. Since by (4.2.13)

$$
AR(z) = [I_{\mathcal{K}} - K(z)]^{-1}AR_0(z), \tag{4.2.19}
$$

$$
BR(z)^* = [I_{\mathcal{K}} - K(z)^*]^{-1}BR_0(z)^*, \tag{4.2.20}
$$

$R(z)f = 0$ implies $AR(z)f = 0$ and hence by (4.2.19) $AR_0(z)f = 0$. The latter implies $R_0(z)f = 0$ by (4.2.13) and thus $f = 0$. Consequently,

$$\ker(R(z)) = \{0\}. \tag{4.2.21}$$

Similarly, (4.2.20) implies

$$\ker(R(z)^*) = \{0\} \text{ and hence } \overline{\operatorname{ran}(R(z))} = \mathcal{H}. \tag{4.2.22}$$

Next, combining (4.2.13), the resolvent equation for H_0, (4.2.6), (4.2.7), (4.2.10), and (4.2.11) proves the resolvent equation

$$\begin{gathered} R(z_1) - R(z_2) = (z_1 - z_2)R(z_1)R(z_2), \\ z_1, z_2 \in \{\zeta \in \rho(H_0) \,|\, 1 \in \rho(K(\zeta))\}. \end{gathered} \tag{4.2.23}$$

Thus, $R(z)$ is indeed the resolvent of a densely defined, closed, linear operator H in $\mathcal{H}$ as claimed in connection with (4.2.14).

By (4.2.19) and (4.2.20), $AR(z) \in \mathcal{B}(\mathcal{H}, \mathcal{K})$ and $[BR(\overline{z})^*]^* = \overline{R(z)B^*} \in \mathcal{B}(\mathcal{K}, \mathcal{H})$, proving (4.2.15). A combination of (4.2.13), (4.2.19), and (4.2.20) then proves (4.2.16) and (4.2.17).

Finally, let $f \in \operatorname{dom}(H_0) \cap \operatorname{dom}(B^*A)$ and set $g = (H_0 - zI_{\mathcal{H}})f$. Then $R_0(z)g = f$ and by (4.2.16), $R(z)g - f = -R(z)B^*Af$. Thus, $f \in \operatorname{dom}(H)$ and $(H - zI_{\mathcal{H}})f = g + B^*Af = (H_0 + B^*A - zI_{\mathcal{H}})f$, proving (4.2.18). $\square$

Remark 4.2.4. (i) Assume that H_0 is self-adjoint in $\mathcal{H}$. Then H is also self-adjoint if

$$(Af, Bg)_{\mathcal{K}} = (Bf, Ag)_{\mathcal{K}} \text{ for all } f, g \in \operatorname{dom}(A) \cap \operatorname{dom}(B). \tag{4.2.24}$$

(ii) The formalism is symmetric with respect to H_0 and H in the following sense: The densely defined operator $-AR(z)B^*$ has a bounded extension to all of $\mathcal{K}$ for all $z \in \{\zeta \in \rho(H_0) \,|\, 1 \in \rho(K(\zeta))\}$, in particular,

$$I_{\mathcal{K}} - \overline{AR(z)B^*} = [I_{\mathcal{K}} - K(z)]^{-1}, \quad z \in \{\zeta \in \rho(H_0) \,|\, 1 \in \rho(K(\zeta))\}. \tag{4.2.25}$$

Moreover,

$$\begin{gathered} R_0(z) = R(z) + \overline{R(z)B^*}[I_{\mathcal{K}} - \overline{AR(z)B^*}]^{-1}AR(z), \\ z \in \{\zeta \in \rho(H_0) \,|\, 1 \in \rho(K(\zeta))\} \end{gathered} \tag{4.2.26}$$

and

$$H_0 \supseteq (H - B^*A)|_{\mathrm{dom}(H)\cap\mathrm{dom}(B^*A)}. \tag{4.2.27}$$

(iii) The basic hypotheses (4.2.2) which amount to

$$AR_0(z) \in \mathcal{B}(\mathcal{H},\mathcal{K}), \quad \overline{R_0(z)B^*} = [B(H_0^* - \overline{z})^{-1}]^* \in \mathcal{B}(\mathcal{K},\mathcal{H}), \quad z \in \rho(H_0) \tag{4.2.28}$$

(cf. (4.2.5)) are more general than a quadratic form perturbation approach which would result in conditions of the form

$$AR_0(z)^{1/2} \in \mathcal{B}(\mathcal{H},\mathcal{K}), \quad \overline{R_0(z)^{1/2}B^*} = [B(H_0^* - \overline{z})^{-1/2}]^* \in \mathcal{B}(\mathcal{K},\mathcal{H}), \quad z \in \rho(H_0), \tag{4.2.29}$$

or even an operator perturbation approach which would involve conditions of the form

$$[B^*A]R_0(z) \in \mathcal{B}(\mathcal{H}), \quad z \in \rho(H_0). \tag{4.2.30}$$

4.3 A General Birman–Schwinger Principle

The principal result in this section represents an abstract version of (a variant of) the Birman–Schwinger principle due to Birman [19] and Schwinger [159] (cf. also [21], [67], [111], [112], [143], [149], [160], and [164]).

We need to strengthen our hypotheses a bit and hence introduce the following assumption:

Hypothesis 4.3.1. In addition to Hypothesis 4.2.1 we suppose the condition:

(iv) $K(z) \in \mathcal{B}_\infty(\mathcal{K})$ for all $z \in \rho(H_0)$.

Since by (4.2.25)

$$-\overline{AR(z)B^*} = [I_{\mathcal{K}} - K(z)]^{-1}K(z) \tag{4.3.1}$$

$$= -I_{\mathcal{K}} + [I_{\mathcal{K}} - K(z)]^{-1}, \tag{4.3.2}$$

Hypothesis 4.3.1 implies that $-\overline{AR(z)B^*}$ extends to a compact operator in $\mathcal{K}$ as long as the right-hand side of (4.3.2) exists.

The following general result is due to Konno and Kuroda [113] in the case where H_0 is self-adjoint. (The more general case presented here requires no modifications but we present a proof for completeness.)

Theorem 4.3.2 ([113])**.** *Assume Hypothesis 4.3.1 and let $\lambda_0 \in \rho(H_0)$. Then,*

$$Hf = \lambda_0 f, \quad 0 \neq f \in \mathrm{dom}(H) \ \textit{implies} \ K(\lambda_0)g = g \tag{4.3.3}$$

where, for fixed $z_0 \in \{\zeta \in \rho(H_0) \,|\, 1 \in \rho(K(\zeta))\}$, $z_0 \neq \lambda_0$,

$$0 \neq g = [I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)f \tag{4.3.4}$$

$$= (\lambda_0 - z_0)^{-1}Af. \tag{4.3.5}$$

Conversely,

$$K(\lambda_0)g = g, \quad 0 \neq g \in \mathcal{K} \ \textit{implies} \ Hf = \lambda_0 f, \tag{4.3.6}$$

where

$$0 \neq f = -\overline{R_0(\lambda_0)B^*}g \in \mathrm{dom}(H). \tag{4.3.7}$$

Moreover,

$$\dim(\ker(H - \lambda_0 I_{\mathcal{H}})) = \dim(\ker(I_{\mathcal{K}} - K(\lambda_0))) < \infty. \tag{4.3.8}$$

In particular, let $z \in \rho(H_0)$, then

$$z \in \rho(H) \text{ if and only if } 1 \in \rho(K(z)). \tag{4.3.9}$$

Proof. $Hf = \lambda_0 f$, $0 \neq f \in \mathrm{dom}(H)$, is equivalent to $f = (\lambda_0 - z_0)R(z_0)f$ and applying (4.2.13) one obtains after a simple rearrangement that

$$(H_0 - \lambda_0 I_{\mathcal{H}})R_0(z_0)f = -(\lambda_0 - z_0)\overline{R_0(z_0)B^*}[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)f. \tag{4.3.10}$$

Next, define $g = [I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)f$. Then $g \neq 0$ since otherwise

$$(H_0 - \lambda_0 I_{\mathcal{H}})R_0(z_0)f = 0, \quad 0 \neq R_0(z_0)f \in \mathrm{dom}(H_0), \text{ and hence } \lambda_0 \in \sigma(H_0), \tag{4.3.11}$$

would contradict our hypothesis $\lambda_0 \in \rho(H_0)$. Applying $[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(\lambda_0)$ to (4.3.10) then yields

$$\begin{aligned}
&[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(\lambda_0)(H_0 - \lambda_0 I_{\mathcal{H}})R_0(z_0)f = [I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)f = g \\
&\quad = -(\lambda_0 - z_0)[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(\lambda_0)\overline{R_0(z_0)B^*}[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)f \\
&\quad = -(\lambda_0 - z_0)[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(\lambda_0)\overline{R_0(z_0)B^*}g.
\end{aligned} \tag{4.3.12}$$

Thus, based on (4.2.10), one infers

$$g = -(\lambda_0 - z_0)[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(\lambda_0)\overline{R_0(z_0)B^*}g$$

$$= [I_{\mathcal{K}} - K(z_0)]^{-1}[K(\lambda_0) - K(z_0)]g$$

$$= g - [I_{\mathcal{K}} - K(z_0)]^{-1}[I_{\mathcal{K}} - K(\lambda_0)]g \tag{4.3.13}$$

and hence $K(\lambda_0)g = g$, proving (4.3.3). Since $f = (\lambda_0 - z_0)R(z_0)f$, using (4.2.19) one computes

$$Af = (\lambda_0 - z_0)AR(z_0)f$$

$$= (\lambda_0 - z_0)[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)f$$

$$= (\lambda_0 - z_0)g, \tag{4.3.14}$$

proving (4.3.5).

Conversely, suppose $K(\lambda_0)g = g$, $0 \neq g \in \mathcal{K}$ and define $f = -\overline{R_0(\lambda_0)B^*}g$. Then a simple computation using (4.2.10) shows

$$g = g - [I_{\mathcal{K}} - K(z_0)]^{-1}[I_{\mathcal{K}} - K(\lambda_0)]g$$

$$= [I_{\mathcal{K}} - K(z_0)]^{-1}[K(\lambda_0) - K(z_0)]g$$

$$= (\lambda_0 - z_0)[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)f. \tag{4.3.15}$$

Thus, $f \neq 0$ since $f = 0$ would imply the contradiction $g = 0$. Next, inserting the definition of f into (4.3.15) yields

$$g = (\lambda_0 - z_0)[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)f$$

$$= -(\lambda_0 - z_0)[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)\overline{R_0(\lambda_0)B^*}g. \tag{4.3.16}$$

Applying $\overline{R_0(z_0)B^*}$ to (4.3.16) and taking into account

$$\overline{R_0(z_0)B^*}g = \overline{[R_0(\lambda_0) - (\lambda_0 - z_0)R_0(z_0)R_0(\lambda_0)]B^*}g$$

$$= -f + (\lambda_0 - z_0)R_0(z_0)f, \tag{4.3.17}$$

a combination of (4.3.17) and (4.2.13) yields that

$$\begin{aligned} -f - (z_0 - \lambda_0)R_0(z_0)f &= (\lambda_0 - z_0)\overline{R_0(z_0)B^*}[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)f \\ &= (\lambda_0 - z_0)[R_0(z_0) - R(z_0)]f. \end{aligned} \tag{4.3.18}$$

The latter is equivalent to $(\lambda_0 - z_0)(H - z_0 I_{\mathcal{H}})^{-1}f = f$. Thus, $f \in \operatorname{dom}(H)$ and $Hf = \lambda_0 f$, proving (4.3.6).

Since $K(\lambda_0) \in \mathcal{B}_\infty(\mathcal{K})$, the eigenspace of $K(\lambda_0)$ corresponding to the eigenvalue 1 is finite-dimensional. The previous considerations established a one-to-one correspondence between the geometric eigenspace of $K(\lambda_0)$ corresponding to the eigenvalue 1 and the geometric eigenspace of H corresponding to the eigenvalue λ_0. This proves (4.3.8).

Finally, (4.3.8), (4.2.13), and (4.2.25) prove (4.3.9). □

Remark 4.3.3. It is possible to avoid the compactness assumption in Hypothesis 4.3.1 in Theorem 4.3.2 provided that (4.3.8) is replaced by the statement

$$\text{the subspaces } \ker(H - \lambda_0 I_{\mathcal{H}}) \text{ and } \ker(I_{\mathcal{K}} - K(\lambda_0)) \text{ are isomorphic.} \tag{4.3.19}$$

(Of course, (4.3.8) follows from (4.3.19) provided $\ker(I_{\mathcal{K}} - K(\lambda_0))$ is finite-dimensional, which in turn follows from Hypothesis 4.3.1). Indeed, by formula (4.2.19), we have $AR(z_0) = [I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)$. By formula (4.3.4), if $f \neq 0$, then $g = AR(z_0)f \neq 0$, and thus the operator

$$AR(z_0) = [I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0) \colon \ker(H - \lambda_0 I) \to \ker(K(\lambda_0) - I) \tag{4.3.20}$$

is injective. By formula (4.3.16) this operator is also surjective, since each $g \in \ker(K(\lambda_0) - I)$ belongs to its range,

$$g = (\lambda_0 - z_0)[I_{\mathcal{K}} - K(z_0)]^{-1} A R_0(z_0) f = A R(z_0) f, \tag{4.3.21}$$

where $f \in \ker(H - \lambda_0 I)$.

4.4 Essential Spectra and a Local Weinstein–Aronszajn Formula

In this section, we closely follow Howland [96] and prove a result which demonstrates the invariance of the essential spectrum. However, since we will extend Howland's result to the non-self-adjoint case, this requires further explanation. Moreover, we will also re-derive Howland's local Weinstein–Aronszajn formula.

Definition 4.4.1. Let $\Omega \subseteq \mathbb{C}$ be open and connected. Suppose $\{L(z)\}_{z\in\Omega}$ is a family of compact operators in $\mathcal{K}$, which is analytic on Ω except for isolated singularities. Following Howland we call $\{L(z)\}_{z\in\Omega}$ *completely meromorphic* on Ω if L is meromorphic on Ω and the principal part of L at each of its poles is of finite rank.

We start with an auxiliary result due to Steinberg [176] with a modification by Howland [96].

Lemma 4.4.2 ([96], [176]). *Let $\{L(z)\}_{z\in\Omega}$ be an analytic (resp., completely meromorphic) family in $\mathcal{K}$ on an open connected set $\Omega \subseteq \mathbb{C}$. Then for each $z_0 \in \Omega$ there is a neighborhood $U(z_0)$ of z_0, and an analytic $\mathcal{B}(\mathcal{K})$-valued function M on $U(z_0)$, such that $M(z)^{-1} \in \mathcal{B}(\mathcal{K})$ for all $z \in U(z_0)$ and*

$$M(z)[I_{\mathcal{K}} - L(z)] = I_{\mathcal{K}} - F(z), \quad z \in U(z_0), \tag{4.4.1}$$

where F is analytic (resp., meromorphic) on $U(z_0)$ with $F(z)$ of finite rank (except at poles) for all $z \in U(z_0)$.

The next auxiliary result is due to Ribaric and Vidav [152].

Lemma 4.4.3 ([152]). *Let $\{L(z)\}_{z\in\Omega}$ be a completely meromorphic family in $\mathcal{K}$ on an open connected set $\Omega \subseteq \mathbb{C}$. Then either*

(i) $I_{\mathcal{K}} - L(z)$ is not boundedly invertible for all $z \in \Omega$,

or

(ii) $\{[I_{\mathcal{K}} - L(z)]^{-1} - I_{\mathcal{K}}\}_{z\in\Omega}$ is completely meromorphic on Ω.

Moreover, we state the following result due to Howland [97].

Lemma 4.4.4 ([97]). *Let $\{L(z)\}_{z\in\Omega}$ be an analytic (resp., meromorphic) family in $\mathcal{K}$ on an open connected set $\Omega \subseteq \mathbb{C}$ and suppose that $L(z)$ has finite rank for each $z \in \Omega$ (except at poles). Then the following assertions hold:*

(i) The rank of $L(z)$ is constant for all $z \in \Omega$, except for isolated points where it decreases.

(ii) $\Delta(z) = \det(I_{\mathcal{K}} - L(z))$ and $\operatorname{tr}(L(z))$ are analytic (resp., meromorphic) for all $z \in \Omega$.

(iii) Whenever $\Delta(z) \neq 0$,

$$\Delta'(z)/\Delta(z) = -\operatorname{tr}([I_{\mathcal{K}} - L(z)]^{-1}L'(z)), \quad z \in \Omega. \tag{4.4.2}$$

We note that it can of course happen that Δ vanishes identically on Ω.

Next, we introduce the multiplicity function $m(\cdot, T)$ on $\mathbb{C}$ associated with a closed, densely defined, linear operator T in $\mathcal{H}$ as follows. Suppose $\lambda_0 \in \mathbb{C}$ is an isolated point in $\sigma(T)$ and introduce the Riesz projection $P(\lambda_0, T)$ of T corresponding to λ_0 by

$$P(\lambda_0, T) = -\frac{1}{2\pi i} \oint_{C(\lambda_0;\varepsilon)} d\zeta \, (T - \zeta I_{\mathcal{H}})^{-1}, \tag{4.4.3}$$

where $C(\lambda_0; \varepsilon)$ is a counterclockwise oriented circle centered at λ_0 with sufficiently small radius $\varepsilon > 0$ (excluding the rest of $\sigma(T)$). Then $m(z, T)$, $z \in \mathbb{C}$, is defined by

$$m(z,T) = \begin{cases} 0, & \text{if } z \in \rho(T), \\ \dim(\operatorname{ran}(P(z,T))), & \text{if } z \text{ is an isolated eigenvalue of } T \\ & \text{of finite algebraic multiplicity,} \\ +\infty, & \text{otherwise.} \end{cases} \tag{4.4.4}$$

We note that the dimension of the Riesz projection in (4.4.3) is finite if and only if λ_0 is an isolated eigenvalue of T of finite algebraic multiplicity (cf. [109, p. 181]). In analogy to the self-adjoint case (but deviating from most definitions in the non-self-adjoint case, see [46, Sect. I.4, Ch. IX]) we now introduce the set

$$\begin{aligned} \widetilde{\sigma}_{\mathrm{e}}(T) = \{\lambda \in \mathbb{C} \,|\, \lambda \in \sigma(T),\ \lambda \text{ is not an isolated eigenvalue of } T \\ \text{of finite algebraic multiplicity}\}. \end{aligned} \tag{4.4.5}$$

Of course, $\widetilde{\sigma}_{\mathrm{e}}(T)$ coincides with the essential spectrum of T if T is self-adjoint in $\mathcal{H}$. In the non-self-adjoint case at hand, the set $\widetilde{\sigma}_{\mathrm{e}}(T)$ is most natural in our study of H_0 and H as will subsequently be shown. It will also be convenient to introduce the complement of $\widetilde{\sigma}_{\mathrm{e}}(T)$ in $\mathbb{C}$,

$$\begin{aligned} \widetilde{\Phi}(T) &= \mathbb{C} \backslash \widetilde{\sigma}_{\mathrm{e}}(T) \\ &= \rho(T) \cup \{\lambda \in \mathbb{C} \,|\, \lambda \text{ is an eigenvalue of } T \text{ of finite algebraic multiplicity}\}. \end{aligned} \tag{4.4.6}$$

If T is self-adjoint in $\mathcal{H}$, $\widetilde{\Phi}(T)$ is the Fredholm domain of T.

If $\lambda_0 \in \mathbb{C}$ is an isolated eigenvalue of T of finite algebraic multiplicity, then the singularity structure of the resolvent of T is of the type

$$\begin{aligned}(T - zI_{\mathcal{H}})^{-1} = (\lambda_0 - z)^{-1}P(\lambda_0, T) + \sum_{k=1}^{\mu(\lambda_0,T)} (\lambda_0 - z)^{-k-1}(-1)^k D(\lambda_0, T)^k \\ + \sum_{k=0}^{\infty}(\lambda_0 - z)^k(-1)^k S(\lambda_0, T)^{k+1}\end{aligned} \tag{4.4.7}$$

for z in a sufficiently small neighborhood of λ_0. Here

$$D(\lambda_0, T) = (T - \lambda_0 I_{\mathcal{H}})P(\lambda_0, T) = \frac{1}{2\pi i}\oint_{C(\lambda_0;\varepsilon)} d\zeta\, (\lambda_0 - \zeta)(T - \zeta I_{\mathcal{H}})^{-1} \in \mathcal{B}(\mathcal{H}), \tag{4.4.8}$$

$$S(\lambda_0, T) = -\frac{1}{2\pi i}\oint_{C(\lambda_0;\varepsilon)} d\zeta\, (\lambda_0 - \zeta)^{-1}(T - \zeta I_{\mathcal{H}})^{-1} \in \mathcal{B}(\mathcal{H}), \tag{4.4.9}$$

and $D(\lambda_0, T)$ is nilpotent with its range contained in that of $P(\lambda_0, T)$,

$$D(\lambda_0, T) = P(\lambda_0, T)D(\lambda_0, T) = D(\lambda_0, T)P(\lambda_0, T). \tag{4.4.10}$$

Moreover,

$$\begin{aligned}&S(\lambda_0, T)T \subset TS(\lambda_0, T), \quad (T - \lambda_0 I_{\mathcal{H}})S(\lambda_0, T) = I_{\mathcal{H}} - P(\lambda_0, T), \\ &S(\lambda_0, T)P(\lambda_0, T) = P(\lambda_0, T)S(\lambda_0, T) = 0.\end{aligned} \tag{4.4.11}$$

Finally,

$$\mu(\lambda_0, T) \leq m(\lambda_0, T) = \dim(\operatorname{ran}(P(\lambda_0, T))), \tag{4.4.12}$$

$$\operatorname{tr}(P(\lambda_0, T)) = m(\lambda_0, T), \quad \operatorname{tr}(D(\lambda_0, T)^k) = 0 \text{ for some } k \in \mathbb{N}. \tag{4.4.13}$$

Next, we need one more notation: Let $\Omega \subseteq \mathbb{C}$ be open and connected, and let $f\colon \Omega \to \mathbb{C}\cup\{\infty\}$ be meromorphic and not identically vanishing on Ω. The multiplicity function $m(z; f)$, $z \in \Omega$, is then defined by

$$m(z; f) = \begin{cases} k, & \text{if } z \text{ is a zero of } f \text{ of order } k, \\ -k, & \text{if } z \text{ is a pole of order } k, \\ 0, & \text{otherwise.} \end{cases} \tag{4.4.14}$$

$$= \frac{1}{2\pi i} \oint_{C(z;\varepsilon)} d\zeta \, \frac{f'(\zeta)}{f(\zeta)}, \quad z \in \Omega \tag{4.4.15}$$

for $\varepsilon > 0$ sufficiently small. If f vanishes identically on Ω, one defines

$$m(z; f) = +\infty, \quad z \in \Omega. \tag{4.4.16}$$

Here the circle $C(z;\varepsilon)$ is chosen sufficiently small such that $C(z;\varepsilon)$ contains no other singularities or zeros of f except, possibly, z.

The following result is due to Howland in the case where H_0 and H are self-adjoint. We will closely follow his strategy of proof and present detailed arguments in the more general situation considered here.

Theorem 4.4.5. *Assume Hypothesis 4.3.1. Then,*

$$\widetilde{\sigma}_{\mathrm{e}}(H) = \widetilde{\sigma}_{\mathrm{e}}(H_0). \tag{4.4.17}$$

In addition, let $\lambda_0 \in \mathbb{C}\backslash\widetilde{\sigma}_{\mathrm{e}}(H_0)$. Then there exists a neighborhood $U(\lambda_0)$ of λ_0 and a function $\Delta(\cdot)$ meromorphic on $U(\lambda_0)$, which does not vanish identically, such that the local Weinstein–Aronszajn formula

$$m(z, H) = m(z, H_0) + m(z; \Delta), \quad z \in U(\lambda_0) \tag{4.4.18}$$

holds.

Proof. By (4.2.10), $K(\cdot)$ is analytic on $\rho(H_0)$ and

$$K'(z) = -AR_0(z)[BR_0(z)^*]^*, \quad z \in \rho(H_0). \tag{4.4.19}$$

Let $z_0 \in \widetilde{\Phi}(H_0)$, then by (4.4.7),

$$R_0(z) = (z_0 - z)^{-1} P_0 + \sum_{k=1}^{\mu_0} (z_0 - z)^{-k-1} (-1)^k D_0^k + G_0(z), \tag{4.4.20}$$

where $G_0(\cdot)$ is analytic in a neighborhood of z_0. Since

$$\operatorname{ran}(D_0) \subseteq \operatorname{ran}(P_0) \subset \operatorname{dom}(H_0) \subset \operatorname{dom}(A), \tag{4.4.21}$$

AP_0B^*, AD_0B^*, and $AG_0(z)B^*$ have compact extensions from $\operatorname{dom}(B^*)$ to $\mathcal{K}$, and the extensions of AP_0B^* and AD_0B^* are given by the finite-rank operators $AP_0[BP_0^*]^*$ and $\overline{AP_0D_0P_0B^*}$, respectively. Moreover, it is easy to see that the extension of $AG_0(z)B^*$ is analytic near z_0. Consequently, $K(\cdot)$ is completely meromorphic on $\widetilde{\Phi}(H_0)$.

Similarly, by (4.3.2) and Lemma 4.4.3, $-\overline{AR(z)B^*}$ is completely meromorphic on $\widetilde{\Phi}(H_0)$. Moreover, by (4.3.2), any singularity z_0 of $-\overline{AR(z)B^*}$ is an isolated point of $\sigma(H)$. Since $R_0(z)$, $AR_0(z)$, and $BR_0(z)$ all have finite-rank principal parts at their poles, (4.2.13) and (4.3.2) show that $R(z)$ also has a finite-rank principal part at z_0. The latter implies that z_0 is an eigenvalue of H of finite algebraic multiplicity. Thus, $\widetilde{\Phi}(H_0) \subseteq \widetilde{\Phi}(H)$. Since by Remark 4.2.4 (ii) this formalism is symmetric with respect to H_0 and H, one also obtains $\widetilde{\Phi}(H_0) \supseteq \widetilde{\Phi}(H)$, and hence (4.4.17).

Next, by Lemma 4.4.2, let U_0 be a neighborhood of λ_0 such that

$$M(z)[I_{\mathcal{K}} - K(z)] = I_{\mathcal{K}} - F(z), \tag{4.4.22}$$

with M analytic and boundedly invertible on U_0 and some F meromorphic and of finite rank on U_0. One defines

$$\Delta(z) = \det(I_{\mathcal{K}} - F(z)), \quad z \in U_0. \tag{4.4.23}$$

Since by Lemma 4.4.3, $[I_{\mathcal{K}} - K(z)]^{-1}$ is meromorphic and $M(z)$ is boundedly invertible for all $z \in U_0$, $[I_{\mathcal{K}} - F(z)]^{-1}$ is also meromorphic on U_0, and hence, $\Delta(\cdot)$ is not identically zero on U_0. By Lemma 4.4.4 (iii) and cyclicity of the trace (i.e., $\operatorname{tr}(ST) = \operatorname{tr}(TS)$ for S and T bounded operators such that ST and TS lie in the trace class, cf. [165, Corollary 3.8]),

$$\begin{aligned}
\Delta'(z)/\Delta(z) &= -\operatorname{tr}([I_{\mathcal{K}} - F(z)]^{-1}F'(z)) \\
&= \operatorname{tr}([I_{\mathcal{K}} - K(z)]^{-1}M(z)^{-1}M'(z)[I_{\mathcal{K}} - K(z)] - [I_{\mathcal{K}} - K(z)]^{-1}K'(z)) \\
&= \operatorname{tr}(M(z)^{-1}M'(z) - K'(z)[I_{\mathcal{K}} - K(z)]^{-1}). \qquad (4.4.24)
\end{aligned}$$

Let $z_0 \in U_0$ and $C(z_0;\varepsilon)$ be a clockwise oriented circle centered at z_0 with sufficiently small radius ε (excluding all singularities of $[I_{\mathcal{K}} - F(z)]^{-1}$, except, possibly, z_0) contained in U_0. Then,

$$\begin{aligned}
m(z_0;\Delta) &= \frac{1}{2\pi i}\oint_{C(z_0;\varepsilon)} d\zeta\, \frac{\Delta'(\zeta)}{\Delta(\zeta)} \\
&= \frac{1}{2\pi i}\oint_{C(z_0;\varepsilon)} d\zeta\, \operatorname{tr}(M(\zeta)^{-1}M'(\zeta) - K'(\zeta)[I_{\mathcal{K}} - K(\zeta)]^{-1}). \qquad (4.4.25)
\end{aligned}$$

Since M is analytic and boundedly invertible on U_0, an interchange of the trace and the integral, using

$$\oint_{C(z_0;\varepsilon)} d\zeta\, M(\zeta)^{-1}M'(\zeta) = 0 \qquad (4.4.26)$$

and (4.4.19), then yields

$$\begin{aligned}
m(z_0;\Delta) &= \frac{1}{2\pi i}\operatorname{tr}\bigg(\oint_{C(z_0;\varepsilon)} d\zeta\, AR_0(\zeta)[BR_0(\zeta)^*]^*[I_{\mathcal{K}} - K(\zeta)]^{-1}\bigg) \\
&= \frac{1}{2\pi i}\operatorname{tr}\bigg(\oint_{C(z_0;\varepsilon)} d\zeta\, AR_0(\zeta)[BR(\zeta)^*]^*\bigg). \qquad (4.4.27)
\end{aligned}$$

Next, for $\varepsilon > 0$ sufficiently small, one infers from [109, p. 178] (cf. (4.4.13)) that

$$m(z_0,H) - m(z_0,H_0) = -\frac{1}{2\pi i}\operatorname{tr}\bigg(\oint_{C(z_0;\varepsilon)} d\zeta\, [R(\zeta) - R_0(\zeta)]\bigg)$$

$$= \frac{1}{2\pi i} \operatorname{tr}\bigg(\oint_{C(z_0;\varepsilon)} d\zeta\, [BR_0(\zeta)^*]^* [I_{\mathcal{K}} - K(\zeta)]^{-1} AR_0(\zeta) \bigg)$$
$$= \frac{1}{2\pi i} \operatorname{tr}\bigg(\oint_{C(z_0;\varepsilon)} d\zeta\, [BR(\zeta)^*]^* AR_0(\zeta) \bigg). \tag{4.4.28}$$

At this point we cannot simply change back the order of the trace and the integral and use the cyclicity of the trace to prove equality of (4.4.27) and (4.4.28) since now the integrand is not necessarily trace class. But one can prove the equality of (4.4.27) and (4.4.28) directly as follows. Writing (cf. (4.4.7)),

$$AR_0(z) = (z_0 - z)^{-1} \widetilde{P}_0 + \sum_{k=1}^{\mu_0} (z_0 - z)^{-k-1} (-1)^k \widetilde{D}_0^k + \sum_{k=0}^{\infty} (z_0 - z)^k (-1)^k \widetilde{S}_0^{k+1}, \tag{4.4.29}$$

$$[BR(z)^*]^* = (z_0 - z)^{-1} \widetilde{Q}_0 + \sum_{k=1}^{\nu_0} (z_0 - z)^{-k-1} (-1)^k \widetilde{E}_0^k + \sum_{k=0}^{\infty} (z_0 - z)^k (-1)^k \widetilde{T}_0^{k+1}, \tag{4.4.30}$$

one obtains

$$\operatorname{res}_{z=z_0}(AR_0(z)[BR(z)^*]^*) = \widetilde{P}_0 \widetilde{T}_0 + \widetilde{S}_0 \widetilde{Q}_0 + \sum_{k=1}^{\mu_0} \widetilde{D}_0^k \widetilde{T}_0^{k+1} + \sum_{k=1}^{\nu_0} \widetilde{S}_0^{k+1} \widetilde{E}_0^k, \tag{4.4.31}$$

$$\operatorname{res}_{z=z_0}([BR(z)^*]^* AR_0(z)) = \widetilde{T}_0 \widetilde{P}_0 + \widetilde{Q}_0 \widetilde{S}_0 + \sum_{k=1}^{\mu_0} \widetilde{T}_0^{k+1} \widetilde{D}_0^k + \sum_{k=1}^{\nu_0} \widetilde{E}_0^k \widetilde{S}_0^{k+1}. \tag{4.4.32}$$

Using the cyclicity of the trace and Cauchy's theorem then proves equality of (4.4.27) and (4.4.28) and hence (4.4.18). $\square$

Remark 4.4.6. Let H_0 be as in Hypothesis 4.2.1.

(*i*) Let $V \in \mathcal{B}_\infty(\mathcal{H})$ and define $H = H_0 + V$, $\operatorname{dom}(H) = \operatorname{dom}(H_0)$. Then (4.4.18) holds identifying $A = V$, $B = I_{\mathcal{H}}$, and $K(z) = VR_0(z)$ in connection with (4.2.13).

(*ii*) Let V be of finite-rank and define $H = H_0 + V$, $\operatorname{dom}(H) = \operatorname{dom}(H_0)$. Then (4.4.18) holds on $\widetilde{\Phi}(H_0)$ with $\Delta(z) = \det(I_{\mathcal{K}} - K(z))$, $K(z) = VR_0(z)$, $z \in \rho(H_0)$, and $U(\lambda_0) = \widetilde{\Phi}(H_0)$.

With the exception of the case discussed in Remark 4.4.6 (ii), Theorem 4.4.5 has the drawback that it yields a Weinstein–Aronszajn-type formula only locally on $U(\lambda_0)$. However, by the same token, the great generality of this formalism, basically assuming only compactness of $K(\cdot)$, must be emphasized. In the following section we will present Howland's global Aronszajn–Weinstein formula.

4.5 A Global Weinstein–Aronszajn Formula

To this end we introduce a new hypothesis on K:

Hypothesis 4.5.1. In addition to Hypothesis 4.3.1 we suppose the condition:

(v) For some $p \in \mathbb{N}$, $K(z) \in \mathcal{B}_p(\mathcal{K})$ for all $z \in \rho(H_0)$.

We denote by $\|\cdot\|_p$ the norm in $\mathcal{B}_p(\mathcal{K})$ and by $\det_p(\cdot)$ the regularized determinant of operators of the type $I_{\mathcal{K}} - L$, $L \in \mathcal{B}_p(\mathcal{K})$ (cf. [86], [87], [88, Chs. IX–XI], [89, Sect. 4.2], [163], [165, Ch. 9]).

We start by recalling the following result (cf. [89, p. 162–163], [165, p. 107]).

Lemma 4.5.2. *Let $p \in \mathbb{N}$ and assume that $\{L(z)\}_{z\in\Omega} \in \mathcal{B}_p(\mathcal{K})$ is a family of $\mathcal{B}_p(\mathcal{K})$-analytic operators on Ω, $\Omega \subseteq \mathbb{C}$ open. Let $\{P_n\}_{n\in\mathbb{N}}$ be a sequence of orthogonal projections in $\mathcal{K}$ converging strongly to $I_{\mathcal{K}}$ as $n \to \infty$. Then, the following limits hold uniformly with respect to z as z varies in compact subsets of Ω,*

$$\lim_{n\to\infty} \|P_n L(z) P_n - L(z)\|_p = 0, \tag{4.5.1}$$

$$\lim_{n\to\infty} \det{}_p(I_{\mathcal{K}} - P_n L(z) P_n) = \det{}_p(I_{\mathcal{K}} - L(z)), \tag{4.5.2}$$

$$\lim_{n\to\infty} \frac{d}{dz}\det{}_p(I_{\mathcal{K}} - P_n L(z) P_n) = \frac{d}{dz}\det{}_p(I_{\mathcal{K}} - L(z)). \tag{4.5.3}$$

So while the situation for analytic $\mathcal{B}_p(\mathcal{K})$-valued functions is very satisfactory, there is, however, a problem with meromorphic (even completely meromorphic) $\mathcal{B}_p(\mathcal{K})$ valued functions as pointed out by Howland. Indeed, suppose $L(z)$, $z \in \Omega$, is meromorphic in Ω and of finite rank. Then of course $\det(I_{\mathcal{K}} - L(\cdot))$ is meromorphic in Ω. However, the formula

$$\det{}_p(I_{\mathcal{K}} - L(z)) = \det(I_{\mathcal{K}} - L(z)) \exp\left[\operatorname{tr}\left(-\sum_{j=1}^{p-1} j^{-1} L(z)^j\right)\right], \quad z \in \Omega \qquad (4.5.4)$$

shows that $\det_p(I_{\mathcal{K}} - L(\cdot))$, for $p > 1$, in general, will exhibit essential singularities at poles of L. To sidestep this difficulty, Howland extends the definition of $m(\cdot\,; f)$ in (4.4.14), (4.4.15) to functions f with isolated essential singularities as follows: Suppose f is meromorphic in Ω except at isolated essential singularities. Then we use (4.4.15) again to define

$$m(z; f) = \frac{1}{2\pi i} \oint_{C(z;\varepsilon)} d\zeta \, \frac{f'(\zeta)}{f(\zeta)}, \quad z \in \Omega, \qquad (4.5.5)$$

where $\varepsilon > 0$ is chosen sufficiently small to exclude all singularities and zeros of f except possibly z.

Given Lemma 4.5.2 and the extension of $m(\cdot\,; f)$ to meromorphic functions with isolated essential singularities, Howland [96] then proves the following fundamental result (the proof of which is independent of any self-adjointness hypotheses on H_0 and H and hence omitted here).

Lemma 4.5.3 ([96]). *Let $p \in \mathbb{N}$ and assume that $\{L(z)\}_{z\in\Omega}$ is a family of $\mathcal{B}_p(\mathcal{K})$-valued completely meromorphic operators on Ω, $\Omega \subseteq \mathbb{C}$ open. Let $M(z)\}_{z\in\Omega}$ be a* *boundedly invertible operator-valued analytic function on* Ω *such that*

$$M(z)[I_{\mathcal{K}} - L(z)] = I_{\mathcal{K}} - F(z), \quad z \in \Omega, \tag{4.5.6}$$

where $F(z)$ *is meromorphic and of finite rank for all* $z \in \Omega$*. Define*

$$\Delta(z) = \det(I_{\mathcal{K}} - F(z)), \quad z \in \Omega, \tag{4.5.7}$$

and

$$\Delta_p(z) = \det{}_p(I_{\mathcal{K}} - L(z)), \quad z \in \Omega. \tag{4.5.8}$$

Then,

$$m(z; \Delta) = m(z; \Delta_p), \quad z \in \Omega. \tag{4.5.9}$$

Combining Theorem 4.4.5 and Lemma 4.5.3 yields Howland's global Weinstein–Aronszajn formula [96] extended to the non-self-adjoint case.

Theorem 4.5.4. *Assume Hypothesis 4.5.1. Then the global Weinstein–Aronszajn formula*

$$m(z, H) = m(z, H_0) + m(z; \det{}_p(I_{\mathcal{K}} - K(z))), \quad z \in \widetilde{\Phi}(H_0), \tag{4.5.10}$$

holds.

Remark 4.5.5. Let H_0 be as in Hypothesis 4.2.1, fix $p \in \mathbb{N}$, and assume $VR_0(z) \in \mathcal{B}_p(\mathcal{H})$. Define $H = H_0 + V$, $\mathrm{dom}(H) = \mathrm{dom}(H_0)$. Then (4.5.10) holds on $\widetilde{\Phi}(H_0)$ with $K(z) = VR_0(z)$. In the special case $p = 1$ this was first obtained by Kuroda [122].

4.6 An Application of Perturbation Determinants to Schrödinger Operators in Dimension $n = 1, 2, 3$

In dimension one on a half-line $(0,\infty)$, the perturbation determinant associated with the Birman–Schwinger kernel corresponding to a Schrödinger operator with an integrable potential on $(0,\infty)$ is known to coincide with the corresponding Jost function and hence with a simple Wronski determinant (cf. Lemmas 4.6.2 and 4.6.3). This reduction of an infinite-dimensional determinant to a finite-dimensional one is quite remarkable and in this section we intend to give some ideas as to how this fact can be generalized to dimensions two and three.

We start with the one-dimensional situation on the half-line $\Omega = (0,\infty)$ and introduce the Dirichlet and Neumann Laplacians $H_{0,+}^D$ and $H_{0,+}^N$ in $L^2((0,\infty);dx)$ by

$$\begin{aligned}
&H_{0,+}^D f = -f'', \\
&f \in \operatorname{dom}\big(H_{0,+}^D\big) = \{g \in L^2((0,\infty);dx) \,|\, g, g' \in AC([0,R]) \text{ for all } R>0, \\
&\qquad\qquad g(0)=0,\ g'' \in L^2((0,\infty);dx)\},
\end{aligned} \tag{4.6.1}$$

$$\begin{aligned}
&H_{0,+}^N f = -f'', \\
&f \in \operatorname{dom}\big(H_{0,+}^N\big) = \{g \in L^2((0,\infty);dx) \,|\, g, g' \in AC([0,R]) \text{ for all } R>0, \\
&\qquad\qquad g'(0)=0,\ g'' \in L^2((0,\infty);dx)\}.
\end{aligned} \tag{4.6.2}$$

Next, we make the following assumption on the potential V:

Hypothesis 4.6.1. Suppose $V \in L^1((0,\infty);dx)$.

Given Hypothesis 4.6.1, we introduce the perturbed operators H_Ω^D and H_Ω^N in

$L^2((0,\infty);dx)$ by

$$
\begin{aligned}
&H_+^D f = -f'' + Vf, \\
&f \in \mathrm{dom}\big(H_{0,+}^D\big) = \{g \in L^2((0,\infty);dx) \,|\, g, g' \in AC([0,R]) \text{ for all } R>0, \\
&\qquad\qquad g(0) = 0,\ (-g'' + Vg) \in L^2((0,\infty);dx)\},
\end{aligned} \tag{4.6.3}
$$

$$
\begin{aligned}
&H_+^N f = -f'' + Vf, \\
&f \in \mathrm{dom}\big(H_{0,+}^N\big) = \{g \in L^2((0,\infty);dx) \,|\, g, g' \in AC([0,R]) \text{ for all } R>0, \\
&\qquad\qquad g'(0) = 0,\ (-g'' + Vg) \in L^2((0,\infty);dx)\}.
\end{aligned} \tag{4.6.4}
$$

A fundamental system of solutions $\phi_+^D(z,\cdot)$, $\theta_+^D(z,\cdot)$, and the Jost solution $f_+(z,\cdot)$ of

$$
-\psi''(z,x) + V\psi(z,x) = z\psi(z,x), \quad z \in \mathbb{C}\backslash\{0\},\ x \geq 0, \tag{4.6.5}
$$

are introduced by

$$
\phi_+^D(z,x) = z^{-1/2}\sin(z^{1/2}x) + \int_0^x dx' g_+^{(0)}(z,x,x')V(x')\phi_+^D(z,x'), \tag{4.6.6}
$$

$$
\theta_+^D(z,x) = \cos(z^{1/2}x) + \int_0^x dx' g_+^{(0)}(z,x,x')V(x')\theta_+^D(z,x'), \tag{4.6.7}
$$

$$
\begin{aligned}
f_+(z,x) = e^{iz^{1/2}x} - \int_x^\infty dx' g_+^{(0)}(z,x,x')V(x')f_+(z,x'), \\
\mathrm{Im}(z^{1/2}) \geq 0,\ z \in \mathbb{C}\backslash\{0\},\ x \geq 0,
\end{aligned} \tag{4.6.8}
$$

where

$$
g_+^{(0)}(z,x,x') = z^{-1/2}\sin(z^{1/2}(x-x')). \tag{4.6.9}
$$

We introduce

$$
u = \exp(i\arg(V))|V|^{1/2}, \quad v = |V|^{1/2}, \text{ so that } V = u\,v, \tag{4.6.10}
$$

and denote by I_+ the identity operator in $L^2((0,\infty);dx)$. In addition, we let

$$W(f,g)(x) = f(x)g'(x) - f'(x)g(x), \quad x \geq 0, \tag{4.6.11}$$

denote the Wronskian of f and g, where $f, g \in C^1([0,\infty))$. We also recall our convention to denote by M_f the operator of multiplication in $L^2((0,\infty);dx)$ by an element $f \in L^1_{\text{loc}}((0,\infty);dx)$ (and similarly in the higher-dimensional context in the main part of this section).

The following is a modern formulation of a classical result by Jost and Pais [104].

Lemma 4.6.2 ([74, Theorem 4.3])**.** *Assume Hypothesis 4.6.1 and $z \in \mathbb{C}\backslash[0,\infty)$ with $\operatorname{Im}(z^{1/2}) > 0$. Then $\overline{M_u(H_{0,+}^D - zI_+)^{-1}M_v} \in \mathcal{B}_1(L^2((0,\infty);dx))$ and*

$$\begin{aligned}\det\big(I_+ + \overline{M_u(H_{0,+}^D - zI_+)^{-1}M_v}\big) &= 1 + z^{-1/2}\int_0^\infty dx\, \sin(z^{1/2}x)V(x)f_+(z,x) \\ &= W(f_+(z,\cdot),\phi_+^D(z,\cdot)) = f_+(z,0).\end{aligned} \tag{4.6.12}$$

Performing calculations similar to Section 4 in [74] for the pair of operators $H_{0,+}^N$ and H_+^N, one also obtains the following result.

Lemma 4.6.3. *Assume Hypothesis 4.6.1 and $z \in \mathbb{C}\backslash[0,\infty)$ with $\operatorname{Im}(z^{1/2}) > 0$. Then $\overline{M_u(H_{0,+}^N - zI_+)^{-1}M_v} \in \mathcal{B}_1\big(L^2((0,\infty);dx)\big)$ and*

$$\begin{aligned}\det\big(I_+ + \overline{M_u(H_{0,+}^N - zI_+)^{-1}M_v}\big) &= 1 + iz^{-1/2}\int_0^\infty dx\, \cos(z^{1/2}x)V(x)f_+(z,x) \\ &= -\frac{W(f_+(z,\cdot),\theta_+^D(z,\cdot))}{iz^{1/2}} = \frac{f'_+(z,0)}{iz^{1/2}}.\end{aligned} \tag{4.6.13}$$

We emphasize that (4.6.12) and (4.6.13) exhibit the remarkable fact that the Fredholm determinant associated with trace class operators in the infinite-dimensional space $L^2((0,\infty);dx)$ is reduced to a simple Wronski determinant of $\mathbb{C}$-valued distributional solutions of (4.6.5). This fact goes back to Jost and Pais [104] (see also [74], [140], [142], [144, Sect. 12.1.2], [165, Proposition 5.7], [168], and the extensive literature cited in these references). The principal aim of this section is to explore possibilities to extend this fact to higher dimensions $n = 2, 3$. While a straightforward generalization of (4.6.12), (4.6.13) appears to be difficult, we will next derive a formula for the ratio of such determinants which permits a direct extension to dimensions $n = 2, 3$.

For this purpose we introduce the boundary trace operators γ_D (Dirichlet trace) and γ_N (Neumann trace) which, in the current one-dimensional half-line situation, are just the functionals,

$$\gamma_D\colon \begin{cases} C([0,\infty)) \to \mathbb{C} \\ \qquad\qquad g \mapsto g(0) \end{cases}, \quad \gamma_N\colon \begin{cases} C^1([0,\infty)) \to \mathbb{C} \\ \qquad\qquad h \mapsto -h'(0) \end{cases}. \tag{4.6.14}$$

In addition, we denote by $m_{0,+}^D$, m_+^D, $m_{0,+}^N$, and m_+^N the Weyl–Titchmarsh m-functions corresponding to $H_{0,+}^D$, H_+^D, $H_{0,+}^N$, and H_+^N, respectively,

$$m_{0,+}^D(z) = iz^{1/2}, \quad m_{0,+}^N(z) = -\frac{1}{m_{0,+}^D(z)} = iz^{-1/2}, \tag{4.6.15}$$

$$m_+^D(z) = \frac{f_+'(z,0)}{f_+(z,0)}, \quad m_+^N(z) = -\frac{1}{m_+^D(z)} = -\frac{f_+(z,0)}{f_+'(z,0)}. \tag{4.6.16}$$

Theorem 4.6.4. *Assume Hypothesis 4.6.1 and let $z \in \mathbb{C}\backslash\sigma(H_+^D)$ with $\operatorname{Im}(z^{1/2}) > 0$. Then,*

$$\begin{aligned} &\frac{\det\big(I_+ + \overline{M_u(H_{0,+}^N - zI_+)^{-1}M_v}\big)}{\det\big(I_+ + \overline{M_u(H_{0,+}^D - zI_+)^{-1}M_v}\big)} \\ &\quad = \frac{W(f_+(z),\phi_+^N(z))}{iz^{1/2}W(f_+(z),\phi_+^D(z))} = \frac{f_+'(z,0)}{iz^{1/2}f_+(z,0)} = \frac{m_+^D(z)}{m_{0,+}^D(z)} = \frac{m_{0,+}^N(z)}{m_+^N(z)} \end{aligned} \tag{4.6.17}$$

$$= 1 - \overline{\left(\gamma_N (H_+^D - zI_+)^{-1} M_V \left[\gamma_D (H_{0,+}^N - \overline{z} I_+)^{-1}\right]^*\right)} 1. \tag{4.6.18}$$

Proof. We start by noting that $\sigma(H_{0,+}^D) = \sigma(H_{0,+}^N) = [0, \infty)$. Applying Lemmas 4.6.2 and 4.6.3 and equations (4.6.15) and (4.6.16) proves (4.6.17).

To verify the equality of (4.6.17) and (4.6.18) requires some preparations. First we recall that the Green's functions (i.e., integral kernels) of the resolvents of $H_{0,+}^D$ and $H_{0,+}^N$ are given by

$$(H_{0,+}^D - zI_+)^{-1}(x, x') = \begin{cases} \frac{\sin(z^{1/2}x)}{z^{1/2}} e^{iz^{1/2}x'}, & 0 \le x \le x', \\ \frac{\sin(z^{1/2}x')}{z^{1/2}} e^{iz^{1/2}x}, & 0 \le x' \le x, \end{cases} \tag{4.6.19}$$

$$(H_{0,+}^N - zI_+)^{-1}(x, x') = \begin{cases} \frac{\cos(z^{1/2}x)}{-iz^{1/2}} e^{iz^{1/2}x'}, & 0 \le x \le x', \\ \frac{\cos(z^{1/2}x')}{-iz^{1/2}} e^{iz^{1/2}x}, & 0 \le x' \le x, \end{cases} \tag{4.6.20}$$

and hence Krein's formula for the resolvent difference of $H_{0,+}^D$ and $H_{0,+}^N$ takes on the simple form

$$(H_{0,+}^D - zI_+)^{-1} - (H_{0,+}^N - zI_+)^{-1} = -iz^{-1/2} (\overline{\psi_{0,+}(z, \cdot)}, \cdot)_{L^2((0,\infty);dx)} \psi_{0,+}(z, \cdot),$$
$$z \in \rho(H_{0,+}^D) \cap \rho(H_{0,+}^N),\ \mathrm{Im}(z^{1/2}) > 0, \tag{4.6.21}$$

where we abbreviated

$$\psi_{0,+}(z, x) = e^{iz^{1/2}x}, \quad \mathrm{Im}(z^{1/2}) > 0,\ x \ge 0. \tag{4.6.22}$$

We also recall

$$(H_+^D - zI_+)^{-1}(x, x') = \begin{cases} \phi_+^D(z, x)\psi_+(z, x'), & 0 \le x \le x', \\ \phi_+^D(z, x')\psi_+(z, x), & 0 \le x' \le x, \end{cases} \tag{4.6.23}$$

where

$$\psi_+(z, x) = \theta_+^D(z, x) + m_+^D(z)\phi_+^D(z, x), \quad z \in \rho(H_+^D),\ x \ge 0, \tag{4.6.24}$$

and

$$\psi_+(z,\cdot) = \frac{f_+(z,\cdot)}{f_+(z,0)} \in L^2((0,\infty);dx), \quad z \in \rho(H_+^D). \tag{4.6.25}$$

In fact, a standard iteration argument applied to (4.6.8) shows that

$$|\psi_+(z,x)| \leq C(z) e^{-\mathrm{Im}(z^{1/2})x}, \quad \mathrm{Im}(z^{1/2}) > 0,\ x \geq 0. \tag{4.6.26}$$

In addition, we note that

$$\gamma_N (H_{0,+}^D - zI_+)^{-1} g = -\int_0^\infty dx\, e^{iz^{1/2}x} g(x), \quad g \in L^2((0,\infty);dx), \tag{4.6.27}$$

$$\gamma_N (H_+^D - zI_+)^{-1} g = -\int_0^\infty dx\, \psi_+(z,x) g(x), \quad g \in L^2((0,\infty);dx), \tag{4.6.28}$$

$$\gamma_D (H_{0,+}^N - zI_+)^{-1} f = iz^{-1/2} \int_0^\infty dx\, e^{iz^{1/2}x} f(x), \quad f \in L^2((0,\infty);dx), \tag{4.6.29}$$

and hence,

$$\big(\big[\gamma_D (H_{0,+}^N - \overline{z} I_+)^{-1}\big]^* c\big)(\cdot) = icz^{-1/2} \psi_{0,+}(z,\cdot), \quad c \in \mathbb{C}. \tag{4.6.30}$$

Then Krein's formula (4.6.21) can be rewritten as

$$\begin{aligned}(H_{0,+}^D - zI_+)^{-1} - (H_{0,+}^N - zI_+)^{-1} = \big[\gamma_D (H_{0,+}^N - \overline{z} I_+)^{-1}\big]^* \gamma_N (H_{0,+}^D - zI_+)^{-1}, \\ z \in \rho(H_{0,+}^D) \cap \rho(H_{0,+}^N),\ \mathrm{Im}(z^{1/2}) > 0.\end{aligned} \tag{4.6.31}$$

Finally, using the facts (cf. (4.6.8))

$$f_+(z,0) = 1 + z^{-1/2} \int_0^\infty dx\, \sin(z^{1/2}x) V(x) f_+(z,x), \tag{4.6.32}$$

$$f_+'(z,0) = iz^{1/2} - \int_0^\infty dx\, \cos(z^{1/2}) V(x) f_+(z,x), \tag{4.6.33}$$

one computes (since $v \in L^2(\mathbb{R};dx)$ and $\psi_+(z,\cdot) \in L^\infty(\mathbb{R};dx)$)

$$-\big[\overline{\gamma_N (H_+^D - zI_+)^{-1} M_V \big[\gamma_D (H_{0,+}^N - \overline{z} I_+)^{-1}\big]^*}\big] 1$$

$$
\begin{aligned}
&= -iz^{-1/2}\overline{\gamma_N(H_+^D - zI_+)^{-1}M_u}(v\psi_{0,+})(z,\cdot) \\
&= iz^{-1/2}\int_0^\infty dx\, e^{iz^{1/2}x}V(x)\psi_+(z,x) \\
&= iz^{-1/2}\int_0^\infty dx\left[\cos(z^{1/2}x) + iz^{1/2}\frac{\sin(z^{1/2}x)}{z^{1/2}}\right]V(x)\frac{f_+(z,x)}{f_+(z,0)} \\
&= \frac{i}{z^{1/2}f_+(z,0)}[iz^{1/2} - f_+'(z,0) + iz^{1/2}(f_+(z,0)-1)] \\
&= \frac{f_+'(z,0)}{iz^{1/2}f_+(z,0)} - 1. \qquad (4.6.34)
\end{aligned}
$$

$\square$

At first sight it may seem unusual to even attempt to prove (4.6.18) in the one-dimensional case since (4.6.17) already yields the reduction of a Fredholm determinant to a simple Wronski determinant. However, we will see in Theorem 4.6.11 that it is precisely (4.6.18) that permits a straightforward extension to dimensions $n = 2, 3$.

Remark 4.6.5. As in Theorem 4.6.4 we assume Hypothesis 4.6.1 and suppose $z \in \mathbb{C}\backslash\sigma(H_+^D)$. First we note that

$$
(H_{0,+}^D - zI_+)^{-1/2}(H_+^D - zI_+)(H_{0,+}^D - zI_+)^{-1/2} - I_+ \in \mathcal{B}_1\big(L^2((0,\infty);dx)\big), \quad (4.6.35)
$$

$$
(H_{0,+}^N - zI_+)^{-1/2}(H_+^N - zI_+)(H_{0,+}^N - zI_+)^{-1/2} - I_+ \in \mathcal{B}_1\big(L^2((0,\infty);dx)\big). \quad (4.6.36)
$$

Indeed, it follows from the proof of [74, Theorem 4.2] (cf. also Lemma 4.6.8 below), that

$$
\overline{(H_{0,+}^D - zI_+)^{-1/2}M_u},\ M_v(H_{0,+}^D - zI_+)^{-1/2} \in \mathcal{B}_2\big(L^2((0,\infty);dx)\big), \qquad (4.6.37)
$$

and hence,

$$
(H_{0,+}^D - zI_+)^{-1/2}(H_+^D - zI_+)(H_{0,+}^D - zI_+)^{-1/2} - I_+ \qquad (4.6.38)
$$

$$= (H_{0,+}^D - zI_+)^{-1/2} M_V (H_{0,+}^D - zI_+)^{-1/2} \in \mathcal{B}_1\big(L^2((0,\infty); dx)\big). \tag{4.6.39}$$

This proves (4.6.35), and a similar argument yields (4.6.36). Using the cyclicity of $\det(\cdot)$, one can then rewrite the left-hand side of (4.6.17) as follows,

$$\begin{aligned}
&\frac{\det\big(I_+ + \overline{M_u(H_{0,+}^N - zI_+)^{-1}M_v}\big)}{\det\big(I_+ + \overline{M_u(H_{0,+}^D - zI_+)^{-1}M_v}\big)} \\
&\quad = \frac{\det\big(I_+ + (H_{0,+}^N - zI_+)^{-1/2} M_V (H_{0,+}^N - zI_+)^{-1/2}\big)}{\det\big(I_+ + (H_{0,+}^D - zI_+)^{-1/2} M_V (H_{0,+}^D - zI_+)^{-1/2}\big)} \\
&\quad = \frac{\det\big((H_{0,+}^N - zI_+)^{-1/2}(H_+^N - zI_+)(H_{0,+}^N - zI_+)^{-1/2}\big)}{\det\big((H_{0,+}^D - zI_+)^{-1/2}(H_+^D - zI_+)(H_{0,+}^D - zI_+)^{-1/2}\big)}.
\end{aligned} \tag{4.6.40}$$

Equation (4.6.40) illustrates the kind of symmetrized perturbation determinants underlying Theorem 4.6.4.

Now we turn to dimensions $n = 2, 3$. As a general rule, we will have to replace Fredholm determinants by modified ones.

For the remainder of this section we make the following assumptions on the domain $\Omega \subset \mathbb{R}^n$, $n = 2, 3$, and the potential V:

Hypothesis 4.6.6. Let $n = 2, 3$.

(i) Assume that $\Omega \subset \mathbb{R}^n$ is an open nonempty domain of class $C^{1,r}$ for some $(1/2) < r < 1$ with a compact, nonempty boundary, $\partial\Omega$. (For details we refer to Appendix C.)

(ii) Suppose that $V \in L^2(\Omega; d^n x)$.

First we introduce the boundary trace operator γ_D^0 (Dirichlet trace) by

$$\gamma_D^0 \colon C(\overline{\Omega}) \to C(\partial\Omega), \quad \gamma_D^0 u = u|_{\partial\Omega}. \tag{4.6.41}$$

Then there exists a bounded, linear operator γ_D,

$$\gamma_D\colon H^s(\Omega) \to H^{s-1/2}(\partial\Omega) \hookrightarrow L^2(\partial\Omega; d^{n-1}\sigma), \quad 1/2 < s < 3/2, \tag{4.6.42}$$

whose action is compatible with γ_D^0, that is, the two Dirichlet trace operators coincide on the intersection of their domains. It is well-known (see, e.g., [130, Theorem 3.38]), that γ_D is bounded. Here $d^{n-1}\sigma$ denotes the surface measure on $\partial\Omega$ and we refer to Appendix C for our notation in connection with Sobolev spaces.

Next, let $I_{\partial\Omega}$ denote the identity operator in $L^2(\partial\Omega; d^{n-1}\sigma)$, and introduce the operator γ_N (Neumann trace) by

$$\gamma_N = \nu \cdot \gamma_D \nabla\colon H^{s+1}(\Omega) \to L^2(\partial\Omega; d^{n-1}\sigma), \quad 1/2 < s < 3/2, \tag{4.6.43}$$

where ν denotes outward pointing normal unit vector to $\partial\Omega$. It follows from (4.6.42) that γ_N is also a bounded operator.

Given Hypothesis 4.6.6 (i), we introduce the Dirichlet and Neumann Laplacians $H_{0,\Omega}^D$ and $H_{0,\Omega}^N$ associated with the domain Ω as follows,

$$H_{0,\Omega}^D = -\Delta, \quad \mathrm{dom}(H_{0,\Omega}^D) = \{u \in H^2(\Omega) \,|\, \gamma_D u = 0\}, \tag{4.6.44}$$

$$H_{0,\Omega}^N = -\Delta, \quad \mathrm{dom}(H_{0,\Omega}^N) = \{u \in H^2(\Omega) \,|\, \gamma_N u = 0\}. \tag{4.6.45}$$

In the following we denote by I_Ω the identity operator in $L^2(\Omega; d^n x)$.

Lemma 4.6.7. *Assume Hypothesis 4.6.6* (i)*. Then the operators* $H_{0,\Omega}^D$ *and* $H_{0,\Omega}^N$ *introduced in* (4.6.44) *and* (4.6.45) *are nonnegative and self-adjoint in* $\mathcal{H} = L^2(\Omega; d^n x)$ *and the following mapping properties hold for all* $q \in [0,1]$ *and* $z \in \mathbb{C}\backslash[0,\infty)$*,*

$$(H_{0,\Omega}^D - zI_\Omega)^{-q},\, (H_{0,\Omega}^N - zI_\Omega)^{-q} \in \mathcal{B}\big(L^2(\Omega; d^n x), H^{2q}(\Omega)\big). \tag{4.6.46}$$

The fractional powers in (4.6.46) (and in subsequent analogous cases such as in (4.6.52)) are defined via the functional calculus implied by the spectral theorem for self-adjoint operators. For the proof of Lemma 4.6.7 we refer to Lemmas C.1 and C.2 in Appendix C.

Lemma 4.6.8. *Assume that $\Omega \subset \mathbb{R}^n$, $n = 2, 3$, is an open nonempty domain of class $C^{1,r}$ for some $(1/2) < r < 1$ with a compact, nonempty boundary, $\partial\Omega$ and let $p \geq 2$, $(n/2p) < q \leq 1$, $f \in L^p(\Omega; d^n x)$, and $z \in \mathbb{C}\backslash[0, \infty)$. Then,*

$$M_f(H_{0,\Omega}^D - zI_\Omega)^{-q},\, M_f(H_{0,\Omega}^N - zI_\Omega)^{-q} \in \mathcal{B}_p\big(L^2(\Omega; d^n x)\big) \tag{4.6.47}$$

and for some $c > 0$ (independent of z and f)

$$\begin{aligned}
&\big\|M_f(H_{0,\Omega}^D - zI_\Omega)^{-q}\big\|_{\mathcal{B}_p(L^2(\Omega;d^n x))}^2 \\
&\quad \leq c\left(1 + \frac{|z|^{2q}+1}{\operatorname{dist}(z,\sigma(H_{0,\Omega}^D))^{2q}}\right)\|(|\cdot|^2 - z)^{-q}\|_{L^p(\mathbb{R}^n;d^n x)}^2\|f\|_{L^p(\Omega;d^n x)}^2, \\
&\big\|M_f(H_{0,\Omega}^N - zI_\Omega)^{-q}\big\|_{\mathcal{B}_p(L^2(\Omega;d^n x))}^2 \\
&\quad \leq c\left(1 + \frac{|z|^{2q}+1}{\operatorname{dist}(z,\sigma(H_{0,\Omega}^N))^{2q}}\right)\|(|\cdot|^2 - z)^{-q}\|_{L^p(\mathbb{R}^n;d^n x)}^2\|f\|_{L^p(\Omega;d^n x)}^2.
\end{aligned} \tag{4.6.48}$$

Proof. We start by noting that under the assumption that Ω is a Lipschitz domain, there is a bounded extension operator $\mathcal{E}$,

$$\mathcal{E} \in \mathcal{B}\big(H^s(\Omega), H^s(\mathbb{R}^n)\big) \text{ such that } (\mathcal{E}u)|_\Omega = u, \quad u \in H^s(\Omega), \tag{4.6.49}$$

for all $s \in \mathbb{R}$ (see, e.g., [156]). Next, for notational convenience, we denote by $H_{0,\Omega}$ either one of the operators $H_{0,\Omega}^D$ or $H_{0,\Omega}^N$ and by $\mathcal{R}_\Omega$ the restriction operator

$$\mathcal{R}_\Omega\colon \begin{cases} L^2(\mathbb{R}^n; d^n x) \to L^2(\Omega; d^n x), \\ \qquad u \mapsto u|_\Omega. \end{cases} \tag{4.6.50}$$

Moreover, we introduce the following extension $\tilde{f}$ of f,

$$\tilde{f}(x) = \begin{cases} f(x), & x \in \Omega, \\ 0, & x \in \mathbb{R}^n \backslash \Omega, \end{cases} \qquad \tilde{f} \in L^p(\mathbb{R}^n; d^n x). \tag{4.6.51}$$

Then,

$$M_f (H_{0,\Omega} - zI_\Omega)^{-q} = \mathcal{R}_\Omega M_{\tilde{f}} (H_0 - zI)^{-q} (H_0 - zI)^q \mathcal{E} (H_{0,\Omega} - zI_\Omega)^{-q}, \tag{4.6.52}$$

where (for simplicity) I denotes the identity operator in $L^2(\mathbb{R}^n; d^n x)$ and H_0 denotes the nonnegative self-adjoint operator

$$H_0 = -\Delta, \quad \operatorname{dom}(H_0) = H^2(\mathbb{R}^n) \tag{4.6.53}$$

in $L^2(\mathbb{R}^n; d^n x)$.

Let $g \in L^2(\Omega; d^n x)$ and define $h = (H_{0,\Omega} - zI_\Omega)^{-q} g$, then by Lemma C.2 $h \in H^{2q}(\Omega) \subset L^2(\Omega; d^n x)$. Utilizing the spectral theorem for the nonnegative self-adjoint operator $H_{0,\Omega}$ in $L^2(\Omega; d^n x)$, one computes,

$$\begin{aligned} \|h\|^2_{L^2(\Omega; d^n x)} &= \big\| (H_{0,\Omega} - zI_\Omega)^{-q} g \big\|^2_{L^2(\Omega; d^n x)} \\ &= \int_{\sigma(H_{0,\Omega})} |\lambda - z|^{-2q} \big(dE_{H_{0,\Omega}}(\lambda) g, g \big)_{L^2(\Omega; d^n x)} \\ &\leq \operatorname{dist}(z, \sigma(H_{0,\Omega}))^{-2q} \, \|g\|^2_{L^2(\Omega; d^n x)} \end{aligned} \tag{4.6.54}$$

and since $(H_{0,\Omega} + I_\Omega)^{-q} \in \mathcal{B}(L^2(\Omega; d^n x), H^{2q}(\Omega))$,

$$\begin{aligned} \|h\|^2_{H^{2q}(\Omega)} &= \big\| (H_{0,\Omega} + I_\Omega)^{-q} (H_{0,\Omega} + I_\Omega)^q h \big\|^2_{H^{2q}(\Omega)} \leq c \, \| (H_{0,\Omega} + I_\Omega)^q h \|^2_{L^2(\Omega; d^n x)} \\ &= c \int_{\sigma(H_{0,\Omega})} |\lambda + 1|^{2q} \big(dE_{H_{0,\Omega}}(\lambda) h, h \big)_{L^2(\Omega; d^n x)} \\ &\leq 2c \int_{\sigma(H_{0,\Omega})} \big(|\lambda - z|^{2q} + |z + 1|^{2q} \big) \big(dE_{H_{0,\Omega}}(\lambda) h, h \big)_{L^2(\Omega; d^n x)} \end{aligned} \tag{4.6.55}$$

$$= 2c\big(\|(H_{0,\Omega} - zI_\Omega)^q h\|_{H^{2q}(\Omega)}^2 + |z+1|^{2q} \|h\|_{L^2(\Omega;d^nx)}^2 \big)$$
$$\leq 2c\big(1 + |z+1|^{2q}\text{dist}(z, \sigma(H_{0,\Omega}))^{-2q}\big) \|g\|_{L^2(\Omega;d^nx)}^2,$$

where $E_{H_{0,\Omega}}(\cdot)$ denotes the spectral family of $H_{0,\Omega}$. Moreover, utilizing the representation of $(H_0 - zI)^q$ as the operator of multiplication by $\big(|\xi|^2 - z\big)^q$ in the Fourier space $L^2(\mathbb{R}^n; d^n\xi)$ and the fact that by (4.6.49)

$$\mathcal{E} \in \mathcal{B}(H^{2q}(\Omega), H^{2q}(\mathbb{R}^n)) \cap \mathcal{B}(L^2(\Omega; d^nx), L^2(\mathbb{R}^n; d^nx)), \tag{4.6.56}$$

one computes

$$\begin{aligned}
\|(H_0 - zI)^q \mathcal{E}h\|_{L^2(\mathbb{R}^n;d^nx)}^2 &= \int_{\mathbb{R}^n} d^n\xi \, \big||\xi|^2 - z\big|^{2q} \, |(\widehat{\mathcal{E}h})(\xi)|^2 \\
&\leq 2 \int_{\mathbb{R}^n} d\xi \big(|\xi|^{4q} + |z|^{2q}\big) |(\widehat{\mathcal{E}h})(\xi)|^2 \\
&\leq 2\big(\|\mathcal{E}h\|_{H^{2q}(\mathbb{R}^n)}^2 + |z|^{2q} \|\mathcal{E}h\|_{L^2(\mathbb{R}^n;d^nx)}^2 \big) \\
&\leq 2c\big(\|h\|_{H^{2q}(\Omega)}^2 + |z|^{2q} \|h\|_{L^2(\Omega;d^nx)}^2 \big).
\end{aligned} \tag{4.6.57}$$

Combining the estimates (4.6.54), (4.6.55), and (4.6.57), one obtains

$$(H_0 - zI)^q \mathcal{E} (H_{0,\Omega} - zI_\Omega)^{-q} \in \mathcal{B}\big(L^2(\Omega; d^nx), L^2(\mathbb{R}^n; d^nx)\big) \tag{4.6.58}$$

and the following norm estimate with some $c > 0$,

$$\big\|(H_0 - zI)^q \mathcal{E} (H_{0,\Omega} - zI_\Omega)^{-q}\big\|_{\mathcal{B}\left(L^2(\Omega;d^nx), L^2(\mathbb{R}^n;d^nx)\right)}^2 \leq c + \frac{c(|z|^{2q} + 1)}{\text{dist}(z, \sigma(H_{0,\Omega}))^{2q}}. \tag{4.6.59}$$

Next, by [165, Theorem 4.1] (or [150, Theorem XI.20]) one obtains

$$M_{\tilde{f}} (H_0 - zI)^{-q} \in \mathcal{B}_p\big(L^2(\mathbb{R}^n; d^nx)\big) \tag{4.6.60}$$

and

$$\begin{aligned}
\big\|M_{\tilde{f}} (H_0 - zI)^{-q}\big\|_{\mathcal{B}_p(L^2(\mathbb{R}^n;d^nx))} &\leq c \, \|(|\cdot|^2 - z)^{-q}\|_{L^p(\mathbb{R}^n;d^nx)} \|\tilde{f}\|_{L^p(\mathbb{R}^n;d^nx)} \\
&= c \, \|(|\cdot|^2 - z)^{-q}\|_{L^p(\mathbb{R}^n;d^nx)} \|f\|_{L^p(\Omega;d^nx)}.
\end{aligned} \tag{4.6.61}$$

Thus, (4.6.47) follows from (4.6.52), (4.6.58), (4.6.60), and (4.6.48) follows from (4.6.52), (4.6.59), and (4.6.61). □

Lemma 4.6.9. *Assume Hypothesis 4.6.6(i) and let* $\varepsilon \in (0,1]$, $n = 2,3$, *and* $z \in \mathbb{C}\backslash[0,\infty)$. *Then,*

$$\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-\frac{3+\varepsilon}{4}}, \gamma_D(H_{0,\Omega}^N - zI_\Omega)^{-\frac{1+\varepsilon}{4}} \in \mathcal{B}\big(L^2(\Omega; d^n x), L^2(\partial\Omega; d^{n-1}\sigma)\big). \quad (4.6.62)$$

Proof. It follows from (4.6.46), that

$$(H_{0,\Omega}^D - zI_\Omega)^{-\frac{3+\varepsilon}{4}} \in \mathcal{B}\big(L^2(\Omega; d^n x), H^{\frac{3+\varepsilon}{2}}(\Omega)\big), \quad (4.6.63)$$

$$(H_{0,\Omega}^N - zI_\Omega)^{-\frac{1+\varepsilon}{4}} \in \mathcal{B}\big(L^2(\Omega; d^n x), H^{\frac{1+\varepsilon}{2}}(\Omega)\big), \quad (4.6.64)$$

and hence one infers the result from (4.6.42) and (4.6.43). □

Corollary 4.6.10. *Let* $f_1 \in L^{p_1}(\Omega; d^n x)$, $p_1 \geq 2$, $p_1 > 2n/3$, $f_2 \in L^{p_2}(\Omega; d^n x)$, $p_2 > 2n$, $n = 2,3$, *and* $z \in \mathbb{C}\backslash[0,\infty)$. *Then,*

$$\overline{\gamma_D(H_{0,\Omega}^N - zI_\Omega)^{-1} M_{f_1}} \in \mathcal{B}_{p_1}\big(L^2(\Omega; d^n x), L^2(\partial\Omega; d^{n-1}\sigma)\big), \quad (4.6.65)$$

$$\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1} M_{f_2}} \in \mathcal{B}_{p_2}\big(L^2(\Omega; d^n x), L^2(\partial\Omega; d^{n-1}\sigma)\big) \quad (4.6.66)$$

and for some $c_j(z) > 0$ (*independent of* f_j), $j = 1,2$,

$$\Big\|\overline{\gamma_D(H_{0,\Omega}^N - zI_\Omega)^{-1} M_{f_1}}\Big\|_{\mathcal{B}_{p_1}(L^2(\Omega; d^n x), L^2(\partial\Omega; d^{n-1}\sigma))} \leq c_1(z) \left\|f_1\right\|_{L^{p_1}(\Omega; d^n x)}, \quad (4.6.67)$$

$$\Big\|\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1} M_{f_2}}\Big\|_{\mathcal{B}_{p_2}(L^2(\Omega; d^n x), L^2(\partial\Omega; d^{n-1}\sigma))} \leq c_2(z) \left\|f_2\right\|_{L^{p_2}(\Omega; d^n x)}. \quad (4.6.68)$$

Proof. Let $\varepsilon_1, \varepsilon_2 \in (0,1)$ be such that $0 < \varepsilon_1 < \min\{1, 3 - (2n/p_1)\}$ and $0 < \varepsilon_2 < 1 - (2n/p_2)$. Then,

$$\overline{\gamma_D(H_{0,\Omega}^N - zI_\Omega)^{-1} M_{f_1}} = \gamma_D(H_{0,\Omega}^N - zI_\Omega)^{-\frac{1+\varepsilon_1}{4}} \overline{(H_{0,\Omega}^N - zI_\Omega)^{-\frac{3-\varepsilon_1}{4}} M_{f_1}}, \quad (4.6.69)$$

$$\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{f_2}} = \gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-\frac{3+\varepsilon_2}{4}}\overline{(H_{0,\Omega}^D - zI_\Omega)^{-\frac{1-\varepsilon_2}{4}}M_{f_2}} \tag{4.6.70}$$

together with Lemmas 4.6.8 and 4.6.9 prove the corollary. □

Next, we introduce the perturbed operators H_Ω^D and H_Ω^N in $L^2(\Omega; d^n x)$ as follows. We denote by $A = M_u$ and $B = B^* = M_v$ the operators of multiplication by $u = \exp(i\arg(V))|V|^{1/2}$ and $v = |V|^{1/2}$ in $L^2(\Omega; d^n x)$, respectively, so that $M_V = BA = M_u M_v$. Applying Lemma 4.6.8 to $f = u \in L^4(\Omega; d^n x)$ with $q = 1/2$ yields

$$M_u(H_{0,\Omega}^D - zI_\Omega)^{-1/2}, \overline{(H_{0,\Omega}^D - zI_\Omega)^{-1/2}M_v} \in \mathcal{B}_4\big(L^2(\Omega; d^n x)\big), \quad z \in \mathbb{C}\backslash[0,\infty), \tag{4.6.71}$$

$$M_u(H_{0,\Omega}^N - zI_\Omega)^{-1/2}, \overline{(H_{0,\Omega}^N - zI_\Omega)^{-1/2}M_v} \in \mathcal{B}_4\big(L^2(\Omega; d^n x)\big), \quad z \in \mathbb{C}\backslash[0,\infty), \tag{4.6.72}$$

and hence, in particular,

$$\operatorname{dom}(A) = \operatorname{dom}(B) \supseteq H^1(\Omega) \supset H^2(\Omega) \supseteq \operatorname{dom}(H_{0,\Omega}^N), \tag{4.6.73}$$

$$\operatorname{dom}(A) = \operatorname{dom}(B) \supseteq H^1(\Omega) \supseteq H_0^1(\Omega) \supseteq \operatorname{dom}(H_{0,\Omega}^D). \tag{4.6.74}$$

Thus, Hypothesis 4.2.1 (i) is satisfied for $H_{0,\Omega}^D$ and $H_{0,\Omega}^N$. Moreover, (4.6.71) and (4.6.72) imply

$$\overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}, \overline{M_u(H_{0,\Omega}^N - zI_\Omega)^{-1}M_v} \in \mathcal{B}_2\big(L^2(\Omega; d^n x)\big), \quad z \in \mathbb{C}\backslash[0,\infty), \tag{4.6.75}$$

which verifies Hypothesis 4.2.1 (ii) for $H_{0,\Omega}^D$ and $H_{0,\Omega}^N$. One verifies Hypothesis 4.2.1 (iii) by utilizing (4.6.48) with sufficiently negative $z < 0$, such that the $\mathcal{B}_4$-norms of the operators in (4.6.71) and (4.6.72) are less than 1, and hence the Hilbert–Schmidt norms of the operators in (4.6.75) are less than 1. Thus, applying Theorem 4.2.3 one obtains the densely defined, closed operators H_Ω^D and H_Ω^N (which are extensions of $H^D_{0,\Omega} + M_V$ on $\mathrm{dom}(H^D_{0,\Omega}) \cap \mathrm{dom}(M_V)$ and $H^N_{0,\Omega} + M_V$ on $\mathrm{dom}(H^N_{0,\Omega}) \cap \mathrm{dom}(M_V)$, respectively).

We note in passing that (4.6.46)–(4.6.48), (4.6.62), (4.6.65)–(4.6.68), (4.6.71)–(4.6.75), etc., extend of course to all z in the resolvent set of the corresponding operators $H^D_{0,\Omega}$ and $H^N_{0,\Omega}$.

The following result is a direct extension of the one-dimensional result in Theorem 4.6.4.

Theorem 4.6.11. *Assume Hypothesis 4.6.6 and* $z \in \mathbb{C}\backslash\big(\sigma(H^D_{\Omega}) \cup \sigma(H^D_{0,\Omega}) \cup \sigma(H^N_{0,\Omega})\big)$. *Then,*

$$\overline{\gamma_N (H^D_{0,\Omega} - zI_\Omega)^{-1} M_V (H^D_{\Omega} - zI_\Omega)^{-1} M_V \big[\gamma_D (H^N_{0,\Omega} - \overline{z} I_\Omega)^{-1}\big]^*} \in \mathcal{B}_1\big(L^2(\partial\Omega; d^{n-1}\sigma)\big), \tag{4.6.76}$$

$$\overline{\gamma_N (H^D_{\Omega} - zI_\Omega)^{-1} M_V \big[\gamma_D (H^N_{0,\Omega} - \overline{z} I_\Omega)^{-1}\big]^*} \in \mathcal{B}_2\big(L^2(\partial\Omega; d^{n-1}\sigma)\big), \tag{4.6.77}$$

and

$$\begin{aligned}
&\frac{\det{}_2\big(I_\Omega + \overline{M_u (H^N_{0,\Omega} - zI_\Omega)^{-1} M_v}\big)}{\det{}_2\big(I_\Omega + \overline{M_u (H^D_{0,\Omega} - zI_\Omega)^{-1} M_v}\big)} \\
&\quad = \det{}_2\Big(I_{\partial\Omega} - \overline{\gamma_N (H^D_{\Omega} - zI_\Omega)^{-1} M_V \big[\gamma_D (H^N_{0,\Omega} - \overline{z} I_\Omega)^{-1}\big]^*}\Big) \qquad (4.6.78) \\
&\qquad \times \exp\Big(\mathrm{tr}\Big(\overline{\gamma_N (H^D_{0,\Omega} - zI_\Omega)^{-1} M_V (H^D_{\Omega} - zI_\Omega)^{-1} M_V \big[\gamma_D (H^N_{0,\Omega} - \overline{z} I_\Omega)^{-1}\big]^*}\Big)\Big).
\end{aligned}$$

Proof. From the outset we note that the left-hand side of (4.6.78) is well-defined by (4.6.75). Let $z \in \mathbb{C}\backslash\big(\sigma(H^D_{\Omega}) \cup \sigma(H^D_{0,\Omega}) \cup \sigma(H^N_{0,\Omega})\big)$ and

$$u(x) = \exp(i \arg(V(x)))|V(x)|^{1/2}, \quad v(x) = |V(x)|^{1/2}, \tag{4.6.79}$$

$$\widetilde{u}(x) = \exp(i \arg(V(x)))|V(x)|^{5/6}, \quad \widetilde{v}(x) = |V(x)|^{1/6}. \tag{4.6.80}$$

Next, we introduce

$$K_D(z) = -\overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}, \quad K_N(z) = -\overline{M_u(H_{0,\Omega}^N - zI_\Omega)^{-1}M_v} \tag{4.6.81}$$

(cf. (4.2.4)) and note that

$$[I_\Omega - K_D(z)]^{-1} \in \mathcal{B}(L^2(\Omega; d^n x)), \quad z \in \mathbb{C}\backslash\big(\sigma(H_\Omega^D) \cup \sigma(H_{0,\Omega}^D)\big), \tag{4.6.82}$$

by Theorem 4.3.2. Thus, utilizing the following facts,

$$[I_\Omega - K_D(z)]^{-1} = I_\Omega + K_D(z)[I_\Omega - K_D(z)]^{-1} \tag{4.6.83}$$

and

$$\begin{aligned} 1 &= \det{}_2(I_\Omega) = \det{}_2\big([I_\Omega - K_D(z)][I - K_D(z)]^{-1}\big) \\ &= \det{}_2\big(I_\Omega - K_D(z)\big) \det{}_2\big([I_\Omega - K_D(z)]^{-1}\big) \exp\big(\operatorname{tr}\big(K_D(z)^2[I_\Omega - K_D(z)]^{-1}\big)\big), \end{aligned} \tag{4.6.84}$$

one obtains

$$\begin{aligned} &\det{}_2\big([I_\Omega - K_N(z)][I_\Omega - K_D(z)]^{-1}\big) \\ &\quad = \det{}_2\big(I_\Omega - K_N(z)\big) \det{}_2\big([I_\Omega - K_D(z)]^{-1}\big) \\ &\qquad \times \exp\big(\operatorname{tr}\big(K_N(z)K_D(z)[I_\Omega - K_D(z)]^{-1}\big)\big) \\ &\quad = \frac{\det{}_2\big(I_\Omega - K_N(z)\big)}{\det{}_2\big(I_\Omega - K_D(z)\big)} \exp\big(\operatorname{tr}\big((K_N(z) - K_D(z))K_D(z)[I_\Omega - K_D(z)]^{-1}\big)\big). \end{aligned} \tag{4.6.85}$$

At this point, the left-hand side of (4.6.78) can be rewritten as

$$\begin{aligned} \frac{\det{}_2\big(I_\Omega + \overline{M_u(H_{0,\Omega}^N - zI_\Omega)^{-1}M_v}\big)}{\det{}_2\big(I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}\big)} &= \frac{\det{}_2\big(I_\Omega - K_N(z)\big)}{\det{}_2\big(I_\Omega - K_D(z)\big)} \\ = \det{}_2\big([I_\Omega - K_N(z)][I_\Omega - K_D(z)]^{-1}\big)& \\ \times \exp\big(\operatorname{tr}\big((K_D(z) - K_N(z))K_D(z)[I_\Omega - K_D(z)]^{-1}\big)\big)& \end{aligned}$$

$$= \det{}_2\big(I_\Omega + (K_D(z) - K_N(z))[I_\Omega - K_D(z)]^{-1}\big) \qquad (4.6.86)$$
$$\times \exp\big(\operatorname{tr}\big((K_D(z) - K_N(z))K_D(z)[I_\Omega - K_D(z)]^{-1}\big)\big).$$

Next, temporarily suppose that $V \in L^2(\Omega; d^n x) \cap L^6(\Omega; d^n x)$. Using Lemma C.3 (an extension of a result of Nakamura [136, Lemma 6]) and Remark C.5, one finds

$$\begin{aligned} K_D(z) - K_N(z) &= -\overline{M_u\big[(H_{0,\Omega}^D - zI_\Omega)^{-1} - (H_{0,\Omega}^N - zI_\Omega)^{-1}\big]M_v} \\ &= -\overline{M_u\big[\gamma_D(H_{0,\Omega}^N - \overline{z}I_\Omega)^{-1}\big]^*}\,\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}, \qquad (4.6.87) \\ &= -\big[\overline{\gamma_D(H_{0,\Omega}^N - \overline{z}I_\Omega)^{-1}M_{\overline{u}}}\big]^*\,\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}. \end{aligned}$$

Thus, inserting (4.6.87) into (4.6.86) yields,

$$\begin{aligned} &\frac{\det{}_2\big(I_\Omega + \overline{M_u(H_{0,\Omega}^N - zI_\Omega)^{-1}M_v}\big)}{\det{}_2\big(I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}\big)} \\ &\quad = \det{}_2\Big(I_\Omega - \big[\overline{\gamma_D(H_{0,\Omega}^N - \overline{z}I_\Omega)^{-1}M_{\overline{u}}}\big]^*\,\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v} \\ &\qquad\qquad \times \big[I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}\big]^{-1}\Big) \\ &\qquad \times \exp\Big(\operatorname{tr}\Big(\big[\overline{\gamma_D(H_{0,\Omega}^N - \overline{z}I_\Omega)^{-1}M_{\overline{u}}}\big]^*\,\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v} \qquad (4.6.88) \\ &\qquad \times \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}\big[I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}\big]^{-1}\Big)\Big). \end{aligned}$$

Then, utilizing Corollary 4.6.10 with $p_1 = 12/5$ and $p_2 = 12$, one finds,

$$\overline{\gamma_D(H_{0,\Omega}^N - \overline{z}I_\Omega)^{-1}M_{\overline{u}}} \in \mathcal{B}_{12/5}\big(L^2(\Omega; d^n x), L^2(\partial\Omega; d^{n-1}\sigma)\big), \qquad (4.6.89)$$

$$\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v} \in \mathcal{B}_{12}\big(L^2(\Omega; d^n x), L^2(\partial\Omega; d^{n-1}\sigma)\big), \qquad (4.6.90)$$

and hence using the fact that,

$$\big[I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}\big]^{-1} \in \mathcal{B}\big(L^2(\Omega; d^n x)\big), \quad z \in \mathbb{C}\backslash\big(\sigma(H_\Omega^D) \cup \sigma(H_{0,\Omega}^D)\big), \qquad (4.6.91)$$

one rearranges the terms in (4.6.88) as follows,

$$\begin{aligned}
&\frac{\det{}_2\big(I_\Omega + \overline{M_u(H_{0,\Omega}^N - zI_\Omega)^{-1}M_v}\big)}{\det{}_2\big(I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}\big)} \\
&\quad = \det{}_2\Big(I_{\partial\Omega} - \overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}\big[I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}\big]^{-1} \\
&\qquad\qquad \times \big[\overline{\gamma_D(H_{0,\Omega}^N - \overline{z}I_\Omega)^{-1}M_{\overline{u}}}\big]^*\Big) \\
&\qquad \times \exp\Big(\operatorname{tr}\Big(\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}\;\overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v} \\
&\qquad \times \big[I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}\big]^{-1}\big[\overline{\gamma_D(H_{0,\Omega}^N - \overline{z}I_\Omega)^{-1}M_{\overline{u}}}\big]^*\Big)\Big) \\
&\quad = \det{}_2\Big(I_{\partial\Omega} - \overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\widetilde{v}}}\big[I_\Omega + \overline{M_{\widetilde{u}}(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\widetilde{v}}}\big]^{-1} \\
&\qquad\qquad \times \big[\overline{\gamma_D(H_{0,\Omega}^N - \overline{z}I_\Omega)^{-1}M_{\overline{\widetilde{u}}}}\big]^*\Big) \\
&\qquad \times \exp\Big(\operatorname{tr}\Big(\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\widetilde{v}}}\;\overline{M_{\widetilde{u}}(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\widetilde{v}}} \\
&\qquad \times \big[I_\Omega + \overline{M_{\widetilde{u}}(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\widetilde{v}}}\big]^{-1}\big[\overline{\gamma_D(H_{0,\Omega}^N - \overline{z}I_\Omega)^{-1}M_{\overline{\widetilde{u}}}}\big]^*\Big)\Big).
\end{aligned} \tag{4.6.92}$$

In the last equality we employed the following simple identities,

$$M_V = M_u M_v = M_{\widetilde{u}} M_{\widetilde{v}}, \tag{4.6.93}$$

$$M_v\big[I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}\big]^{-1}M_u = M_{\widetilde{v}}\big[I + \overline{M_{\widetilde{u}}(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\widetilde{v}}}\big]^{-1}M_{\widetilde{u}}. \tag{4.6.94}$$

Utilizing (4.6.92) and the following analog of formula (4.2.20),

$$\overline{(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\widetilde{v}}}\big[I_\Omega + \overline{M_{\widetilde{u}}(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\widetilde{v}}}\big]^{-1} = \overline{(H_\Omega^D - zI_\Omega)^{-1}M_{\widetilde{v}}}, \tag{4.6.95}$$

one arrives at (4.6.78), subject to the extra assumption $V \in L^2(\Omega; d^nx) \cap L^6(\Omega; d^nx)$.

Finally, assuming only $V \in L^2(\Omega; d^nx)$ and utilizing Theorem 4.3.2, Lemma 4.6.8, and Corollary 4.6.10 once again, one obtains

$$\big[I_\Omega + \overline{M_{\widetilde{u}}(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\widetilde{v}}}\big]^{-1} \in \mathcal{B}\big(L^2(\Omega; d^nx)\big), \tag{4.6.96}$$

$$M_{\widetilde{u}}(H_{0,\Omega}^D - zI_\Omega)^{-5/6} \in \mathcal{B}_{12/5}\big(L^2(\Omega; d^n x)\big), \tag{4.6.97}$$

$$M_{\widetilde{v}}(H_{0,\Omega}^D - zI_\Omega)^{-1/6} \in \mathcal{B}_{12}\big(L^2(\Omega; d^n x)\big), \tag{4.6.98}$$

$$\overline{\gamma_D(H_{0,\Omega}^N - zI_\Omega)^{-1}M_{\widetilde{u}}} \in \mathcal{B}_{12/5}\big(L^2(\Omega; d^n x), L^2(\partial\Omega; d^{n-1}\sigma)\big), \tag{4.6.99}$$

$$\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\widetilde{v}}} \in \mathcal{B}_{12}\big(L^2(\Omega; d^n x), L^2(\partial\Omega; d^{n-1}\sigma)\big), \tag{4.6.100}$$

and hence

$$\overline{M_{\widetilde{u}}(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\widetilde{v}}} \in \mathcal{B}_2(L^2(\Omega; d^n x)). \tag{4.6.101}$$

Relations (4.6.95)–(4.6.101) prove (4.6.76) and (4.6.77), and hence, the left- and the right-hand sides of (4.6.78) are well-defined for $V \in L^2(\Omega; d^n x)$. Thus, using (4.6.48), (4.6.67), (4.6.68), the continuity of $\det{}_2(\cdot)$ with respect to the Hilbert–Schmidt norm $\|\cdot\|_{\mathcal{B}_2(L^2(\Omega;d^n x))}$, the continuity of $\operatorname{tr}(\cdot)$ with respect to the trace norm $\|\cdot\|_{\mathcal{B}_1(L^2(\Omega;d^n x))}$, and an approximation of $V \in L^2(\Omega; d^n x)$ by a sequence of potentials $V_k \in L^2(\Omega; d^n x) \cap L^6(\Omega; d^n x)$, $k \in \mathbb{N}$, in the norm of $L^2(\Omega; d^n x)$ as $k \uparrow \infty$, then extends the result from $V \in L^2(\Omega; d^n x) \cap L^6(\Omega; d^n x)$ to $V \in L^2(\Omega; d^n x)$, $n = 2, 3$. $\square$

Remark 4.6.12. Thus, a comparison of Theorem 4.6.11 with the one-dimensional case in Theorem 4.6.4 shows that the reduction of Fredholm determinants associated with operators in $L^2((0,\infty); dx)$ to simple Wronski determinants, and hence to Jost functions as first observed by Jost and Pais [104], can be properly extended to higher dimensions and results in a reduction of appropriate ratios of Fredholm determinants associated with operators in $L^2(\Omega; d^n x)$ to an appropriate Fredholm determinant associated with an operator in $L^2(\partial\Omega; d^{n-1}\sigma)$.

Remark 4.6.13. As in Theorem 4.6.11 we assume Hypothesis 4.6.6 and suppose $z \in \mathbb{C} \backslash \big(\sigma(H_\Omega^D) \cup \sigma(H_{0,\Omega}^D) \cup \sigma(H_{0,\Omega}^N)\big)$. First we note that

$$\big[(H_{0,\Omega}^D - zI_\Omega)^{-1/2}(H_\Omega^D - zI_\Omega)(H_{0,\Omega}^D - zI_\Omega)^{-1/2} - I_\Omega\big] \in \mathcal{B}_2\big(L^2(\Omega; d^n x)\big), \quad (4.6.102)$$

$$\big[(H_{0,\Omega}^N - zI_\Omega)^{-1/2}(H_\Omega^N - zI_\Omega)(H_{0,\Omega}^N - zI_\Omega)^{-1/2} - I_\Omega\big] \in \mathcal{B}_2\big(L^2(\Omega; d^n x)\big). \quad (4.6.103)$$

Indeed, by (4.6.71) and (4.6.72), one obtains

$$\begin{aligned}
&(H_{0,\Omega}^D - zI_\Omega)^{-1/2}(H_\Omega^D - zI_\Omega)(H_{0,\Omega}^D - zI_\Omega)^{-1/2} - I_\Omega \\
&\quad = (H_{0,\Omega}^D - zI_\Omega)^{-1/2} M_V (H_{0,\Omega}^D - zI_\Omega)^{-1/2} \in \mathcal{B}_2\big(L^2(\Omega; d^n x)\big), \quad (4.6.104)\\
&(H_{0,\Omega}^N - zI_\Omega)^{-1/2}(H_\Omega^N - zI_\Omega)(H_{0,\Omega}^N - zI_\Omega)^{-1/2} - I_\Omega \\
&\quad = (H_{0,\Omega}^N - zI_\Omega)^{-1/2} M_V (H_{0,\Omega}^N - zI_\Omega)^{-1/2} \in \mathcal{B}_2\big(L^2(\Omega; d^n x)\big). \quad (4.6.105)
\end{aligned}$$

Thus, using (4.6.71)–(4.6.75) and the cyclicity of ${\det}_2(\cdot)$, one rearranges the left-hand side of (4.6.78) as follows,

$$\begin{aligned}
&\frac{{\det}_2\big(I_\Omega + \overline{M_u (H_{0,\Omega}^N - zI_\Omega)^{-1} M_v}\big)}{{\det}_2\big(I_\Omega + \overline{M_u (H_{0,\Omega}^D - zI_\Omega)^{-1} M_v}\big)} \\
&\quad = \frac{{\det}_2\big(I_\Omega + (H_{0,\Omega}^N - zI_\Omega)^{-1/2} M_V (H_{0,\Omega}^N - zI_\Omega)^{-1/2}\big)}{{\det}_2\big(I_\Omega + (H_{0,\Omega}^D - zI_\Omega)^{-1/2} M_V (H_{0,\Omega}^D - zI_\Omega)^{-1/2}\big)} \\
&\quad = \frac{{\det}_2\big((H_{0,\Omega}^N - zI_\Omega)^{-1/2}(H_\Omega^N - zI_\Omega)(H_{0,\Omega}^N - zI_\Omega)^{-1/2}\big)}{{\det}_2\big((H_{0,\Omega}^D - zI_\Omega)^{-1/2}(H_\Omega^D - zI_\Omega)(H_{0,\Omega}^D - zI_\Omega)^{-1/2}\big)}. \quad (4.6.106)
\end{aligned}$$

Again (4.6.106) illustrates that symmetrized perturbation determinants underly Theorem 4.6.11.

Remark 4.6.14. The following observation yields a simple application of formula (4.6.78). Since by Theorem 4.3.2, for any $z \in \mathbb{C} \backslash \big(\sigma(H_\Omega^D) \cup \sigma(H_{0,\Omega}^D) \cup \sigma(H_{0,\Omega}^N)\big)$, one has $z \in \sigma(H_\Omega^N)$ if and only if $\det{}_2\big(I_\Omega + \overline{M_u(H_{0,\Omega}^N - zI_\Omega)^{-1}M_v}\big) = 0$, it follows from (4.6.78) that

$$\begin{aligned}&\text{for all } z \in \mathbb{C}\backslash\big(\sigma(H_\Omega^D) \cup \sigma(H_{0,\Omega}^D) \cup \sigma(H_{0,\Omega}^N)\big), \text{ one has } z \in \sigma(H_\Omega^N)\\ &\quad \text{if and only if } \det{}_2\Big(I_{\partial\Omega} - \overline{\gamma_N(H_\Omega^D - zI_\Omega)^{-1}M_V\big[\gamma_D(H_{0,\Omega}^N - \overline{z}I_\Omega)^{-1}\big]^*}\Big) = 0.\end{aligned} \tag{4.6.107}$$

One can also prove the following analog of (4.6.78):

$$\begin{aligned}&\frac{\det{}_2\big(I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}\big)}{\det{}_2\big(I_\Omega + \overline{M_u(H_{0,\Omega}^N - zI_\Omega)^{-1}M_v}\big)}\\ &\quad = \det{}_2\Big(I_{\partial\Omega} + \overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_V\big[\gamma_D((H_\Omega^N - zI_\Omega)^{-1})^*\big]^*}\Big) \qquad (4.6.108)\\ &\qquad \times \exp\Big(-\operatorname{tr}\Big(\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_V(H_\Omega^N - zI_\Omega)^{-1}M_V\big[\gamma_D((H_{0,\Omega}^N - zI_\Omega)^{-1})^*\big]^*}\Big)\Big).\end{aligned}$$

Then, proceeding as before, one obtains

$$\begin{aligned}&\text{for all } z \in \mathbb{C}\backslash\big(\sigma(H_\Omega^N) \cup \sigma(H_{0,\Omega}^N) \cup \sigma(H_{0,\Omega}^D)\big), \text{ one has } z \in \sigma(H_\Omega^D) \qquad (4.6.109)\\ &\quad \text{if and only if } \det{}_2\Big(I_{\partial\Omega} + \overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_V\big[\gamma_D((H_\Omega^N - zI_\Omega)^{-1})^*\big]^*}\Big) = 0.\end{aligned}$$

4.7 Further Improvement of the Reduction Formula in Dimensions $n = 2, 3$

Hypothesis 4.7.1. Let $n = 2, 3$.

(i) Assume that $\Omega \subset \mathbb{R}^n$ is an open nonempty domain of class $C^{1,r}$ for some $(1/2) < r < 1$ with a compact, nonempty boundary, $\partial\Omega$. (For details we refer to Appendix C.)

(ii) Suppose that $V \in L^p(\Omega; d^nx)$ for some p satisfying $\frac{4}{3} < p \leq 2$, in the case $n = 2$, and $\frac{3}{2} < p \leq 2$, in the case $n = 3$.

The perturbed operators H_Ω^D and H_Ω^N in $L^2(\Omega;d^nx)$ are now introduced as follows. We denote by $A = M_u$ and $B = B^* = M_v$ the operators of multiplication by $u = \exp(i\arg(V))|V|^{1/2}$ and $v = |V|^{1/2}$ in $L^2(\Omega;d^nx)$, respectively, so that $M_V = BA = M_uM_v$. Applying Lemma 4.6.8 to $f = u \in L^{2p}(\Omega;d^nx)$ with $q = 1/2$ yields

$$M_u(H_{0,\Omega}^D - zI_\Omega)^{-1/2},\ \overline{(H_{0,\Omega}^D - zI_\Omega)^{-1/2}M_v} \in \mathcal{B}_{2p}\big(L^2(\Omega;d^nx)\big), \quad z \in \mathbb{C}\backslash[0,\infty), \tag{4.7.1}$$

$$M_u(H_{0,\Omega}^N - zI_\Omega)^{-1/2},\ \overline{(H_{0,\Omega}^N - zI_\Omega)^{-1/2}M_v} \in \mathcal{B}_{2p}\big(L^2(\Omega;d^nx)\big), \quad z \in \mathbb{C}\backslash[0,\infty), \tag{4.7.2}$$

and hence, in particular,

$$\operatorname{dom}(A) = \operatorname{dom}(B) \supseteq H^1(\Omega) \supset H^2(\Omega) \supseteq \operatorname{dom}(H_{0,\Omega}^N), \tag{4.7.3}$$

$$\operatorname{dom}(A) = \operatorname{dom}(B) \supseteq H^1(\Omega) \supseteq H_0^1(\Omega) \supseteq \operatorname{dom}(H_{0,\Omega}^D). \tag{4.7.4}$$

Thus, Hypothesis 4.2.1 (i) is satisfied for $H_{0,\Omega}^D$ and $H_{0,\Omega}^N$. Moreover, (4.7.1) and (4.7.2) imply

$$\overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v},\ \overline{M_u(H_{0,\Omega}^N - zI_\Omega)^{-1}M_v} \in \mathcal{B}_p\big(L^2(\Omega;d^nx)\big) \subset \mathcal{B}_2\big(L^2(\Omega;d^nx)\big),$$
$$z \in \mathbb{C}\backslash[0,\infty), \tag{4.7.5}$$

which verifies Hypothesis 4.2.1 (ii) for $H_{0,\Omega}^D$ and $H_{0,\Omega}^N$. One verifies Hypothesis 4.2.1 (iii) by utilizing (4.6.48) with sufficiently negative $z < 0$, such that the $\mathcal{B}_{2p}$-norms of the operators in (4.7.1) and (4.7.2) are less than 1, and hence the Hilbert–Schmidt norms of the operators in (4.7.5) are less than 1. Thus, applying Theorem 4.2.3 one obtains the densely defined, closed operators H_Ω^D and H_Ω^N (which are extensions of $H_{0,\Omega}^D + M_V$ on $\operatorname{dom}(H_{0,\Omega}^D) \cap \operatorname{dom}(M_V)$ and $H_{0,\Omega}^N + M_V$ on $\operatorname{dom}(H_{0,\Omega}^N) \cap \operatorname{dom}(M_V)$, respectively).

We note in passing that (4.7.1)–(4.7.5) extend of course to all z in the resolvent set of the corresponding operators $H_{0,\Omega}^D$ and $H_{0,\Omega}^N$.

The following result is an extension of the reduction principle that was obtained in Theorem 4.6.11.

Theorem 4.7.2. *Assume Hypothesis 4.7.1 and* $z \in \mathbb{C}\backslash\big(\sigma(H_\Omega^D) \cup \sigma(H_{0,\Omega}^D) \cup \sigma(H_{0,\Omega}^N)\big)$. *Then,*

$$\overline{\gamma_N (H_{0,\Omega}^D - zI_\Omega)^{-1} M_V (H_\Omega^D - zI_\Omega)^{-1} M_V \big[\gamma_D (H_{0,\Omega}^N - \overline{z} I_\Omega)^{-1}\big]^*} \in \mathcal{B}_1\big(L^2(\partial\Omega; d^{n-1}\sigma)\big), \tag{4.7.6}$$

$$\overline{\gamma_N (H_\Omega^D - zI_\Omega)^{-1} M_V \big[\gamma_D (H_{0,\Omega}^N - \overline{z} I_\Omega)^{-1}\big]^*} \in \mathcal{B}_2\big(L^2(\partial\Omega; d^{n-1}\sigma)\big), \tag{4.7.7}$$

and

$$\begin{aligned}
&\frac{\det{}_2\big(I_\Omega + \overline{M_u (H_{0,\Omega}^N - zI_\Omega)^{-1} M_v}\big)}{\det{}_2\big(I_\Omega + \overline{M_u (H_{0,\Omega}^D - zI_\Omega)^{-1} M_v}\big)} \\
&\quad = \det{}_2\Big(I_{\partial\Omega} - \overline{\gamma_N (H_\Omega^D - zI_\Omega)^{-1} M_V \big[\gamma_D (H_{0,\Omega}^N - \overline{z} I_\Omega)^{-1}\big]^*}\Big) \\
&\qquad \times \exp\Big(\operatorname{tr}\Big(\overline{\gamma_N (H_{0,\Omega}^D - zI_\Omega)^{-1} M_V (H_\Omega^D - zI_\Omega)^{-1} M_V \big[\gamma_D (H_{0,\Omega}^N - \overline{z} I_\Omega)^{-1}\big]^*}\Big)\Big).
\end{aligned} \tag{4.7.8}$$

Proof. From the outset we note that the left-hand side of (4.7.8) is well-defined by (4.7.5). Let $z \in \mathbb{C}\backslash\big(\sigma(H_\Omega^D) \cup \sigma(H_{0,\Omega}^D) \cup \sigma(H_{0,\Omega}^N)\big)$ and

$$u(x) = \exp(i \arg(V(x)))|V(x)|^{1/2}, \quad v(x) = |V(x)|^{1/2}, \tag{4.7.9}$$

$$\widetilde{u}(x) = \exp(i \arg(V(x)))|V(x)|^{p/p_1}, \quad \widetilde{v}(x) = |V(x)|^{p/p_2}, \tag{4.7.10}$$

where

$$p_1 = \begin{cases} \frac{3}{2}p, & n = 2 \\ \frac{4}{3}p, & n = 3, \end{cases} \qquad p_2 = \begin{cases} 3p, & n = 2, \\ 4p, & n = 3. \end{cases} \tag{4.7.11}$$

Then it follows that $\frac{1}{p_1} + \frac{1}{p_2} = \frac{1}{p}$, in both cases $n = 2, 3$, and hence $V = uv = \widetilde{u}\widetilde{v}$.

Next, we introduce

$$K_D(z) = -\overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}, \quad K_N(z) = -\overline{M_u(H_{0,\Omega}^N - zI_\Omega)^{-1}M_v} \qquad (4.7.12)$$

(cf. (4.2.4)) and note that

$$[I_\Omega - K_D(z)]^{-1} \in \mathcal{B}(L^2(\Omega; d^n x)), \quad z \in \mathbb{C}\backslash\big(\sigma(H_\Omega^D) \cup \sigma(H_{0,\Omega}^D)\big), \qquad (4.7.13)$$

by Theorem 4.3.2. Thus, utilizing the following facts,

$$[I_\Omega - K_D(z)]^{-1} = I_\Omega + K_D(z)[I_\Omega - K_D(z)]^{-1} \qquad (4.7.14)$$

and

$$\begin{aligned} 1 &= {\det}_2(I_\Omega) = {\det}_2\big([I_\Omega - K_D(z)][I - K_D(z)]^{-1}\big) \qquad (4.7.15) \\ &= {\det}_2\big(I_\Omega - K_D(z)\big)\,{\det}_2\big([I_\Omega - K_D(z)]^{-1}\big)\exp\big(\operatorname{tr}\big(K_D(z)^2[I_\Omega - K_D(z)]^{-1}\big)\big), \end{aligned}$$

one obtains

$$\begin{aligned} &{\det}_2\big([I_\Omega - K_N(z)][I_\Omega - K_D(z)]^{-1}\big) \\ &\quad = {\det}_2\big(I_\Omega - K_N(z)\big)\,{\det}_2\big([I_\Omega - K_D(z)]^{-1}\big) \\ &\qquad \times \exp\big(\operatorname{tr}\big(K_N(z)K_D(z)[I_\Omega - K_D(z)]^{-1}\big)\big) \qquad (4.7.16) \\ &\quad = \frac{{\det}_2\big(I_\Omega - K_N(z)\big)}{{\det}_2\big(I_\Omega - K_D(z)\big)}\exp\big(\operatorname{tr}\big((K_N(z) - K_D(z))K_D(z)[I_\Omega - K_D(z)]^{-1}\big)\big). \end{aligned}$$

At this point, the left-hand side of (4.7.8) can be rewritten as

$$\frac{{\det}_2\big(I_\Omega + \overline{M_u(H_{0,\Omega}^N - zI_\Omega)^{-1}M_v}\big)}{{\det}_2\big(I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}\big)} = \frac{{\det}_2\big(I_\Omega - K_N(z)\big)}{{\det}_2\big(I_\Omega - K_D(z)\big)}$$

$$
\begin{aligned}
&= \det{}_2\big([I_\Omega - K_N(z)][I_\Omega - K_D(z)]^{-1}\big) \\
&\quad \times \exp\big(\operatorname{tr}\big((K_D(z) - K_N(z))K_D(z)[I_\Omega - K_D(z)]^{-1}\big)\big) \\
&= \det{}_2\big(I_\Omega + (K_D(z) - K_N(z))[I_\Omega - K_D(z)]^{-1}\big) \\
&\quad \times \exp\big(\operatorname{tr}\big((K_D(z) - K_N(z))K_D(z)[I_\Omega - K_D(z)]^{-1}\big)\big).
\end{aligned} \tag{4.7.17}
$$

Next, temporarily suppose that $V \in L^p(\Omega; d^n x) \cap L^\infty(\Omega; d^n x)$. Using Lemma C.3 (an extension of a result of Nakamura [136, Lemma 6]) and Remark C.5, one finds

$$
\begin{aligned}
K_D(z) - K_N(z) &= -\overline{M_u\big[(H_{0,\Omega}^D - zI_\Omega)^{-1} - (H_{0,\Omega}^N - zI_\Omega)^{-1}\big]M_v} \\
&= -\overline{M_u\big[\gamma_D(H_{0,\Omega}^N - \overline{z}I_\Omega)^{-1}\big]^*}\,\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}, \\
&= -\big[\overline{\gamma_D(H_{0,\Omega}^N - \overline{z}I_\Omega)^{-1}M_{\overline{u}}}\big]^*\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}.
\end{aligned} \tag{4.7.18}
$$

Thus, inserting (4.7.18) into (4.7.17) yields,

$$
\begin{aligned}
&\frac{\det{}_2\big(I_\Omega + \overline{M_u(H_{0,\Omega}^N - zI_\Omega)^{-1}M_v}\big)}{\det{}_2\big(I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}\big)} \\
&\quad = \det{}_2\Big(I_\Omega - \big[\overline{\gamma_D(H_{0,\Omega}^N - \overline{z}I_\Omega)^{-1}M_{\overline{u}}}\big]^*\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v} \\
&\qquad\qquad \times \big[I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}\big]^{-1}\Big) \\
&\quad\times \exp\Big(\operatorname{tr}\Big(\big[\overline{\gamma_D(H_{0,\Omega}^N - \overline{z}I_\Omega)^{-1}M_{\overline{u}}}\big]^*\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v} \\
&\quad\times \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}\big[I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}\big]^{-1}\Big)\Big).
\end{aligned} \tag{4.7.19}
$$

Then, utilizing Corollary 4.6.10 with p_1 and p_2 as in (4.7.11), one finds,

$$
\overline{\gamma_D(H_{0,\Omega}^N - \overline{z}I_\Omega)^{-1}M_{\overline{u}}} \in \mathcal{B}_{p_1}\big(L^2(\Omega; d^n x), L^2(\partial\Omega; d^{n-1}\sigma)\big), \tag{4.7.20}
$$

$$
\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v} \in \mathcal{B}_{p_2}\big(L^2(\Omega; d^n x), L^2(\partial\Omega; d^{n-1}\sigma)\big), \tag{4.7.21}
$$

and hence,

$$
\big[\overline{\gamma_D(H_{0,\Omega}^N - \overline{z}I_\Omega)^{-1}M_{\overline{u}}}\big]^*\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v} \in \mathcal{B}_p\big(L^2(\Omega; d^n x)\big)
$$

$$\subset \mathcal{B}_2\big(L^2(\Omega; d^n x)\big), \tag{4.7.22}$$

$$\overline{\gamma_N (H_{0,\Omega}^D - zI_\Omega)^{-1} M_v}\big[\overline{\gamma_D (H_{0,\Omega}^N - \overline{z} I_\Omega)^{-1} M_{\overline{u}}}\big]^* \in \mathcal{B}_p\big(L^2(\partial\Omega; d^{n-1}\sigma)\big)$$

$$\subset \mathcal{B}_2\big(L^2(\partial\Omega; d^{n-1}\sigma)\big). \tag{4.7.23}$$

Moreover, using the fact that,

$$\big[I_\Omega + \overline{M_u (H_{0,\Omega}^D - zI_\Omega)^{-1} M_v}\big]^{-1} \in \mathcal{B}\big(L^2(\Omega; d^n x)\big), \quad z \in \mathbb{C}\backslash\big(\sigma(H_\Omega^D) \cup \sigma(H_{0,\Omega}^D)\big), \tag{4.7.24}$$

one rearranges the terms in (4.7.19) as follows:

$$\begin{aligned}
&\frac{\det{}_2\big(I_\Omega + \overline{M_u (H_{0,\Omega}^N - zI_\Omega)^{-1} M_v}\big)}{\det{}_2\big(I_\Omega + \overline{M_u (H_{0,\Omega}^D - zI_\Omega)^{-1} M_v}\big)} \\
&\quad = \det{}_2\Big(I_{\partial\Omega} - \overline{\gamma_N (H_{0,\Omega}^D - zI_\Omega)^{-1} M_v}\big[I_\Omega + \overline{M_u (H_{0,\Omega}^D - zI_\Omega)^{-1} M_v}\big]^{-1} \\
&\qquad\qquad \times \big[\overline{\gamma_D (H_{0,\Omega}^N - \overline{z} I_\Omega)^{-1} M_{\overline{u}}}\big]^*\Big) \\
&\qquad \times \exp\Big(\operatorname{tr}\Big(\overline{\gamma_N (H_{0,\Omega}^D - zI_\Omega)^{-1} M_v}\; \overline{M_u (H_{0,\Omega}^D - zI_\Omega)^{-1} M_v} \\
&\qquad \times \big[I_\Omega + \overline{M_u (H_{0,\Omega}^D - zI_\Omega)^{-1} M_v}\big]^{-1} \big[\overline{\gamma_D (H_{0,\Omega}^N - \overline{z} I_\Omega)^{-1} M_{\overline{u}}}\big]^*\Big)\Big) \\
&\quad = \det{}_2\Big(I_{\partial\Omega} - \overline{\gamma_N (H_{0,\Omega}^D - zI_\Omega)^{-1} M_{\widetilde{v}}}\big[I_\Omega + \overline{M_{\widetilde{u}} (H_{0,\Omega}^D - zI_\Omega)^{-1} M_{\widetilde{v}}}\big]^{-1} \\
&\qquad\qquad \times \big[\overline{\gamma_D (H_{0,\Omega}^N - \overline{z} I_\Omega)^{-1} M_{\overline{\widetilde{u}}}}\big]^*\Big) \\
&\qquad \times \exp\Big(\operatorname{tr}\Big(\overline{\gamma_N (H_{0,\Omega}^D - zI_\Omega)^{-1} M_{\widetilde{v}}}\; \overline{M_{\widetilde{u}} (H_{0,\Omega}^D - zI_\Omega)^{-1} M_{\widetilde{v}}} \\
&\qquad \times \big[I_\Omega + \overline{M_{\widetilde{u}} (H_{0,\Omega}^D - zI_\Omega)^{-1} M_{\widetilde{v}}}\big]^{-1} \big[\overline{\gamma_D (H_{0,\Omega}^N - \overline{z} I_\Omega)^{-1} M_{\overline{\widetilde{u}}}}\big]^*\Big)\Big).
\end{aligned} \tag{4.7.25}$$

In the last equality we employed the following simple identities,

$$M_V = M_u M_v = M_{\widetilde{u}} M_{\widetilde{v}}, \tag{4.7.26}$$

$$M_v\big[I_\Omega + \overline{M_u (H_{0,\Omega}^D - zI_\Omega)^{-1} M_v}\big]^{-1} M_u = M_{\widetilde{v}}\big[I + \overline{M_{\widetilde{u}} (H_{0,\Omega}^D - zI_\Omega)^{-1} M_{\widetilde{v}}}\big]^{-1} M_{\widetilde{u}}. \tag{4.7.27}$$

Utilizing (4.7.25) and the following analog of formula (4.2.20),

$$\overline{(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\widetilde{v}}}\big[I_\Omega + \overline{M_{\widetilde{u}}(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\widetilde{v}}}\big]^{-1} = \overline{(H_\Omega^D - zI_\Omega)^{-1}M_{\widetilde{v}}}, \qquad (4.7.28)$$

one arrives at (4.7.8), subject to the extra assumption $V \in L^p(\Omega; d^nx) \cap L^\infty(\Omega; d^nx)$.

Finally, assuming only $V \in L^p(\Omega; d^nx)$ and utilizing Theorem 4.3.2, Lemma 4.6.8, and Corollary 4.6.10 once again, one obtains

$$\big[I_\Omega + \overline{M_{\widetilde{u}}(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\widetilde{v}}}\big]^{-1} \in \mathcal{B}\big(L^2(\Omega; d^nx)\big), \qquad (4.7.29)$$

$$M_{\widetilde{u}}(H_{0,\Omega}^D - zI_\Omega)^{-p/p_1} \in \mathcal{B}_{p_1}\big(L^2(\Omega; d^nx)\big), \qquad (4.7.30)$$

$$M_{\widetilde{v}}(H_{0,\Omega}^D - zI_\Omega)^{-p/p_2} \in \mathcal{B}_{p_2}\big(L^2(\Omega; d^nx)\big), \qquad (4.7.31)$$

$$\overline{\gamma_D(H_{0,\Omega}^N - zI_\Omega)^{-1}M_{\widetilde{u}}} \in \mathcal{B}_{p_1}\big(L^2(\Omega; d^nx), L^2(\partial\Omega; d^{n-1}\sigma)\big), \qquad (4.7.32)$$

$$\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\widetilde{v}}} \in \mathcal{B}_{p_2}\big(L^2(\Omega; d^nx), L^2(\partial\Omega; d^{n-1}\sigma)\big), \qquad (4.7.33)$$

and hence

$$\overline{M_{\widetilde{u}}(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\widetilde{v}}} \in \mathcal{B}_p(L^2(\Omega; d^nx)) \subset \mathcal{B}_2(L^2(\Omega; d^nx)). \qquad (4.7.34)$$

Relations (4.7.28)–(4.7.34) prove (4.7.6) and (4.7.7), and hence, the left- and the right-hand sides of (4.7.8) are well-defined for $V \in L^p(\Omega; d^nx)$. Thus, using (4.6.48), (4.6.67), (4.6.68), the continuity of $\det{}_2(\cdot)$ with respect to the Hilbert–Schmidt norm $\|\cdot\|_{\mathcal{B}_2(L^2(\Omega;d^nx))}$, the continuity of $\operatorname{tr}(\cdot)$ with respect to the trace norm $\|\cdot\|_{\mathcal{B}_1(L^2(\Omega;d^nx))}$, and an approximation of $V \in L^p(\Omega; d^nx)$ by a sequence of potentials $V_k \in L^p(\Omega; d^nx) \cap L^\infty(\Omega; d^nx)$, $k \in \mathbb{N}$, in the norm of $L^p(\Omega; d^nx)$ as $k \uparrow \infty$, then extends the result from $V \in L^p(\Omega; d^nx) \cap L^\infty(\Omega; d^nx)$ to $V \in L^p(\Omega; d^nx)$, $n = 2, 3$. $\square$

4.8 An Application to Scattering Theory

In this section we relate Krein's spectral shift function and hence the determinant of the scattering operator in connection with quantum mechanical scattering theory in dimensions $n = 2, 3$ with appropriate modified Fredholm determinants.

The results of this section are not new, they were first derived for $n = 3$ by Newton [141] and subsequently for $n = 2$ by Cheney [29]. However, since our method of proof nicely illustrates the use of infinite determinants in connection with scattering theory and is different from that in [141] and [29], and moreover, since our derivation in the case $n = 3$ is performed under slightly more general hypotheses than in [141], we thought it worthwhile to include it at this point.

Hypothesis 4.8.1. Fix $\delta > 0$. Suppose $V \in \mathcal{R}_{2,\delta}$ for $n = 2$ and $V \in L^1(\mathbb{R}^3; d^3x) \cap \mathcal{R}_3$ for $n = 3$, where

$$\mathcal{R}_{2,\delta} = \big\{V : \mathbb{R}^2 \to \mathbb{R} \text{ measurable} \,\big|\, V^{1+\delta}, (1 + |\cdot|^{\delta})V \in L^1(\mathbb{R}^2; d^2x)\big\}, \tag{4.8.1}$$

$$\mathcal{R}_3 = \left\{V : \mathbb{R}^3 \to \mathbb{R} \text{ measurable} \,\middle|\, \int_{\mathbb{R}^6} d^3x d^3x' \, |V(x)||V(x')||x - x'|^{-2} < \infty\right\}. \tag{4.8.2}$$

We introduce H_0 as the following nonnegative self-adjoint operator in the Hilbert space $L^2(\mathbb{R}^n; d^nx)$,

$$H_0 = -\Delta, \quad \operatorname{dom}(H_0) = H^2(\mathbb{R}^n), \quad n = 2, 3. \tag{4.8.3}$$

Moreover, let $A = M_u$ and $B = B^* = M_v$ denote the operators of multiplication by $u = \operatorname{sign}(V)|V|^{1/2}$ and $v = |V|^{1/2}$ in $L^2(\mathbb{R}^n; d^nx)$, respectively, so that $M_V = BA =$

$M_u M_v$. Then, (cf. [161, Theorem I.21] for $n=3$ and [162] for $n=2$),

$$\operatorname{dom}(A) = \operatorname{dom}(B) \supseteq H^1(\mathbb{R}^n) \supset \operatorname{dom}(H_0), \tag{4.8.4}$$

and hence, Hypothesis 4.2.1 (i) is satisfied for H_0. It follows from Hypothesis 4.8.1 that

$$\overline{M_u (H_0 - zI)^{-1} M_v} \in \mathcal{B}_2\big(L^2(\mathbb{R}^n; d^n x)\big), \quad z \in \mathbb{C}\backslash[0,\infty), \tag{4.8.5}$$

where I now denotes the identity operator in $L^2(\mathbb{R}^n; d^n x)$, and hence, Hypothesis 4.2.1 (ii) is satisfied. Taking $z \in \mathbb{C}\backslash[0,\infty)$ with a sufficiently large absolute value, one also verifies Hypothesis 4.2.1 (iii). Thus, applying Theorem 4.2.3 and Remark 4.2.4 (i), one obtains a self-adjoint operator H (which is an extension of $H_0 + V$ on $\operatorname{dom}(H_0) \cap \operatorname{dom}(V)$).

Theorem 4.8.2. *Assume Hypothesis 4.8.1 and let $z \in \mathbb{C}\backslash\sigma(H)$ and $n = 2, 3$. Then,*

$$(H - zI)^{-1} - (H_0 - zI)^{-1} \in \mathcal{B}_1\big(L^2(\mathbb{R}^n; d^n x)\big), \tag{4.8.6}$$

and there is a unique real-valued spectral shift function

$$\xi(\cdot, H, H_0) \in L^1\big(\mathbb{R}; (1+\lambda^2)^{-1} d\lambda\big) \tag{4.8.7}$$

such that $\xi(\lambda, H, H_0) = 0$ for $\lambda < \inf(\sigma(H))$, and

$$\operatorname{tr}\big((H - zI)^{-1} - (H_0 - zI)^{-1}\big) = -\int_{\sigma(H)} \frac{d\lambda\, \xi(\lambda, H, H_0)}{(\lambda - z)^2}. \tag{4.8.8}$$

We recall that $\xi(\cdot, H, H_0)$ is called the spectral shift function for the pair of self-adjoint operators (H, H_0). For background information on $\xi(\cdot, H, H_0)$ and its connection with the scattering operator at fixed energy, we refer, for instance, to [15, Sect. 19.1], [20], [22], [193, Ch. 8].

Lemma 4.8.3. *Assume Hypothesis 4.8.1 and let $z \in \mathbb{C}\backslash\sigma(H)$ and $n = 2, 3$. Then,*

$$\overline{M_u(H_0 - zI)^{-1}M_v} \in \mathcal{B}_2\big(L^2(\mathbb{R}^n; d^n x)\big), \tag{4.8.9}$$

$$(H_0 - zI)^{-1}M_V(H_0 - zI)^{-1} \in \mathcal{B}_1\big(L^2(\mathbb{R}^n; d^n x)\big), \tag{4.8.10}$$

and

$$\begin{aligned} &\frac{d}{dz}\ln\big(\det{}_2\big(I + \overline{M_u(H_0 - zI)^{-1}M_v}\big)\big) \\ &\quad = -\operatorname{tr}\big((H - zI)^{-1} - (H_0 - zI)^{-1} + (H_0 - zI)^{-1}M_V(H_0 - zI)^{-1}\big). \end{aligned} \tag{4.8.11}$$

The key ingredient in proving (4.8.6) is the fact that

$$M_u(H_0 - zI)^{-1}, \overline{(H_0 - zI)^{-1}M_v} \in \mathcal{B}_2\big(L^2(\mathbb{R}^n; d^n x)\big), \quad z \in \mathbb{C}\backslash[0, \infty),\ n = 2, 3. \tag{4.8.12}$$

This follows from either [165, Theorem 4.1] (or [150, Theorem XI.20]), or explicitly by an inspection of the corresponding integral kernels. For instance, the one for $M_u(H_0 - zI)^{-1}$ reads:

$$\big(M_u(H_0 - zI)^{-1}\big)(x, x') = \begin{cases} u(x)(i/4)H_0^{(1)}(z^{1/2}|x - x'|), & x \neq x',\ x, x' \in \mathbb{R}^2, \\ u(x)e^{iz^{1/2}|x-x'|}/[4\pi|x - x'|], & x \neq x',\ x, x' \in \mathbb{R}^3, \end{cases}$$
$$z \in \mathbb{C}\backslash[0, \infty),\ \operatorname{Im}(z^{1/2}) > 0, \tag{4.8.13}$$

where $H_0^{(1)}(\cdot)$ denotes the Hankel function of order zero and first kind (see, e.g., [3, Sect. 9.1]). Hence, one only needs to apply equation (4.2.13) to conclude (4.8.6) and hence (4.8.10) (by factoring $M_V = M_u M_v$). (We note that (4.8.6) is proved in [150, Sect. XI.6] and [161, Theorem II.37] for $n = 3$.) Relation (4.8.9) is then clear from $V \in \mathcal{R}_3$ for $n = 3$ and follows from [162] for $n = 2$. Equation (4.8.11) is discussed in [23] for $n = 2, 3$. The trace formula (4.8.8) is a celebrated result of Krein [119], [120]; detailed accounts of it can be found in [15, Sect. 19.1.5], [22], [121], [193, Ch. 8].

Lemma 4.8.4. *Assume Hypothesis 4.8.1. Then the following formula holds for a.e. $\lambda \in \mathbb{R}$,*

$$\begin{aligned}
2\pi i \xi(\lambda, H, H_0) = \ln\left(\frac{{\det}_2\big(I + \overline{M_u(H_0 - (\lambda + i0)I)^{-1}M_v}\big)}{{\det}_2\big(I + \overline{M_u(H_0 - (\lambda - i0)I)^{-1}M_v}\big)}\right) \\
+ \frac{i}{2\pi}\int_{\mathbb{R}^n} d^n x\, V(x) \times \begin{cases} \pi, & \lambda > 0,\ n = 2, \\ \lambda^{1/2}, & \lambda > 0,\ n = 3, \\ 0, & \lambda \leq 0,\ n = 2, 3. \end{cases}
\end{aligned} \tag{4.8.14}$$

Proof. It follows from Theorem 4.8.2 and Lemma 4.8.3, that for $z \in \mathbb{C}\backslash\sigma(H)$,

$$\begin{aligned}
\int_{\mathbb{R}} \frac{d\lambda\, \xi(\lambda, H, H_0)}{(\lambda - z)^2} =& \frac{d}{dz}\ln\big({\det}_2\big(I + \overline{M_u(H_0 - zI)^{-1}M_v}\big)\big) \\
&+ \operatorname{tr}\big((H_0 - zI)^{-1}M_V(H_0 - zI)^{-1}\big).
\end{aligned} \tag{4.8.15}$$

First, we rewrite the left-hand side of (4.8.15). Since $\xi(\cdot, H, H_0) \in L^1\big(\mathbb{R}; \frac{d\lambda}{1+\lambda^2}\big)$, one has the following formula,

$$\int_{\mathbb{R}} \frac{d\lambda\, \xi(\lambda, H, H_0)}{(\lambda - z)^2} = \frac{d}{dz}\int_{\mathbb{R}} d\lambda\, \xi(\lambda, H, H_0)\left(\frac{1}{\lambda - z} - \frac{\lambda}{1 + \lambda^2}\right), \quad z \in \mathbb{C}\backslash\sigma(H). \tag{4.8.16}$$

Next, we compute the second term on the right-hand side of (4.8.15). By (4.8.12) and the cyclicity of the trace,

$$\operatorname{tr}\big((H_0 - zI)^{-1}M_V(H_0 - zI)^{-1}\big) = \operatorname{tr}\big(\overline{M_u(H_0 - zI)^{-2}M_v}\big), \quad z \in \mathbb{C}\backslash[0, \infty). \tag{4.8.17}$$

Then $\overline{M_u(H_0 - zI)^{-2}M_v} = \overline{M_u\frac{d}{dz}(H_0 - zI)^{-1}M_v}$ has the integral kernel

$$\big(\overline{M_u(H_0 - zI)^{-2}M_v}\big)(x, x') = \begin{cases} u(x)\frac{iH_0^{(1)'}(z^{1/2}|x-x'|)|x-x'|}{8z^{1/2}}v(x'), & x, x' \in \mathbb{R}^2, \\ u(x)\frac{i\exp(iz^{1/2}|x-x'|)}{8\pi z^{1/2}}v(x'), & x, x' \in \mathbb{R}^3, \end{cases}$$
$$x \neq x',\ z \in \mathbb{C}\backslash[0, \infty),\ \operatorname{Im}(z^{1/2}) > 0, \tag{4.8.18}$$

and hence, utilizing [43, p. 1086], one computes for $z \in \mathbb{C}\backslash[0,\infty)$,

$$\begin{aligned}\operatorname{tr}\big((H_0 - zI)^{-1} M_V (H_0 - zI)^{-1}\big) &= \frac{1}{4\pi}\int_{\mathbb{R}^n} d^n x\, V(x) \times \begin{cases} -z^{-1}, & n=2 \\ i(2z^{1/2})^{-1}, & n=3 \end{cases} \\ &= \frac{1}{4\pi}\int_{\mathbb{R}^n} d^n x\, V(x) \times \frac{d}{dz}\begin{cases} -\ln(z), & n=2, \\ iz^{1/2}, & n=3. \end{cases}\end{aligned} \tag{4.8.19}$$

Finally, using (4.8.15), (4.8.16), and (4.8.19), one obtains for $z \in \mathbb{C}\backslash\sigma(H)$,

$$\begin{aligned}&\int_{\mathbb{R}} d\lambda\, \xi(\lambda, H, H_0)\left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\right) + C \\ &\quad = \ln\big(\det{}_2\big(I + \overline{M_u (H_0 - zI)^{-1} M_v}\big)\big) + \frac{1}{4\pi}\int_{\mathbb{R}^n} d^n x\, V(x) \times \begin{cases} -\ln(z), & n=2, \\ iz^{1/2}, & n=3, \end{cases}\end{aligned} \tag{4.8.20}$$

where $C \in \mathbb{C}$ denotes an appropriate constant. To complete the proof we digress for a moment and recall the Stieltjes inversion formula for Herglotz functions m (i.e., analytic maps $m\colon \mathbb{C}_+ \to \mathbb{C}_+$, where $\mathbb{C}_+$ denotes the open complex upper half-plane). Such functions m permit the Nevanlinna, respectively, Riesz-Herglotz representation

$$\begin{aligned}&m(z) = c + dz + \int_{\mathbb{R}} d\omega(\lambda)\left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\right), \quad z \in \mathbb{C}_+, \\ &c = \operatorname{Re}[m(i)], \quad d = \lim_{\eta\uparrow\infty} m(i\eta)/(i\eta) \geq 0,\end{aligned} \tag{4.8.21}$$

with a nonnegative measure $d\omega$ on $\mathbb{R}$ satisfying

$$\int_{\mathbb{R}} \frac{d\omega(\lambda)}{1+\lambda^2} < \infty. \tag{4.8.22}$$

The absolutely continuous part $d\omega_{ac}$ of $d\omega$ with respect to Lebesgue measure $d\lambda$ on $\mathbb{R}$ is then known to be given by

$$d\omega_{ac}(\lambda) = \pi^{-1}\operatorname{Im}[m(\lambda + i0)]\, d\lambda. \tag{4.8.23}$$

In addition, one extends m to the open lower complex half-plane $\mathbb{C}_-$ by

$$m(z) = \overline{m(\overline{z})}, \quad z \in \mathbb{C}_-. \tag{4.8.24}$$

(We refer, e.g., to [5, Sect. 69] for details on (4.8.21)–(4.8.24).) Thus, in order to apply (4.8.21)–(4.8.24) to the computation of $\xi(\cdot, H, H_0)$ in (4.8.20) it suffices to decompose $\xi(\cdot, H, H_0) = \xi_+(\cdot, H, H_0) - \xi_-(\cdot, H, H_0)$ into its positive and negative parts $\xi_\pm(\cdot, H, H_0) \geq 0$ and separately consider the absolutely continuous measures $\xi_\pm(\cdot, H, H_0)d\lambda$. Thus, letting $z = \lambda \pm i\varepsilon$, taking the limit $\varepsilon \downarrow 0$ in (4.8.20), and subtracting the corresponding results, yields (4.8.14). $\square$

We conclude with the following result:

Corollary 4.8.5. *Assume Hypothesis 4.8.1. Then, for a.e. $\lambda > 0$,*

$$\det(S(\lambda)) = \frac{\det{}_2\big(I + \overline{M_u(H_0 - (\lambda - i0)I)^{-1}M_v}\big)}{\det{}_2\big(I + \overline{M_u(H_0 - (\lambda + i0)I)^{-1}M_v}\big)} \times \begin{cases} \exp\big(-\frac{i}{2}\int_{\mathbb{R}^n} d^n x\, V(x)\big), & n = 2, \\ \exp\big(-\frac{i\lambda^{1/2}}{2\pi}\int_{\mathbb{R}^n} d^n x\, V(x)\big), & n = 3. \end{cases} \tag{4.8.25}$$

Proof. Hypothesis 4.8.1 implies that the scattering operator $S(\lambda)$ at fixed energy $\lambda > 0$ in $L^2(S^{n-1}; d^{n-1}\omega)$ satisfies

$$[S(\lambda) - I] \in \mathcal{B}_1\big(L^2(S^{n-1}; d^{n-1}\omega)\big) \text{ for a.e. } \lambda > 0 \tag{4.8.26}$$

and

$$\det(S(\lambda)) = \exp(-2\pi i\xi(\lambda, H, H_0)) \text{ for a.e. } \lambda > 0 \tag{4.8.27}$$

(cf., e.g., [15, Sects. 19.1.4, 19.1.5], [20], [22], [193, Ch. 8]), where S^{n-1} denotes the unit sphere in $\mathbb{R}^n$ and $d^{n-1}\omega$ the corresponding surface measure on S^{n-1}. Relation (4.8.25) then follows from Lemma 4.8.4 and (4.8.27). $\square$

We note again that Corollary 7.5 was derived earlier using different means by Cheney [29] for $n = 2$ and by Newton [141] for $n = 3$. (The stronger conditions $V \in L^2(\mathbb{R}^3; dx^3)$ and the existence of $a > 0$ and $0 < C < \infty$ such that for all $y \in \mathbb{R}^3$, $\int_{\mathbb{R}^3} d^3x \, |V(x)| [(|x| + |y| + a)/(|x - y|)]^2 \leq C$, are assumed in [141].)

Appendix A

Basic Facts on Caratheodory and Schur Functions

In this appendix we summarize a few basic properties of Caratheodory and Schur functions used in Chapters 1 and 2.

We denote by $\mathbb{D}$ and $\partial\mathbb{D}$ the open unit disk and the counterclockwise oriented unit circle in the complex plane $\mathbb{C}$,

$$\mathbb{D} = \{z \in \mathbb{C} \,|\, |z| < 1\}, \quad \partial\mathbb{D} = \{\zeta \in \mathbb{C} \,|\, |\zeta| = 1\}, \tag{A.1}$$

and by

$$\mathbb{C}_\ell = \{z \in \mathbb{C} \,|\, \mathrm{Re}(z) < 0\}, \quad \mathbb{C}_r = \{z \in \mathbb{C} \,|\, \mathrm{Re}(z) > 0\} \tag{A.2}$$

the open left and right complex half-planes, respectively.

Definition A.1. Let $f_\pm$, φ_+, and $1/\varphi_-$ be analytic in $\mathbb{D}$.

(i) f_+ is called a *Caratheodory function* if $f_+ \colon \mathbb{D} \to \mathbb{C}_r$ and f_- is called an *anti-Caratheodory function* if $-f_-$ is a Caratheodory function.

(ii) φ_+ is called a *Schur function* if $\varphi_+ \colon \mathbb{D} \to \mathbb{D}$. φ_- is called an *anti-Schur function* if $1/\varphi_-$ is a Schur function.

Theorem A.2 ([4], Sect. 3.1; [5], Sect. 69; [171], Sect. 1.3)**.**

Let f be a Caratheodory function. Then f admits the Herglotz representation

$$f(z) = ic + \oint_{\partial\mathbb{D}} d\mu(\zeta)\, \frac{\zeta + z}{\zeta - z}, \quad z \in \mathbb{D}, \tag{A.3}$$

$$c = \mathrm{Im}(f(0)), \quad \oint_{\partial\mathbb{D}} d\mu(\zeta) = \mathrm{Re}(f(0)) < \infty, \tag{A.4}$$

where $d\mu$ denotes a nonnegative measure on $\partial\mathbb{D}$. The measure $d\mu$ can be reconstructed from f by the formula

$$\mu\big(\mathrm{Arc}\big(\big(e^{i\theta_1}, e^{i\theta_2}\big]\big)\big) = \lim_{\delta\downarrow 0} \lim_{r\uparrow 1} \frac{1}{2\pi} \oint_{\theta_1+\delta}^{\theta_2+\delta} d\theta\, \mathrm{Re}\big(f\big(re^{i\theta}\big)\big), \tag{A.5}$$

where

$$\mathrm{Arc}\big(\big(e^{i\theta_1}, e^{i\theta_2}\big]\big) = \big\{e^{i\theta} \in \partial\mathbb{D} \,|\, \theta_1 < \theta \le \theta_2\big\}, \quad \theta_1 \in [0, 2\pi),\ \theta_1 < \theta_2 \le \theta_1 + 2\pi. \tag{A.6}$$

Conversely, the right-hand side of (A.3) *with $c \in \mathbb{R}$ and $d\mu$ a finite* (*nonnegative*) *measure on $\partial\mathbb{D}$ defines a Caratheodory function.*

We note that additive nonnegative constants on the right-hand side of (A.3) can be absorbed into the measure $d\mu$ since

$$\oint_{\partial\mathbb{D}} d\mu_0(\zeta)\, \frac{\zeta + z}{\zeta - z} = 1, \quad z \in \mathbb{D}, \tag{A.7}$$

where

$$d\mu_0(\zeta) = \frac{d\theta}{2\pi}, \quad \zeta = e^{i\theta},\ \theta \in [0, 2\pi] \tag{A.8}$$

denotes the normalized Lebesgue measure on the unit circle $\partial\mathbb{D}$.

A useful fact on Caratheodory functions f is a certain monotonicity property they exhibit on open connected arcs of the unit circle away from the support of the measure

$d\mu$ in the Herglotz representation (A.3). More precisely, suppose $\mathrm{Arc}\big((e^{i\theta_1}, e^{i\theta_2})\big) \subset (\partial\mathbb{D}\backslash\mathrm{supp}(d\mu))$, $\theta_1 < \theta_2$, then f has an analytic continuation through $\mathrm{Arc}\big((e^{i\theta_1}, e^{i\theta_2})\big)$ and it is purely imaginary on $\mathrm{Arc}\big((e^{i\theta_1}, e^{i\theta_2})\big)$. Moreover,

$$\frac{d}{d\theta} f\big(e^{i\theta}\big) = -\frac{i}{2} \int_{[0,2\pi]\backslash(\theta_1,\theta_2)} d\mu\big(e^{it}\big) \frac{1}{\sin^2((t-\theta)/2)}, \quad \theta \in (\theta_1, \theta_2). \tag{A.9}$$

In particular,

$$-i \frac{d}{d\theta} f\big(e^{i\theta}\big) < 0, \quad \theta \in (\theta_1, \theta_2). \tag{A.10}$$

We recall that any Caratheodory function f has finite radial limits to the unit circle μ_0-almost everywhere, that is,

$$f(\zeta) = \lim_{r\uparrow 1} f(r\zeta) \text{ exists and is finite for } \mu_0\text{-a.e. } \zeta \in \partial\mathbb{D}. \tag{A.11}$$

The absolutely continuous part $d\mu_{\mathrm{ac}}$ of the measure $d\mu$ in the Herglotz representation (A.3) of the Caratheodory function f is given by

$$d\mu_{\mathrm{ac}}(\zeta) = \lim_{r\uparrow 1} \mathrm{Re}(f(r\zeta))\, d\mu_0(\zeta), \quad \zeta \in \partial\mathbb{D}. \tag{A.12}$$

The set

$$S_{\mu_{\mathrm{ac}}} = \{\zeta \in \partial\mathbb{D} \,|\, \lim_{r\uparrow 1} \mathrm{Re}(f(r\zeta)) = \mathrm{Re}(f(\zeta)) > 0 \text{ exists finitely}\} \tag{A.13}$$

is an essential support of $d\mu_{\mathrm{ac}}$ and its essential closure, $\overline{S_{\mu_{\mathrm{ac}}}}^e$, coincides with the topological support, $\mathrm{supp}(d\mu_{\mathrm{ac}})$ (the smallest closed support), of $d\mu_{\mathrm{ac}}$,

$$\overline{S_{\mu_{\mathrm{ac}}}}^e = \mathrm{supp}\,(d\mu_{\mathrm{ac}}). \tag{A.14}$$

Moreover, the set

$$S_{\mu_{\mathrm{s}}} = \{\zeta \in \partial\mathbb{D} \,|\, \lim_{r\uparrow 1} \mathrm{Re}(f(r\zeta)) = \infty\} \tag{A.15}$$

is an essential support of the singular part $d\mu_{\mathrm{s}}$ of the measure $d\mu$, and

$$\lim_{r\uparrow 1}(1-r)f(r\zeta) = \lim_{r\uparrow 1}(1-r)\mathrm{Re}(f(r\zeta)) \geq 0 \text{ exists for all } \zeta \in \partial\mathbb{D}. \tag{A.16}$$

In particular, $\zeta_0 \in \partial\mathbb{D}$ is a pure point of $d\mu$ if and only if

$$\mu(\{\zeta_0\}) = \lim_{r\uparrow 1}\left(\frac{1-r}{2}\right) f(r\zeta_0) > 0. \tag{A.17}$$

Given a Caratheodory (resp., anti-Caratheodory) function f_+ (resp. f_-) defined in $\mathbb{D}$ as in (A.3), one extends $f_\pm$ to all of $\mathbb{C}\backslash\partial\mathbb{D}$ by

$$f_\pm(z) = ic_\pm \pm \oint_{\partial\mathbb{D}} d\mu_\pm(\zeta)\,\frac{\zeta+z}{\zeta-z}, \quad z \in \mathbb{C}\backslash\partial\mathbb{D},\ c_\pm \in \mathbb{R}. \tag{A.18}$$

In particular,

$$f_\pm(z) = -\overline{f_\pm(1/\overline{z})}, \quad z \in \mathbb{C}\backslash\overline{\mathbb{D}}. \tag{A.19}$$

Of course, this continuation of $f_\pm|_{\mathbb{D}}$ to $\mathbb{C}\backslash\overline{\mathbb{D}}$, in general, is not an analytic continuation of $f_\pm|_{\mathbb{D}}$. With $f_\pm$ defined on $\mathbb{C}\backslash\partial\mathbb{D}$ by (A.18) one infers the mapping properties

$$f_+ \colon \mathbb{D} \to \mathbb{C}_r, \quad f_+ \colon \mathbb{C}\backslash\overline{\mathbb{D}} \to \mathbb{C}_\ell, \quad f_- \colon \mathbb{D} \to \mathbb{C}_\ell, \quad f_- \colon \mathbb{C}\backslash\overline{\mathbb{D}} \to \mathbb{C}_r. \tag{A.20}$$

Next, given the functions $f_\pm$ defined in $\mathbb{C}\backslash\partial\mathbb{D}$ as in (A.18), we introduce the functions $\varphi_\pm$ by

$$\varphi_\pm(z) = \frac{f_\pm(z)-1}{f_\pm(z)+1}, \quad z \in \mathbb{C}\backslash\partial\mathbb{D}. \tag{A.21}$$

Then $\varphi_\pm$ have the mapping properties

$$\begin{aligned} &\varphi_+ \colon \mathbb{D} \to \mathbb{D}, \quad 1/\varphi_+ \colon \mathbb{C}\backslash\overline{\mathbb{D}} \to \mathbb{D} \quad (\varphi_+ \colon \mathbb{C}\backslash\overline{\mathbb{D}} \to (\mathbb{C}\backslash\overline{\mathbb{D}}) \cup \{\infty\}), \\ &\varphi_- \colon \mathbb{C}\backslash\overline{\mathbb{D}} \to \mathbb{D}, \quad 1/\varphi_- \colon \mathbb{D} \to \mathbb{D} \quad (\varphi_- \colon \mathbb{D} \to (\mathbb{C}\backslash\overline{\mathbb{D}}) \cup \{\infty\}), \end{aligned} \tag{A.22}$$

in particular, $\varphi_+|_{\mathbb{D}}$ (resp., $\varphi_-|_{\mathbb{D}}$) is a Schur (resp., anti-Schur) function. Moreover,

$$f_\pm(z) = \frac{1+\varphi_\pm(z)}{1-\varphi_\pm(z)}, \quad z \in \mathbb{C}\backslash\partial\mathbb{D}. \tag{A.23}$$

We also recall the following useful result (see [171, Lemma 10.11.17] and Lemma 2.4.4 for a proof). To fix some notation we denote by f_+ and f_- a Caratheodory and anti-Caratheodory function, respectively, and by φ_+ and φ_- the corresponding Schur and anti-Schur functions as defined in (A.21). We also introduce the following notation for open arcs on the unit circle $\partial\mathbb{D}$,

$$\operatorname{Arc}\big(\big(e^{i\theta_1}, e^{i\theta_2}\big)\big) = \big\{e^{i\theta} \in \partial\mathbb{D} \,|\, \theta_1 < \theta < \theta_2\big\}, \quad \theta_1 \in [0, 2\pi],\ \theta_1 < \theta_2 \leq \theta_1 + 2\pi. \tag{A.24}$$

An open arc $A \subseteq \partial\mathbb{D}$ then either coincides with $\operatorname{Arc}\big(\big(e^{i\theta_1}, e^{i\theta_2}\big)\big)$ for some $\theta_1 \in [0, 2\pi]$, $\theta_1 < \theta_2 \leq \theta_1 + 2\pi$, or else, $A = \partial\mathbb{D}$.

Lemma A.3. *Let $A \subseteq \partial\mathbb{D}$ be an open arc and assume that f_+ (resp., f_-) is a Caratheodory (resp., anti-Caratheodory) function satisfying the reflectionless condition*

$$\lim_{r\uparrow 1} \big[f_+(r\zeta) + \overline{f_-(r\zeta)}\big] = 0 \ \ \mu_0\text{-a.e. on } A. \tag{A.25}$$

Then,

(i) $f_+(\zeta) = -\overline{f_-(\zeta)}$ for all $\zeta \in A$.

(ii) For $z \in \mathbb{D}$, $-\overline{f_-(1/\overline{z})}$ is the analytic continuation of $f_+(z)$ through the arc A.

(iii) $d\mu_\pm$ are purely absolutely continuous on A and

$$\frac{d\mu_\pm}{d\mu_0}(\zeta) = \operatorname{Re}(f_+(\zeta)) = -\operatorname{Re}(f_-(\zeta)), \quad \zeta \in A. \tag{A.26}$$

In analogy to the exponential representation of Nevanlinna–Herglotz functions (i.e., functions analytic in the open complex upper half-plane $\mathbb{C}_+$ with a strictly positive imaginary part on $\mathbb{C}_+$, cf. [7], [8], [78], [107]) one obtains the following result.

Theorem A.4. *Let f be a Caratheodory function. Then $-i\ln(if)$ is a Caratheodory function and f has the exponential Herglotz representation,*

$$-i\ln(if(z)) = id + \oint_{\partial\mathbb{D}} d\mu_0(\zeta)\,\Upsilon(\zeta)\,\frac{\zeta+z}{\zeta-z}, \quad z \in \mathbb{D}, \tag{A.27}$$

$$d = -\mathrm{Re}(\ln(f(0))), \quad 0 \leq \Upsilon(\zeta) \leq \pi \ \textit{for } \mu_0\textit{-a.e. } \zeta \in \partial\mathbb{D}. \tag{A.28}$$

Υ can be reconstructed from f by

$$\begin{aligned} \Upsilon(\zeta) &= \lim_{r\uparrow 1} \mathrm{Re}[-i\ln(if(r\zeta))] \\ &= (\pi/2) + \lim_{r\uparrow 1} \mathrm{Im}[\ln(f(r\zeta))] \ \textit{for } \mu_0\textit{-a.e. } \zeta \in \partial\mathbb{D}. \end{aligned} \tag{A.29}$$

Next we briefly turn to matrix-valued Caratheodory functions. We denote as usual $\mathrm{Re}(A) = (A + A^*)/2$, $\mathrm{Im}(A) = (A - A^*)/(2i)$, etc., for square matrices A.

Definition A.5. Let $m \in \mathbb{N}$ and $\mathcal{F}$ be an $m \times m$ matrix-valued function analytic in $\mathbb{D}$. $\mathcal{F}$ is called a *Caratheodory matrix* if $\mathrm{Re}(\mathcal{F}(z)) \geq 0$ for all $z \in \mathbb{D}$.

Theorem A.6. *Let $\mathcal{F}$ be an $m \times m$ Caratheodory matrix, $m \in \mathbb{N}$. Then $\mathcal{F}$ admits the Herglotz representation*

$$\mathcal{F}(z) = iC + \oint_{\partial\mathbb{D}} d\Omega(\zeta)\,\frac{\zeta+z}{\zeta-z}, \quad z \in \mathbb{D}, \tag{A.30}$$

$$C = \mathrm{Im}(\mathcal{F}(0)), \quad \oint_{\partial\mathbb{D}} d\Omega(\zeta) = \mathrm{Re}(\mathcal{F}(0)), \tag{A.31}$$

where $d\Omega$ denotes a nonnegative $m \times m$ matrix-valued measure on $\partial\mathbb{D}$. The measure $d\Omega$ can be reconstructed from $\mathcal{F}$ by the formula

$$\Omega\big(\mathrm{Arc}\big(\big(e^{i\theta_1}, e^{i\theta_2}\big]\big)\big) = \lim_{\delta\downarrow 0}\lim_{r\uparrow 1} \frac{1}{2\pi} \oint_{\theta_1+\delta}^{\theta_2+\delta} d\theta\, \mathrm{Re}\big(\mathcal{F}\big(re^{i\theta}\big)\big), \tag{A.32}$$

$$\theta_1 \in [0, 2\pi], \ \theta_1 < \theta_2 \leq \theta_1 + 2\pi.$$

Conversely, the right-hand side of equation (A.30) *with* $C = C^*$ *and* $d\Omega$ *a finite nonnegative* $m \times m$ *matrix-valued measure on* $\partial\mathbb{D}$ *defines a Caratheodory matrix.*

Appendix B

Basic Facts on Herglotz Functions

In this appendix we recall the definition and basic properties of Herglotz functions used extensively in Chapter 3.

Definition B.1. Let $\mathbb{C}_\pm = \{z \in \mathbb{C} \mid \operatorname{Im}(z) \gtrless 0\}$. $m : \mathbb{C}_+ \to \mathbb{C}$ is called a *Herglotz* function (or *Nevanlinna* or *Pick* function) if m is analytic on $\mathbb{C}_+$ and $m(\mathbb{C}_+) \subseteq \mathbb{C}_+$.

One then extends m to $\mathbb{C}_-$ by reflection, that is, one defines

$$m(z) = \overline{m(\overline{z})}, \quad z \in \mathbb{C}_-. \tag{B.1}$$

Of course, generally, (B.1) does not represent the analytic continuation of $m\big|_{\mathbb{C}_+}$ into $\mathbb{C}_-$.

The fundamental result on Herglotz functions and their representations on Borel transforms, in part due to Fatou, Herglotz, Luzin, Nevanlinna, Plessner, Privalov, de la Vallée Poussin, Riesz, and others, then reads as follows.

Theorem B.2. ([5], Sect. 69, [7], [42], Chs. II, IV, [107], [114], Ch. 6, [148], Chs. II, IV, [153], Ch. 5.) Let m be a Herglotz function. Then,

(i) $m(z)$ has finite normal limits $m(\lambda \pm i0) = \lim_{\varepsilon\downarrow 0} m(\lambda \pm i\varepsilon)$ for a.e. $\lambda \in \mathbb{R}$.

(ii) Suppose $m(z)$ has a zero normal limit on a subset of $\mathbb{R}$ having positive Lebesgue measure. Then $m \equiv 0$.

(iii) There exists a Borel measure $d\omega$ on $\mathbb{R}$ satisfying

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

such that the Nevanlinna, respectively, Riesz-Herglotz representation

$$m(z) = c + dz + \int_{\mathbb{R}} d\omega(\lambda) \left[\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2} \right], \quad z \in \mathbb{C}_+, \tag{B.3}$$

$$c = \mathrm{Re}(m(i)), \quad d = \lim_{\eta \uparrow \infty} m(i\eta)/(i\eta) \geq 0$$

holds. Conversely, any function m of the type (B.3) is a Herglotz function.

(iv) Let $\lambda_1, \lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$. Then the Stieltjes inversion formula for $d\omega$ reads

$$\omega((\lambda_1, \lambda_2]) = \pi^{-1} \lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} \int_{\lambda_1 + \delta}^{\lambda_2 + \delta} d\lambda \, \mathrm{Im}(m(\lambda + i\varepsilon)). \tag{B.4}$$

(v) The absolutely continuous (ac) part $d\omega_{ac}$ of $d\omega$ with respect to Lebesgue measure $d\lambda$ on $\mathbb{R}$ is given by

$$d\omega_{ac}(\lambda) = \pi^{-1} \mathrm{Im}(m(\lambda + i0)) \, d\lambda. \tag{B.5}$$

(vi) Local singularities of m and m^{-1} are necessarily real and at most of first order in the sense that

$$\lim_{\epsilon \downarrow 0} (-i\epsilon) \, m(\lambda + i\epsilon) \geq 0, \quad \lambda \in \mathbb{R}, \tag{B.6}$$

$$\lim_{\epsilon \downarrow 0} (i\epsilon) \, m(\lambda + i\epsilon)^{-1} \geq 0, \quad \lambda \in \mathbb{R}. \tag{B.7}$$

Further properties of Herglotz functions are collected in the following theorem. We denote by

$$d\omega = d\omega_{\mathrm{ac}} + d\omega_{\mathrm{sc}} + d\omega_{\mathrm{pp}} \tag{B.8}$$

the decomposition of $d\omega$ into its absolutely continuous (ac), singularly continuous (sc), and pure point (pp) parts with respect to Lebesgue measure on $\mathbb{R}$.

Theorem B.3. ([7], [78], [107], [166], [167].) Let m be a Herglotz function with representation (B.3). Then,

(i)

$$\begin{aligned}
&d = 0 \text{ and } \int_{\mathbb{R}} d\omega(\lambda)(1+|\lambda|^s)^{-1} < \infty \text{ for some } s \in (0,2) \\
&\text{if and only if } \int_1^\infty d\eta\, \eta^{-s}\, \mathrm{Im}(m(i\eta)) < \infty.
\end{aligned} \tag{B.9}$$

(ii) Let $(\lambda_1, \lambda_2) \subset \mathbb{R}$, $\eta_1 > 0$. Then there is a constant $C(\lambda_1, \lambda_2, \eta_1) > 0$ such that

$$\eta|m(\lambda + i\eta)| \leq C(\lambda_1, \lambda_2, \eta_1), \quad (\lambda, \eta) \in [\lambda_1, \lambda_2] \times (0, \eta_1). \tag{B.10}$$

(iii)

$$\sup_{\eta>0} \eta|m(i\eta)| < \infty \text{ if and only if } m(z) = \int_{\mathbb{R}} d\omega(\lambda)(\lambda - z)^{-1} \text{ and } \int_{\mathbb{R}} d\omega(\lambda) < \infty. \tag{B.11}$$

In this case,

$$\int_{\mathbb{R}} d\omega(\lambda) = \sup_{\eta>0} \eta|m(i\eta)| = -i \lim_{\eta\uparrow\infty} \eta m(i\eta). \tag{B.12}$$

(iv) For all $\lambda \in \mathbb{R}$,

$$\lim_{\varepsilon\downarrow 0} \varepsilon \mathrm{Re}(m(\lambda + i\varepsilon)) = 0, \tag{B.13}$$

$$\omega(\{\lambda\}) = \lim_{\varepsilon\downarrow 0} \varepsilon \mathrm{Im}(m(\lambda + i\varepsilon)) = -i \lim_{\varepsilon\downarrow 0} \varepsilon m(\lambda + i\varepsilon). \tag{B.14}$$

(v) Let $L > 0$ and suppose $0 \leq \mathrm{Im}(m(z)) \leq L$ for all $z \in \mathbb{C}_+$. Then $d = 0$, $d\omega$ is purely absolutely continuous, $d\omega = d\omega_{ac}$, and

$$0 \leq \frac{d\omega(\lambda)}{d\lambda} = \pi^{-1} \lim_{\varepsilon\downarrow 0} \mathrm{Im}(m(\lambda + i\varepsilon)) \leq \pi^{-1} L \text{ for a.e. } \lambda \in \mathbb{R}. \tag{B.15}$$

(vi) Let $p \in (1,\infty)$, $[\lambda_3,\lambda_4] \subset (\lambda_1,\lambda_2)$, $[\lambda_1,\lambda_2] \subset (\lambda_5,\lambda_6)$. If

$$\sup_{0<\varepsilon<1} \int_{\lambda_1}^{\lambda_2} d\lambda \, |\mathrm{Im}(m(\lambda+i\varepsilon))|^p < \infty, \tag{B.16}$$

then $d\omega = d\omega_{ac}$ is purely absolutely continuous on (λ_1,λ_2), $\frac{d\omega_{ac}}{d\lambda} \in L^p((\lambda_1,\lambda_2); d\lambda)$, and

$$\lim_{\varepsilon\downarrow 0} \left\| \pi^{-1}\mathrm{Im}(m(\cdot+i\varepsilon)) - \frac{d\omega_{ac}}{d\lambda} \right\|_{L^p((\lambda_3,\lambda_4);d\lambda)} = 0. \tag{B.17}$$

Conversely, if $d\omega$ is purely absolutely continuous on (λ_5,λ_6), and if $\frac{d\omega_{ac}}{d\lambda} \in L^p((\lambda_5,\lambda_6); d\lambda)$, then (B.16) holds.

(vii) Let $(\lambda_1,\lambda_2) \subset \mathbb{R}$. Then a local version of Wiener's theorem reads for $p \in (1,\infty)$,

$$\begin{aligned} &\lim_{\varepsilon\downarrow 0} \varepsilon^{p-1} \int_{\lambda_1}^{\lambda_2} d\lambda \, |\mathrm{Im}(m(\lambda+i\varepsilon))|^p \\ &\quad = \frac{\Gamma(\frac{1}{2})\Gamma(p-\frac{1}{2})}{\Gamma(p)} \left[\frac{1}{2}\omega(\{\lambda_1\})^p + \frac{1}{2}\omega(\{\lambda_2\})^p + \sum_{\lambda\in(\lambda_1,\lambda_2)} \omega(\{\lambda\})^p \right]. \end{aligned} \tag{B.18}$$

Moreover, for $0 < p < 1$,

$$\lim_{\varepsilon\downarrow 0} \int_{\lambda_1}^{\lambda_2} d\lambda \, |\pi^{-1}\mathrm{Im}(m(\lambda+i\varepsilon))|^p = \int_{\lambda_1}^{\lambda_2} d\lambda \left| \frac{d\omega_{ac}(\lambda)}{d\lambda} \right|^p. \tag{B.19}$$

It should be stressed that Theorems B.2 and B.3 record only the tip of an iceberg of results in this area. A substantial number of additional references relevant in this context can be found in [78].

Appendix C

Properties of the Dirichlet and Neumann Laplacians

The purpose of this appendix is to derive some basic domain properties of Dirichlet and Neumann Laplacians on $C^{1,r}$-domains $\Omega \subset \mathbb{R}^n$ as needed in Chapter 4 and to prove Lemma 4.6.7. Throughout this appendix we assume $n \geq 2$, but we note that n is restricted to $n = 2, 3$ in Sections 4.6–4.8.

In this manuscript we use the following notation for the standard Sobolev Hilbert spaces ($s \in \mathbb{R}$),

$$H^s(\mathbb{R}^n) = \left\{ U \in \mathcal{S}(\mathbb{R}^n)^* \mid \|U\|^2_{H^s(\mathbb{R}^n)} = \int_{\mathbb{R}^n} d^n\xi \, \big|\widehat{U}(\xi)\big|^2 \big(1 + |\xi|^{2s}\big) < \infty \right\}, \tag{C.1}$$

$$H^s(\Omega) = \{ u \in C_0^\infty(\Omega)^* \mid u = U|_\Omega \text{ for some } U \in H^s(\mathbb{R}^n) \}, \tag{C.2}$$

$$H_0^s(\Omega) = \text{the closure of } C_0^\infty(\Omega) \text{ in the norm of } H^s(\Omega). \tag{C.3}$$

Here $C_0^\infty(\Omega)^*$ denotes the usual set of distributions on $\Omega \subseteq \mathbb{R}^n$, Ω open and nonempty, $\mathcal{S}(\mathbb{R}^n)^*$ is the space of tempered distributions on $\mathbb{R}^n$, and $\widehat{U}$ denotes the Fourier transform of $U \in \mathcal{S}(\mathbb{R}^n)^*$. It is then immediate that

$$H^{s_0}(\Omega) \hookrightarrow H^{s_1}(\Omega) \quad \text{whenever} \quad -\infty < s_0 \leq s_1 < +\infty, \tag{C.4}$$

continuously and densely.

Before we present a proof of Lemma 4.6.7, we recall the definition of a $C^{1,r}$-domain $\Omega \subseteq \mathbb{R}^n$, Ω open and nonempty, for convenience of the reader: Let $\mathcal{N}$ be a space of real-valued functions in $\mathbb{R}^{n-1}$. One calls a bounded domain $\Omega \subset \mathbb{R}^n$ of class $\mathcal{N}$ if there exists a finite open covering $\{\mathcal{O}_j\}_{1\leq j\leq N}$ of the boundary $\partial\Omega$ of Ω with the property that, for every $j \in \{1, ..., N\}$, $\mathcal{O}_j \cap \Omega$ coincides with the portion of $\mathcal{O}_j$ lying in the over-graph of a function $\varphi_j \in \mathcal{N}$ (considered in a new system of coordinates obtained from the original one via a rigid motion). Two special cases are going to play a particularly important role in the sequel. First, if $\mathcal{N}$ is $\mathrm{Lip}\,(\mathbb{R}^{n-1})$, the space of real-valued functions satisfying a (global) Lipschitz condition in $\mathbb{R}^{n-1}$, we shall refer to Ω as being a Lipschitz domain; cf. [175, p. 189], where such domains are called "minimally smooth". Second, corresponding to the case when $\mathcal{N}$ is the subspace of $\mathrm{Lip}\,(\mathbb{R}^{n-1})$ consisting of functions whose first-order derivatives satisfy a (global) Hölder condition of order $r \in (0, 1)$, we shall say that Ω is of class $C^{1,r}$. The classical theorem of Rademacher of almost everywhere differentiability of Lipschitz functions ensures that, for any Lipschitz domain Ω, the surface measure $d\sigma$ is well-defined on $\partial\Omega$ and that there exists an outward pointing normal vector ν at almost every point of $\partial\Omega$. For a Lipschitz domain $\Omega \subset \mathbb{R}^n$ it is known that

$$\big(H^s(\Omega)\big)^* = H^{-s}(\Omega), \quad -\tfrac{1}{2} < s < \tfrac{1}{2}. \tag{C.5}$$

See [186] for this and other related properties.

Next, assume that $\Omega \subset \mathbb{R}^n$ is the domain lying above the graph of a function $\varphi : \mathbb{R}^{n-1} \to \mathbb{R}$ of class $C^{1,r}$. Then for $0 \leq s < 1+r$, the Sobolev space $H^s(\partial\Omega)$ consists of functions $f \in L^2(\partial\Omega; d^{n-1}\sigma)$ such that $f(x', \varphi(x'))$, as function of $x' \in \mathbb{R}^{n-1}$, belongs to $H^s(\mathbb{R}^{n-1})$. This definition is easily adapted to the case when Ω is domain of class $C^{1,r}$ whose boundary is compact, by using a smooth partition of unity. Finally, for $-1-r < s < 0$, we set $H^s(\partial\Omega) = (H^{-s}(\partial\Omega))^*$. For additional background information in this context we refer, for instance, to [130, Ch. 3], [192, Sect. I.4.2].

Assuming Hypothesis 4.6.6 (i) (i.e., Ω is an open nonempty $C^{1,r}$-domain for some $(1/2) < r < 1$ with compact boundary $\partial\Omega$), we introduce the Dirichlet and Neumann Laplacians $\widetilde{H}^D_{0,\Omega}$ and $\widetilde{H}^N_{0,\Omega}$ associated with the domain Ω as the unique self-adjoint operators on $L^2(\Omega; d^nx)$ whose quadratic form equals $q(f,g) = \int_\Omega d^nx\, \overline{\nabla f} \cdot \nabla g$ with the form domains $H^1_0(\Omega)$ and $H^1(\Omega)$, respectively. Then,

$$\begin{aligned}
\operatorname{dom}(\widetilde{H}^D_{0,\Omega}) = \{u \in H^1_0(\Omega) \,|\, &\text{there exists } f \in L^2(\Omega; d^nx) \text{ such that} \\
&q(u,v) = (f,v)_{L^2(\Omega;d^nx)} \text{ for all } v \in H^1_0(\Omega)\}, \qquad \text{(C.6)} \\
\operatorname{dom}(\widetilde{H}^N_{0,\Omega}) = \{u \in H^1(\Omega) \,|\, &\text{there exists } f \in L^2(\Omega; d^nx) \text{ such that} \\
&q(u,v) = (f,v)_{L^2(\Omega;d^nx)} \text{ for all } v \in H^1(\Omega)\}, \qquad \text{(C.7)}
\end{aligned}$$

with $(\cdot,\cdot)_{L^2(\Omega;d^nx)}$ denoting the scalar product in $L^2(\Omega; d^nx)$. Equivalently, we introduce the densely defined closed linear operators

$$D = \nabla, \ \operatorname{dom}(D) = H^1_0(\Omega) \ \text{ and } \ N = \nabla, \ \operatorname{dom}(N) = H^1(\Omega) \tag{C.8}$$

from $L^2(\Omega; d^nx)$ to $L^2(\Omega; d^nx)^n$ and note that

$$\widetilde{H}^D_{0,\Omega} = D^*D \ \text{ and } \ \widetilde{H}^N_{0,\Omega} = N^*N. \tag{C.9}$$

For details we refer to [151, Sects. XIII.14, XIII.15]. Moreover, with $\operatorname{div}(\cdot)$ denoting the divergence operator,

$$\operatorname{dom}(D^*) = \{w \in L^2(\Omega; d^n x)^n \,|\, \operatorname{div}(w) \in L^2(\Omega; d^n x)\}, \tag{C.10}$$

and hence,

$$\begin{aligned}\operatorname{dom}(\widetilde{H}^D_{0,\Omega}) &= \{u \in \operatorname{dom}(D) \,|\, Du \in \operatorname{dom}(D^*)\} \\ &= \{u \in H^1_0(\Omega) \,|\, \Delta u \in L^2(\Omega; d^n x)\}.\end{aligned} \tag{C.11}$$

One can also define the following map

$$\begin{cases} \{w \in L^2(\Omega; d^n x)^n \,|\, \operatorname{div}(w) \in (H^1(\Omega))^*\} \to H^{-1/2}(\partial\Omega) = \big(H^{1/2}(\partial\Omega)\big)^* \\ \qquad\qquad w \mapsto \nu \cdot w \end{cases} \tag{C.12}$$

by setting

$$\langle \nu \cdot w, \phi \rangle = \int_\Omega d^n x\, w(x) \cdot \nabla\Phi(x) + \langle \operatorname{div}(w)\,,\, \Phi \rangle \tag{C.13}$$

whenever $\phi \in H^{1/2}(\partial\Omega)$ and $\Phi \in H^1(\Omega)$ is such that $\gamma_D \Phi = \phi$. The last paring in (C.13) is in the duality sense (which, in turn, is compatible with the (bilinear) distributional pairing). It should be remarked that the above definition is independent of the particular extension $\Phi \in H^1(\Omega)$ of ϕ. Indeed, by linearity this comes down to proving that

$$\langle \operatorname{div}(w)\,,\, \Phi \rangle = -\int_\Omega d^n x\, w(x) \cdot \nabla\Phi(x) \tag{C.14}$$

if $w \in L^2(\Omega; d^n x)^n$ has $\operatorname{div}(w) \in H^1(\Omega))^*$ and $\Phi \in H^1(\Omega)$ has $\gamma_D \Phi = 0$. To see this, we rely on the existence of a sequence $\Phi_j \in C_0^\infty(\Omega)$ such that $\Phi_j \underset{j\uparrow\infty}{\longrightarrow} \Phi$ in $H^1(\Omega)$. When Ω is a bounded Lipschitz domain, this is well-known (see, e.g., [102, Remark 2.7] for a rather general result of this nature), and this result is easily extended to the case when Ω is an unbounded Lipschitz domain with a compact boundary. For if $\xi \in C_0^\infty(B(0;2))$ is such that $\xi = 1$ on $B(0;1)$ and $\xi_j(x) = \xi(x/j)$, $j \in \mathbb{N}$ (here $B(x_0;r_0)$ denotes the ball in $\mathbb{R}^n$ centered at $x_0 \in \mathbb{R}^n$ of radius $r_0 > 0$), then $\xi_j\Phi \underset{j\uparrow\infty}{\longrightarrow} \Phi$ in $H^1(\Omega)$ and matters are reduced to approximating $\xi_j\Phi$ in $H^1(B(0;2j)\cap\Omega)$ with test functions supported in $B(0;2j)\cap\Omega$, for each fixed $j \in \mathbb{N}$. Since $\gamma_D(\xi_j\Phi) = 0$, the result for bounded Lipschitz domains applies.

Returning to the task of proving (C.14), it suffices to prove a similar identity with Φ_j in place of Φ. This, in turn, follows from the definition of $\operatorname{div}(\cdot)$ in the sense of distributions and the fact that the duality between $(H^1(\Omega))^*$ and $H^1(\Omega)$ is compatible with the duality between distributions and test functions.

Going further, we can introduce a (weak) Neumann trace operator $\widetilde{\gamma}_N$ as follows:

$$\widetilde{\gamma}_N : \{u \in H^1(\Omega) \,|\, \Delta u \in (H^1(\Omega))^*\} \to H^{-1/2}(\partial\Omega), \quad \widetilde{\gamma}_N u = \nu \cdot \nabla u, \tag{C.15}$$

with the dot product understood in the sense of (C.12). We emphasize that the weak Neumann trace operator $\widetilde{\gamma}_N$ in (C.17) is an extension of the operator γ_N introduced in (4.6.43). Indeed, to see that $\operatorname{dom}(\gamma_N) \subset \operatorname{dom}(\widetilde{\gamma}_N)$, we note that if $u \in H^{s+1}(\Omega)$ for some $1/2 < s < 3/2$, then $\Delta u \in H^{-1+s}(\Omega) = \big(H^{1-s}(\Omega)\big)^* \hookrightarrow \big(H^1(\Omega)\big)^*$, by (C.5) and (C.4). With this in hand, it is then easy to shown that $\widetilde{\gamma}_N$ in (C.17) and γ_N in (4.6.43) agree (on the smaller domain), as claimed.

We now return to the mainstream discussion. From the above preamble it follows that

$$\operatorname{dom}(N^*) = \{w \in L^2(\Omega;d^nx)^n \,|\, \operatorname{div}(w) \in L^2(\Omega;d^nx) \text{ and } \nu \cdot w = 0\} \tag{C.16}$$

where the dot product operation is understood in the sense of (C.12). Consequently, with $\widetilde{H}^N_{0,\Omega} = N^*N$, we have

$$\begin{aligned}\operatorname{dom}(\widetilde{H}^N_{0,\Omega}) &= \{u \in \operatorname{dom}(N) \,|\, Nu \in \operatorname{dom}(N^*)\} \\ &= \{u \in H^1(\Omega) \,|\, \Delta u \in L^2(\Omega; d^n x) \text{ and } \widetilde{\gamma}_N u = 0\}. \end{aligned} \tag{C.17}$$

Next, we will prove that $H^D_{0,\Omega} = \widetilde{H}^D_{0,\Omega}$ and $H^N_{0,\Omega} = \widetilde{H}^N_{0,\Omega}$, where $H^D_{0,\Omega}$ and $H^N_{0,\Omega}$ denote the operators introduced in (4.6.44) and (4.6.45), respectively. Since it follows from the first Green's formula (cf., e.g., [130, Theorem 4.4]) that $H^D_{0,\Omega} \subseteq \widetilde{H}^D_{0,\Omega}$ and $H^N_{0,\Omega} \subseteq \widetilde{H}^N_{0,\Omega}$, it remains to show that $H^D_{0,\Omega} \supseteq \widetilde{H}^D_{0,\Omega}$ and $H^N_{0,\Omega} \supseteq \widetilde{H}^N_{0,\Omega}$. Moreover, it follows from comparing (4.6.44) with (C.11) and (4.6.45) with (C.17), that one needs only to show that $\operatorname{dom}(\widetilde{H}^D_{0,\Omega})$, $\operatorname{dom}(\widetilde{H}^N_{0,\Omega}) \subseteq H^2(\Omega)$.

Lemma C.1. *Assume Hypothesis 4.6.6 (i). Then,*

$$\operatorname{dom}(\widetilde{H}^D_{0,\Omega}) \subseteq H^2(\Omega), \quad \operatorname{dom}(\widetilde{H}^N_{0,\Omega}) \subseteq H^2(\Omega). \tag{C.18}$$

In particular,

$$H^D_{0,\Omega} = \widetilde{H}^D_{0,\Omega}, \quad H^N_{0,\Omega} = \widetilde{H}^N_{0,\Omega}. \tag{C.19}$$

Proof. Consider $u \in \operatorname{dom}(\widetilde{H}^N_{0,\Omega})$ and set $f = \Delta u - u \in L^2(\Omega; d^n x)$. Viewing f as an element in $\big(H^1(\Omega)\big)^*$, the classical Lax-Milgram Lemma implies that u is the unique solution of the boundary-value problem

$$\begin{cases} (\Delta - I_\Omega)u = f \in L^2(\Omega) \hookrightarrow \big(H^1(\Omega)\big)^*, \\ u \in H^1(\Omega), \\ \widetilde{\gamma}_N u = 0. \end{cases} \tag{C.20}$$

One convenient way to show that actually

$$u \in H^2(\Omega), \tag{C.21}$$

is to use layer potentials. Specifically, let $E(x)$, $x \in \mathbb{R}^n\backslash\{0\}$, be the fundamental solution of the Helmholtz operator $\Delta - I_\Omega$ in $\mathbb{R}^n$ and denote by $(\Delta - I_\Omega)^{-1}$ the operator of convolution with E. Let us also define the associated single layer potential

$$\mathcal{S}g(x) = \int_{\partial\Omega} d^{n-1}\sigma_y \, E(x-y)g(y), \quad x \in \Omega, \tag{C.22}$$

where g is an arbitrary measurable function on $\partial\Omega$. As is well-known (the interested reader may consult, e.g., [133], [190] for jump relations in the context of Lipschitz domains), if

$$K^{\#}g(x) = \int_{\partial\Omega} d^{n-1}\sigma_y \, \partial_{\nu_x} E(x-y)g(y), \quad x \in \partial\Omega \tag{C.23}$$

stands for the so-called adjoint double layer on $\partial\Omega$, the following jump formula holds

$$\widetilde{\gamma}_N \mathcal{S}g = (\tfrac{1}{2} I_{\partial\Omega} + K^{\#})g. \tag{C.24}$$

Now, the solution u of (C.20) is given by

$$u = (\Delta - I_\Omega)^{-1} f - \mathcal{S}g \tag{C.25}$$

for a suitable chosen g. In order to continue, we recall that the classical Calderón-Zygmund theory yields that, locally, $(\Delta - I_\Omega)^{-1}$ is smoothing of order 2 on the scale of Sobolev spaces, and since E has exponential decay at infinity, it follows that $(\Delta - I_\Omega)^{-1} f \in H^2(\Omega)$ whenever $f \in L^2(\Omega; d^n x)$. We shall then require that

$$\gamma_N \mathcal{S}g = \gamma_N (\Delta - I_\Omega)^{-1} f \text{ or } (\tfrac{1}{2} I_{\partial\Omega} + K^{\#})g = h = \gamma_N (\Delta - I_\Omega)^{-1} f \in H^{1/2}(\partial\Omega). \tag{C.26}$$

Thus, formally, $g = (\frac{1}{2} I_{\partial\Omega} + K^{\#})^{-1} h$ and (C.21) follows as soon as we prove that

$$\tfrac{1}{2} I_{\partial\Omega} + K^{\#} \text{ is invertible on } H^{1/2}(\partial\Omega) \tag{C.27}$$

and that the operator

$$\mathcal{S}\colon H^{1/2}(\partial\Omega) \to H^2(\Omega) \tag{C.28}$$

is well-defined and bounded. That (C.27) holds is essentially well-known. See, for instance, [181, Proposition 4.5] which requires that Ω is of class $C^{1,r}$ for some $(1/2) < r < 1$. As for (C.28), we note, as a preliminary step, that

$$\mathcal{S}\colon H^{-s}(\partial\Omega) \to H^{-s+3/2}(\Omega) \tag{C.29}$$

is well-defined and bounded for each $s \in [0,1]$, even when the boundary of Ω is only Lipschitz. Indeed, with $H^{-s+3/2}(\Omega)$ replaced by $H^{-s+3/2}(\Omega \cap B)$ for a sufficiently large ball $B \subset \mathbb{R}^n$, this is proved in [134] and the behavior at infinity is easily taken care of by employing the exponential decay of E.

For a fixed, arbitrary $j \in \{1,...,n\}$, consider next the operator $\partial_{x_j}\mathcal{S}$ whose kernel is $\partial_{x_j}E(x-y) = -\partial_{y_j}E(x-y)$. We write

$$\partial_{y_j} = \sum_{k=1}^{n} \nu_k(y)\nu_k(y)\partial_{y_j} = \sum_{k=1}^{n} \nu_k(y)\frac{\partial}{\partial\tau_{k,j}(y)} + \nu_j\partial_{\nu_y}, \tag{C.30}$$

where $\partial/\partial\tau_{k,j} = \nu_k\partial_j - \nu_j\partial_k,\ j,k = 1,\dots,n$, is a tangential derivative operator for which we have

$$\int_{\partial\Omega} d^{n-1}\sigma\, \frac{\partial h_1}{\partial\tau_{j,k}} h_2 = -\int_{\partial\Omega} d^{n-1}\sigma\, h_1 \frac{\partial h_2}{\partial\tau_{j,k}}, \quad h_1, h_2 \in H^{1/2}(\partial\Omega). \tag{C.31}$$

It follows that

$$\partial_j\mathcal{S}h = -\mathcal{D}(\nu_j h) + \sum_{k=1}^{n} \mathcal{S}\bigg(\frac{\partial(\nu_k h)}{\partial\tau_{k,j}}\bigg), \tag{C.32}$$

where $\mathcal{D}$, the so-called double layer potential operator, is the integral operator with integral kernel $\partial_{\nu_y}E(x-y)$. Its mappings properties on the scale of Sobolev spaces have been analyzed in [134] and we note here that

$$\mathcal{D}\colon H^s(\partial\Omega) \to H^{s+1/2}(\Omega), \quad 0 \le s \le 1, \tag{C.33}$$

requires only that $\partial\Omega$ is Lipschitz.

Assuming that multiplication by (the components of) normal unit vector ν preserves the space $H^{1/2}(\partial\Omega)$ (which is the case if, e.g., Ω is of class $C^{1,r}$ for some $(1/2) < r < 1$), the desired conclusion about the operator (C.28) follows from (C.29), (C.32) and (C.33). This concludes the proof of the fact that $\mathrm{dom}(\widetilde{H}^N_{0,\Omega}) \subseteq H^2(\Omega)$.

To prove that $\mathrm{dom}(\widetilde{H}^D_{0,\Omega}) \subseteq H^2(\Omega)$ we proceed in an analogous fashion, starting with the same representation (C.25). This time, the requirement on g is that $Sg = h = \gamma_D(\Delta - I_\Omega)^{-1} f \in H^{3/2}(\partial\Omega)$, where $S = \gamma_D \circ \mathcal{S}$ is the trace of the single layer. Thus, in this scenario, it suffices to know that

$$S\colon H^{1/2}(\partial\Omega) \to H^{3/2}(\partial\Omega) \tag{C.34}$$

is an isomorphism. When $\partial\Omega$ is of class C^∞, it has been proved in [181, Proposition 7.9] that $S\colon H^s(\partial\Omega) \to H^{s+1}(\partial\Omega)$ is an isomorphism for each $s \in \mathbb{R}$ and, if Ω is of class $C^{1,r}$ with $(1/2) < r < 1$, the validity range of this result is limited to $-1-r < s < r$, which covers (C.34). The latter fact follows from an inspection of Taylor's original proof of Proposition 7.9 in [181]. Here we just note that the only significant difference is that if $\partial\Omega$ is of class $C^{1,r}$ (instead of class C^∞), then S is a pseudodifferential operator whose symbol exhibits a limited amount of regularity in the space-variable. Such classes of operators have been studied in, e.g., [133], [180, Chs. 1, 2]. $\square$

We note that Lemma C.1 also follows from [36, Theorem 8.2] in the case of C^2-domains Ω with compact boundary. This is proved in [36] by rather different methods and can be viewed as a generalization of the classical result for bounded C^2-domains.

Lemma C.2. *Assume Hypothesis 4.6.6 (i) and let $q \in [0,1]$. Then one has for each $z \in \mathbb{C}\backslash[0,\infty)$,*

$$(H_{0,\Omega}^D - zI_\Omega)^{-q},\, (H_{0,\Omega}^N - zI_\Omega)^{-q} \in \mathcal{B}\big(L^2(\Omega; d^n x), H^{2q}(\Omega)\big). \tag{C.35}$$

Proof. For notational convenience, we denote by $H_{0,\Omega}$ either one of the operators $H_{0,\Omega}^D$ or $H_{0,\Omega}^N$. The operator $H_{0,\Omega}$ is a semibounded self-adjoint operator in $L^2(\Omega; d^n x)$, and thus the resolvent set of $H_{0,\Omega}$ is linearly connected.

Step 1: We claim that it is enough to prove (C.35) for one point z in the resolvent set of $H_{0,\Omega}$. Indeed, suppose that (C.35) holds, and z' is any other point in the resolvent set of $H_{0,\Omega}$. Connecting z and z' by a curve in the resolvent set, and splitting this curve in small segments, without loss of generality we may assume that z' is arbitrarily close to z so that the operator $I_\Omega - (z'-z)(H_{0,\Omega} - zI_\Omega)^{-1}$ is invertible, and thus the operator $(I_\Omega - (z'-z)(H_{0,\Omega} - zI_\Omega)^{-1})^{-q}$ is a bounded operator on $L^2(\Omega; d^n x)$. Then (C.35) and the identity

$$(H_{0,\Omega} - z'I_\Omega)^{-q} = (H_{0,\Omega} - zI_\Omega)^{-q}(I_\Omega - (z'-z)(H_{0,\Omega} - zI_\Omega)^{-1})^{-q} \tag{C.36}$$

imply (C.35) with z replaced by z', proving the claim.

Step 2: By [130, Theorem B.8] (cf. also Theorem 4.3.1.2 and Remark 4.3.1.2 in [185]), if $\Omega \subseteq \mathbb{R}^n$ is a Lipschitz domain, $n \in \mathbb{N}$, and $s_0, s_1 \in \mathbb{R}$, then

$$\Big(H^{s_0}(\Omega), H^{s_1}(\Omega)\Big)_{\theta,2} = H^s(\Omega), \quad s = (1-\theta)s_0 + \theta s_1,\ 0 < \theta < 1. \tag{C.37}$$

Here, for Banach spaces $\mathcal{X}_0$ and $\mathcal{X}_1$, we denote by $\big(\mathcal{X}_0, \mathcal{X}_1\big)_{\theta,p}$ the real interpolation space (obtained by the K-method), as discussed, for instance, in [130, Appendix B] and [185, Sect. 1.3]. Letting $s_0 = 0$, $s_1 = 2$, and $s = 2q$, one then infers

$$\Big(L^2(\Omega; d^n x), H^2(\Omega)\Big)_{q,2} = H^{2q}(\Omega). \tag{C.38}$$

Step 3: Using the claim in Step 1, we may assume without loss of generality that $H_{0,\Omega} - zI_\Omega$ is a strictly positive operator and thus the fractional power $(H_{0,\Omega} - zI_\Omega)^q$ can be defined via its spectral decomposition (see, e.g., [185, Sec.1.18.10]). We remark that the operator $(H_{0,\Omega} - zI_\Omega)^q$ is an isomorphism between the Banach space $\operatorname{dom}(H_{0,\Omega} - zI_\Omega)^q$, equipped with the graph-norm, and the space $L^2(\Omega; d^n x)$, and thus

$$(H_{0,\Omega} - zI_\Omega)^{-q} \in \mathcal{B}\big(L^2(\Omega; d^n x), \operatorname{dom}\big((H_{0,\Omega} - zI_\Omega)^q\big)\big). \tag{C.39}$$

By an abstract interpolation result for strictly positive, self-adjoint operators, see [185, Theorem 1.18.10], for any $\alpha, \beta \in \mathbb{C}$ with $\operatorname{Re}\alpha, \operatorname{Re}\beta \geqslant 0$ and $\theta \in (0,1)$ one has,

$$\Big(\operatorname{dom}\big((H_{0,\Omega} - zI_\Omega)^\alpha\big), \operatorname{dom}\big((H_{0,\Omega} - zI_\Omega)^\beta\big)\Big)_{\theta,2} = \operatorname{dom}\big((H_{0,\Omega} - zI_\Omega)^{\alpha(1-\theta)+\beta\theta}\big). \tag{C.40}$$

Applying this result with $\alpha = 0$ and $\beta = 1$, one infers

$$\Big(L^2(\Omega; d^n x), \operatorname{dom}(H_{0,\Omega} - zI_\Omega)\Big)_{q,2} = \operatorname{dom}\big((H_{0,\Omega} - zI_\Omega)^q\big). \tag{C.41}$$

Noting that $\operatorname{dom}(H_{0,\Omega}) = \operatorname{dom}(H_{0,\Omega} - zI_\Omega)$, and using (C.38), (C.41), and Lemma C.1, one arrives at the continuous imbedding

$$\operatorname{dom}\big((H_{0,\Omega} - zI_\Omega)^q\big) \hookrightarrow H^{2q}(\Omega). \tag{C.42}$$

Thus, (C.35) is a consequence of (C.39) and (C.42). $\square$

Finally, we will prove an extension of a result of Nakamura [136, Lemma 6] from a cube in $\mathbb{R}^n$ to a Lipschitz domain Ω. This requires some preparations. First, we note that (C.15) and (C.13) yield the following Green formula

$$\langle \widetilde{\gamma}_N u, \gamma_D \Phi\rangle = \big(\overline{\nabla u}, \nabla\Phi\big)_{L^2(\Omega;d^nx)^n} + \langle \Delta u, \Phi\rangle, \tag{C.43}$$

valid for any $u \in H^1(\Omega)$ with $\Delta u \in \big(H^1(\Omega)\big)^*$, and any $\Phi \in H^1(\Omega)$. The pairing on the left-hand side of (C.43) is between functionals in $\big(H^{1/2}(\partial\Omega)\big)^*$ and elements in $H^{1/2}(\partial\Omega)$, whereas the last pairing on the right-hand side is between functionals in $\big(H^1(\Omega)\big)^*$ and elements in $H^1(\Omega)$. For further use, we also note that the adjoint of (4.6.42) maps as follows

$$\gamma_D^* : \big(H^{s-1/2}(\partial\Omega)\big)^* \to \big(H^s(\Omega)\big)^*, \quad 1/2 < s < 3/2. \tag{C.44}$$

Next we observe that the operator $(\widetilde{H}^N_{0,\Omega} - zI_\Omega)^{-1}$, $z \in \mathbb{C}\backslash\sigma(\widetilde{H}^N_{0,\Omega})$, originally defined as

$$(\widetilde{H}^N_{0,\Omega} - zI_\Omega)^{-1} : L^2(\Omega;d^nx) \to L^2(\Omega;d^nx), \tag{C.45}$$

can be extended to a bounded operator, mapping $\big(H^1(\Omega)\big)^*$ into $L^2(\Omega;d^nx)$. Specifically, since $(\widetilde{H}^N_{0,\Omega} - \overline{z}I_\Omega)^{-1} : L^2(\Omega;d^nx) \to \operatorname{dom}(\widetilde{H}^N_{0,\Omega})$ is bounded and since the inclusion $\operatorname{dom}(\widetilde{H}^N_{0,\Omega}) \hookrightarrow H^1(\Omega)$ is bounded, we can naturally view $(\widetilde{H}^N_{0,\Omega} - \overline{z}I_\Omega)^{-1}$ as an operator

$$(\widehat{H}^N_{0,\Omega} - \overline{z}I_\Omega)^{-1} \colon L^2(\Omega;d^nx) \to H^1(\Omega) \tag{C.46}$$

mapping in a linear, bounded fashion. Consequently, for its adjoint, we have

$$\big((\widehat{H}^N_{0,\Omega} - \overline{z}I_\Omega)^{-1}\big)^* : \big(H^1(\Omega)\big)^* \to L^2(\Omega;d^nx), \tag{C.47}$$

and it is easy to see that this latter operator extends the one in (C.45). Hence, there is no ambiguity in retaining the same symbol, that is, $(\widetilde{H}^N_{0,\Omega} - \overline{z} I_\Omega)^{-1}$, both for the operator in (C.47) as well as for the operator in (C.45). Similar considerations and conventions apply to $(\widetilde{H}^D_{0,\Omega} - z I_\Omega)^{-1}$.

Lemma C.3. *Let $\Omega \subset \mathbb{R}^n$, $n \geq 2$, be a Lipschitz domain and let $z \in \mathbb{C}\backslash\big(\sigma(\widetilde{H}^D_{0,\Omega}) \cup \sigma(\widetilde{H}^N_{0,\Omega})\big)$. Then, on $L^2(\Omega; d^n x)$,*

$$(\widetilde{H}^D_{0,\Omega} - z I_\Omega)^{-1} - (\widetilde{H}^N_{0,\Omega} - z I_\Omega)^{-1} = (\widetilde{H}^N_{0,\Omega} - z I_\Omega)^{-1} \gamma_D^* \widetilde{\gamma}_N (\widetilde{H}^D_{0,\Omega} - z I_\Omega)^{-1}, \tag{C.48}$$

where γ_D^* is an adjoint operator to γ_D in the sense of (C.44)

Proof. To set the stage, we note that the composition of operators appearing on the right-hand side of (C.48) is meaningful since

$$(\widetilde{H}^D_{0,\Omega} - z I_\Omega)^{-1} \colon L^2(\Omega; d^n x) \to \operatorname{dom}(\widetilde{H}^D_{0,\Omega}) \subset \{u \in H^1(\Omega) \,|\, \Delta u \in (H^1(\Omega))^*\}, \tag{C.49}$$

$$\widetilde{\gamma}_N \colon \{u \in H^1(\Omega) \,|\, \Delta u \in (H^1(\Omega))^*\} \to H^{-1/2}(\partial\Omega) \tag{C.50}$$

$$\gamma_D^* \colon \big(H^{1/2}(\partial\Omega)\big)^* = H^{-1/2}(\partial\Omega) \to \big(H^1(\Omega)\big)^*, \tag{C.51}$$

$$(\widetilde{H}^N_{0,\Omega} - z I_\Omega)^{-1} \colon \big(H^1(\Omega)\big)^* \to L^2(\Omega; d^n x), \tag{C.52}$$

with the convention made just before the statement of the lemma used in the last line. Next, let $\phi_1, \psi_1 \in L^2(\Omega; d^n x)$ be arbitrary and define

$$\begin{aligned} \phi &= (\widetilde{H}^N_{0,\Omega} - \overline{z} I_\Omega)^{-1} \phi_1 \in \operatorname{dom}(\widetilde{H}^N_{0,\Omega}) \subset H^1(\Omega), \\ \psi &= (\widetilde{H}^D_{0,\Omega} - z I_\Omega)^{-1} \psi_1 \in \operatorname{dom}(\widetilde{H}^D_{0,\Omega}) \subset H^1(\Omega). \end{aligned} \tag{C.53}$$

It therefore suffices to show that the following identity holds:

$$\begin{aligned} &\big(\phi_1, (\widetilde{H}^D_{0,\Omega} - z I_\Omega)^{-1} \psi_1\big)_{L^2(\Omega; d^n x)} - \big(\phi_1, (\widetilde{H}^N_{0,\Omega} - z I_\Omega)^{-1} \psi_1\big)_{L^2(\Omega; d^n x)} \\ &\quad = \big(\phi_1, (\widetilde{H}^N_{0,\Omega} - z I_\Omega)^{-1} \gamma_D^* \widetilde{\gamma}_N (\widetilde{H}^D_{0,\Omega} - z I_\Omega)^{-1} \psi_1\big)_{L^2(\Omega; d^n x)}. \end{aligned} \tag{C.54}$$

We note that according to (C.53) one has,

$$\big(\phi_1, (\widetilde{H}^D_{0,\Omega} - zI_\Omega)^{-1}\psi_1\big)_{L^2(\Omega;d^nx)} = \big((\widetilde{H}^N_{0,\Omega} - \overline{z}I_\Omega)\phi, \psi\big)_{L^2(\Omega;d^nx)}, \tag{C.55}$$

$$\begin{aligned}\big(\phi_1, (\widetilde{H}^N_{0,\Omega} - zI_\Omega)^{-1}\psi_1\big)_{L^2(\Omega;d^nx)} &= \big(\big((\widetilde{H}^N_{0,\Omega} - zI_\Omega)^{-1}\big)^*\phi_1, \psi_1\big)_{L^2(\Omega;d^nx)} \\ &= \big((\widetilde{H}^N_{0,\Omega} - \overline{z}I_\Omega)^{-1}\phi_1, \psi_1\big)_{L^2(\Omega;d^nx)} \\ &= \big(\phi, (\widetilde{H}^D_{0,\Omega} - zI_\Omega)\psi\big)_{L^2(\Omega;d^nx)}, \end{aligned} \tag{C.56}$$

and, keeping in mind the convention adopted prior to the statement of the lemma,

$$\begin{aligned}&\big(\phi_1, (\widetilde{H}^N_{0,\Omega} - zI_\Omega)^{-1}\gamma_D^*\widetilde{\gamma}_N(\widetilde{H}^D_{0,\Omega} - zI_\Omega)^{-1}\psi_1\big)_{L^2(\Omega;d^nx)} \\ &\quad = \langle\overline{(\widetilde{H}^N_{0,\Omega} - \overline{z}I_\Omega)^{-1}\phi_1}, \gamma_D^*\widetilde{\gamma}_N(\widetilde{H}^D_{0,\Omega} - zI_\Omega)^{-1}\psi_1\rangle \\ &\quad = \big\langle\overline{\gamma_D(\widetilde{H}^N_{0,\Omega} - \overline{z}I_\Omega)^{-1}\phi_1}, \widetilde{\gamma}_N(\widetilde{H}^D_{0,\Omega} - zI_\Omega)^{-1}\psi_1\big\rangle = \big\langle\overline{\gamma_D\phi}, \widetilde{\gamma}_N\psi\big\rangle \end{aligned} \tag{C.57}$$

where $\langle\cdot\,,\,\cdot\rangle$ stands for pairings between Sobolev spaces (in Ω and $\partial\Omega$) and their duals.

Thus, matters have been reduced to proving that

$$\big((\widetilde{H}^N_{0,\Omega} - \overline{z}I_\Omega)\phi, \psi\big)_{L^2(\Omega;d^nx)} - \big(\phi, (\widetilde{H}^D_{0,\Omega} - zI_\Omega)\psi\big)_{L^2(\Omega;d^nx)} = \big\langle\overline{\gamma_D\phi}, \widetilde{\gamma}_N\psi\big\rangle. \tag{C.58}$$

Using (C.43) for the left-hand side of (C.58) one obtains

$$\begin{aligned}&\big((\widetilde{H}^N_{0,\Omega} - \overline{z}I_\Omega)\phi, \psi\big)_{L^2(\Omega;d^nx)} - \big(\phi, (\widetilde{H}^D_{0,\Omega} - zI_\Omega)\psi\big)_{L^2(\Omega;d^nx)} \\ &\quad = -\big(\Delta\phi, \psi\big)_{L^2(\Omega;d^nx)} + \big(\phi, \Delta\psi\big)_{L^2(\Omega;d^nx)} \\ &\quad = \big(\nabla\phi, \nabla\psi\big)_{L^2(\Omega;d^nx)^n} - \big\langle\overline{\widetilde{\gamma}_N\phi}, \gamma_D\psi\big\rangle - \big(\nabla\phi, \nabla\psi\big)_{L^2(\Omega;d^nx)^n} + \big\langle\overline{\gamma_D\phi}, \widetilde{\gamma}_N\psi\big\rangle \\ &\quad = -\big\langle\overline{\widetilde{\gamma}_N\phi}, \gamma_D\psi\big\rangle + \big\langle\overline{\gamma_D\phi}, \widetilde{\gamma}_N\psi\big\rangle. \end{aligned} \tag{C.59}$$

Observing that $\widetilde{\gamma}_N\phi = 0$ since $\phi \in \mathrm{dom}(H^N_{0,\Omega})$, one concludes (C.58). $\square$

Remark C.4. While it is tempting to view γ_D as an unbounded but densely defined operator on $L^2(\Omega; d^n x)$ whose domain contains the space $C_0^\infty(\Omega)$, one should note that in this case its adjoint γ_D^* is not densely defined: Indeed, the adjoint γ_D^* of γ_D would have to be an unbounded operator from $L^2(\partial\Omega; d^{n-1}\sigma)$ to $L^2(\Omega; d^n x)$ such that

$$(\gamma_D f, g)_{L^2(\partial\Omega; d^{n-1}\sigma)} = (f, \gamma_D^* g)_{L^2(\Omega; d^n x)} \text{ for all } f \in \operatorname{dom}(\gamma_D),\ g \in \operatorname{dom}(\gamma_D^*). \quad \text{(C.60)}$$

In particular, choosing $f \in C_0^\infty(\Omega)$, in which case $\gamma_D f = 0$, one concludes that $(f, \gamma_D^* g)_{L^2(\Omega; d^n x)} = 0$ for all $f \in C_0^\infty(\Omega)$. Thus, one obtains $\gamma_D^* g = 0$ for all $g \in \operatorname{dom}(\gamma_D^*)$. Since obviously $\gamma_D \neq 0$, (C.60) implies $\operatorname{dom}(\gamma_D^*) = \{0\}$ and hence γ_D is not a closable linear operator in $L^2(\Omega; d^n x)$.

Remark C.5. In the case of a domain Ω of class $C^{1,r}$, $(1/2) < r < 1$, the operators $\widetilde{H}_{0,\Omega}^D$ and $\widetilde{H}_{0,\Omega}^N$ coincide with the operators $H_{0,\Omega}^D$ and $H_{0,\Omega}^N$, respectively, and hence one can use the operators $H_{0,\Omega}^D$ and $H_{0,\Omega}^N$ in Lemma C.3. Moreover, since $\operatorname{dom}(H_{0,\Omega}^D) \subseteq H^2(\Omega)$, one can also replace $\widetilde{\gamma}_N$ by γ_N (cf. (4.6.43)) in Lemma C.3. In particular,

$$(H_{0,\Omega}^D - zI_\Omega)^{-1} - (H_{0,\Omega}^N - zI_\Omega)^{-1} = \big[\gamma_D (H_{0,\Omega}^N - \overline{z} I_\Omega)^{-1}\big]^* \gamma_N (H_{0,\Omega}^D - zI_\Omega)^{-1}. \quad \text{(C.61)}$$

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