

DONOGHUE-TYPE m -FUNCTIONS FOR SCHRÖDINGER OPERATORS WITH OPERATOR-VALUED POTENTIALS

By

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Abstract. Given a complex, separable Hilbert space \mathcal{H} , we consider differential expressions of the type $\tau = -(d^2/dx^2)I_{\mathcal{H}} + V(x)$, with $x \in (x_0, \infty)$ for some $x_0 \in \mathbb{R}$, or $x \in \mathbb{R}$ (assuming the limit-point property of τ at $\pm\infty$). Here V denotes a bounded operator-valued potential $V(\cdot) \in \mathcal{B}(\mathcal{H})$ such that $V(\cdot)$ is weakly measurable, the operator norm $\|V(\cdot)\|_{\mathcal{B}(\mathcal{H})}$ is locally integrable, and $V(x) = V(x)^*$ a.e. on $x \in [x_0, \infty)$ or $x \in \mathbb{R}$. We focus on two major cases. First, on m -function theory for self-adjoint half-line L^2 -realizations $H_{+, \alpha}$ in $L^2((x_0, \infty); dx; \mathcal{H})$ (with x_0 a regular endpoint for τ , associated with the self-adjoint boundary condition $\sin(\alpha)u'(x_0) + \cos(\alpha)u(x_0) = 0$, indexed by the self-adjoint operator $\alpha = \alpha^* \in \mathcal{B}(\mathcal{H})$), and second, on m -function theory for self-adjoint full-line L^2 -realizations H of τ in $L^2(\mathbb{R}; dx; \mathcal{H})$.

In a nutshell, a Donoghue-type m -function $M_{A, \mathcal{N}_i}^{Do}(\cdot)$ associated with self-adjoint extensions A of a closed, symmetric operator \dot{A} in \mathcal{H} with deficiency spaces $\mathcal{N}_z = \ker(\dot{A}^* - zI_{\mathcal{H}})$ and corresponding orthogonal projections $P_{\mathcal{N}_z}$ onto \mathcal{N}_z is given by

$$\begin{aligned} M_{A, \mathcal{N}_i}^{Do}(z) &= P_{\mathcal{N}_i}(zA + I_{\mathcal{H}})(A - zI_{\mathcal{H}})^{-1}P_{\mathcal{N}_i}|_{\mathcal{N}_i} \\ &= zI_{\mathcal{N}_i} + (z^2 + 1)P_{\mathcal{N}_i}(A - zI_{\mathcal{H}})^{-1}P_{\mathcal{N}_i}|_{\mathcal{N}_i}, \quad z \in \mathbb{C} \setminus \mathbb{R}. \end{aligned}$$

In the concrete case of half-line and full-line Schrödinger operators, the role of \dot{A} is played by a suitably defined minimal Schrödinger operator $H_{+, \min}$ in $L^2((x_0, \infty); dx; \mathcal{H})$ and H_{\min} in $L^2(\mathbb{R}; dx; \mathcal{H})$, both of which will be proven to be completely non-self-adjoint. The latter property is used to prove that if $H_{+, \alpha}$ in $L^2((x_0, \infty); dx; \mathcal{H})$, respectively, H in $L^2(\mathbb{R}; dx; \mathcal{H})$, are self-adjoint extensions of $H_{+, \min}$, respectively, H_{\min} , then the corresponding operator-valued measures in the Herglotz–Nevanlinna representations of the Donoghue-type m -functions $M_{H_{+, \alpha}, \mathcal{N}_{+, i}}^{Do}(\cdot)$ and $M_{H, \mathcal{N}_i}^{Do}(\cdot)$ encode the entire spectral information of $H_{+, \alpha}$, respectively, H .

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1 Introduction

The principal topic of this paper centers around basic spectral theory for self-adjoint Schrödinger operators with bounded operator-valued potentials on a half-line as well as on the full real line, focusing on Donoghue-type m -function theory, eigenfunction expansions, and a version of the spectral theorem. More precisely, given a complex, separable Hilbert space \mathcal{H} , we consider differential expressions τ of the type

$$(1.1) \quad \tau = -(d^2/dx^2)I_{\mathcal{H}} + V(x),$$

with $x \in (x_0, \infty)$ or $x \in \mathbb{R}$ ($x_0 \in \mathbb{R}$ a reference point), and V a bounded operator-valued potential $V(\cdot) \in \mathcal{B}(\mathcal{H})$ such that $V(\cdot)$ is weakly measurable, the operator norm $\|V(\cdot)\|_{\mathcal{B}(\mathcal{H})}$ is locally integrable, and $V(x) = V(x)^*$ a.e. on $x \in [x_0, \infty)$ or

$x \in \mathbb{R}$. The self-adjoint operators in question are then half-line L^2 -realizations of τ in $L^2((x_0, \infty); dx; \mathcal{H})$, with x_0 assumed to be a regular endpoint for τ , and hence with appropriate boundary conditions at x_0 (cf. (1.24)) on one hand, and full-line L^2 -realizations of τ in $L^2(\mathbb{R}; dx; \mathcal{H})$ on the other.

The case of Schrödinger operators with operator-valued potentials under various continuity or smoothness hypotheses on $V(\cdot)$, and under various self-adjoint boundary conditions on bounded and unbounded open intervals, received considerable attention in the past. In the special case where $\dim(\mathcal{H}) < \infty$, that is, in the case of Schrödinger operators with matrix-valued potentials, the literature is so voluminous that we cannot possibly describe individual references and hence we primarily refer to the monographs [2], [96], and the references cited therein. We note that the finite-dimensional case, $\dim(\mathcal{H}) < \infty$, as discussed in [18], is of considerable interest as it represents an important ingredient in some proofs of Lieb–Thirring inequalities (cf. [71]). For the particular case of Schrödinger-type operators corresponding to the differential expression $\tau = -(d^2/dx^2)I_{\mathcal{H}} + A + V(x)$ on a bounded interval $(a, b) \subset \mathbb{R}$ with either $A = 0$ or A a self-adjoint operator satisfying $A \geq cI_{\mathcal{H}}$ for some $c > 0$, we refer to the list of references in [52]. For earlier results on various aspects of boundary value problems, spectral theory, and scattering theory in the half-line case $(a, b) = (0, \infty)$, we refer, for instance, to [3], [4], [33], [54]–[56], [57, Chs. 3,4], [58], [60], [64], [80], [82], [95], [99], [101] (the case of the real line is discussed in [103]). Our treatment of spectral theory for half-line and full-line Schrödinger operators in $L^2((x_0, \infty); dx; \mathcal{H})$ and in $L^2(\mathbb{R}; dx; \mathcal{H})$, respectively, in [50], [52] represents the most general one to date.

Next, we briefly turn to Donoghue-type m -functions which abstractly can be introduced as follows (cf. [47], [48]). Given a self-adjoint extension A of a densely defined, closed, symmetric operator \dot{A} in \mathcal{K} (a complex, separable Hilbert space) and the deficiency subspace \mathcal{N}_i of \dot{A} in \mathcal{K} , with

$$(1.2) \quad \mathcal{N}_i = \ker(\dot{A}^* - iI_{\mathcal{K}}), \quad \dim(\mathcal{N}_i) = k \in \mathbb{N} \cup \{\infty\},$$

the Donoghue-type m -operator $M_{A, \mathcal{N}_i}^{Do}(z) \in \mathcal{B}(\mathcal{N}_i)$ associated with the pair (A, \mathcal{N}_i) is given by

$$(1.3) \quad \begin{aligned} M_{A, \mathcal{N}_i}^{Do}(z) &= P_{\mathcal{N}_i}(zA + I_{\mathcal{K}})(A - zI_{\mathcal{K}})^{-1}P_{\mathcal{N}_i}|_{\mathcal{N}_i} \\ &= zI_{\mathcal{N}_i} + (z^2 + 1)P_{\mathcal{N}_i}(A - zI_{\mathcal{K}})^{-1}P_{\mathcal{N}_i}|_{\mathcal{N}_i}, \quad z \in \mathbb{C} \setminus \mathbb{R}, \end{aligned}$$

with $I_{\mathcal{N}_i}$ the identity operator in \mathcal{N}_i , and $P_{\mathcal{N}_i}$ the orthogonal projection in \mathcal{K} onto \mathcal{N}_i . Then $M_{A, \mathcal{N}_i}^{Do}(\cdot)$ is a $\mathcal{B}(\mathcal{N}_i)$ -valued Nevanlinna–Herglotz function that admits the representation

$$(1.4) \quad M_{A, \mathcal{N}_i}^{Do}(z) = \int_{\mathbb{R}} d\Omega_{A, \mathcal{N}_i}^{Do}(\lambda) \left[\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2 + 1} \right], \quad z \in \mathbb{C} \setminus \mathbb{R},$$

where the $\mathcal{B}(\mathcal{N}_i)$ -valued measure $\Omega_{A, \mathcal{N}_i}^{Do}(\cdot)$ satisfies (5.9)–(5.11).

In the concrete case of regular half-line Schrödinger operators in $L^2((x_0, \infty); dx)$ with a scalar potential, Donoghue [45] introduced the analogue of (1.3) and used it to settle certain inverse spectral problems. From a historical perspective, operators of the type $M_{A, \mathcal{N}}^{Do}(\cdot)$ appear to go back to Krein [65] (see also [67]) and Saakjan [98]; apparently, Donoghue was unaware of M. Krein’s work in this context, and similarly, M. Krein and his school appeared to have been unaware of Donoghue’s contribution to this subject. For hints to the extensive literature on this topic since these early developments we refer to the paragraph following inequality (5.14).

As has been shown in detail in [47], [48], [49], Donoghue-type m -functions naturally lead to Krein-type resolvent formulas as well as linear fractional transformations relating two different self-adjoint extensions of \dot{A} . However, in this paper we are particularly interested in the question under which conditions on \dot{A} , the spectral information on its self-adjoint extension A , contained in its family of spectral projections $\{E_A(\lambda)\}_{\lambda \in \mathbb{R}}$, is already encoded in the $\mathcal{B}(\mathcal{N}_i)$ -valued measure $\Omega_{A, \mathcal{N}_i}^{Do}(\cdot)$. As shown in Corollary 5.8, this is the case if and only if \dot{A} is completely non-self-adjoint in \mathcal{K} and we will apply this to half-line and full-line Schrödinger operators with $\mathcal{B}(\mathcal{H})$ -valued potentials.

In the general case of $\mathcal{B}(\mathcal{H})$ -valued potentials on the right half-line (x_0, ∞) , assuming Hypothesis 6.1 (i), we introduce minimal and maximal, operators $H_{+, \min}$ and $H_{+, \max}$ in $L^2((x_0, \infty); dx; \mathcal{H})$ associated to τ , and self-adjoint extensions $H_{+, \alpha}$ of $H_{+, \min}$ (cf. (3.2), (3.4), (3.9)) and given the generating property of the deficiency spaces $\mathcal{N}_{+, z} = \ker(H_{+, \min} - zI)$, $z \in \mathbb{C} \setminus \mathbb{R}$, proven in Theorem 6.2, conclude that $H_{+, \min}$ is completely non-self-adjoint (i.e., it has no nontrivial invariant subspace in $L^2((x_0, \infty); dx; \mathcal{H})$ on which it is self-adjoint).

According to (1.3), the right half-line Donoghue-type m -function corresponding to $H_{+, \alpha}$ and $\mathcal{N}_{+, i}$ is given by

$$\begin{aligned}
 (1.5) \quad M_{H_{+, \alpha}, \mathcal{N}_{+, i}}^{Do}(z, x_0) &= P_{\mathcal{N}_{+, i}}(zH_{+, \alpha} + I)(H_{+, \alpha} - zI)^{-1}P_{\mathcal{N}_{+, i}}|_{\mathcal{N}_{+, i}} \\
 &= \int_{\mathbb{R}} d\Omega_{H_{+, \alpha}, \mathcal{N}_{+, i}}^{Do}(\lambda, x_0) \left[\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2 + 1} \right], \quad z \in \mathbb{C} \setminus \mathbb{R},
 \end{aligned}$$

where $\Omega_{H_{+, \alpha}, \mathcal{N}_{+, i}}^{Do}(\cdot, x_0)$ satisfies the analogues of (5.9)–(5.11).

Combining Corollary 5.8 with the complete non-self-adjointness of $H_{+, \min}$ proves that the entire spectral information for $H_{+, \alpha}$, contained in the corresponding family of spectral projections $\{E_{H_{+, \alpha}}(\lambda)\}_{\lambda \in \mathbb{R}}$ in $L^2((x_0, \infty); dx; \mathcal{H})$, is already encoded in the $\mathcal{B}(\mathcal{N}_{+, i})$ -valued measure $\Omega_{H_{+, \alpha}, \mathcal{N}_{+, i}}^{Do}(\cdot, x_0)$ (including multiplicity properties of the spectrum of $H_{+, \alpha}$).

An explicit computation of $M_{H_{+, \alpha}, \mathcal{N}_{\pm, i}}^{Do}(z, x_0)$ then yields

$$\begin{aligned}
 M_{H_{+, \alpha}, \mathcal{N}_{\pm, i}}^{Do}(z, x_0) &= \pm \sum_{j, k \in \mathcal{J}} (e_j, m_{+, \alpha}^{Do}(z, x_0) e_k)_{\mathcal{H}} \\
 &\quad \times (\psi_{+, \alpha}(i, \cdot, x_0) [\text{Im}(m_{+, \alpha}(i, x_0))]^{-1/2} e_k, \cdot)_{L^2((x_0, \infty); dx; \mathcal{H})} \\
 (1.6) \quad &\quad \times \psi_{+, \alpha}(i, \cdot, x_0) [\text{Im}(m_{+, \alpha}(i, x_0))]^{-1/2} e_j|_{\mathcal{N}_{\pm, i}}, \quad z \in \mathbb{C} \setminus \mathbb{R},
 \end{aligned}$$

where $\{e_j\}_{j \in \mathcal{J}}$ is an orthonormal basis in \mathcal{H} ($\mathcal{J} \subseteq \mathbb{N}$ an appropriate index set) and the $\mathcal{B}(\mathcal{H})$ -valued Nevanlinna–Herglotz functions $m_{+, \alpha}^{Do}(\cdot, x_0)$ are given by

$$\begin{aligned}
 m_{+, \alpha}^{Do}(z, x_0) &= [\text{Im}(m_{+, \alpha}(i, x_0))]^{-1/2} [m_{+, \alpha}(z, x_0) - \text{Re}(m_{+, \alpha}(i, x_0))] \\
 (1.7) \quad &\quad \times [\text{Im}(m_{+, \alpha}(i, x_0))]^{-1/2} \\
 (1.8) \quad &= d_{+, \alpha} + \int_{\mathbb{R}} d\omega_{+, \alpha}^{Do}(\lambda, x_0) \left[\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2 + 1} \right], \quad z \in \mathbb{C} \setminus \mathbb{R}.
 \end{aligned}$$

Here $d_{+, \alpha} = \text{Re}(m_{+, \alpha}^{Do}(i, x_0)) \in \mathcal{B}(\mathcal{H})$, and

$$(1.9) \quad \omega_{+, \alpha}^{Do}(\cdot, x_0) = [\text{Im}(m_{+, \alpha}(i, x_0))]^{-1/2} \rho_{+, \alpha}(\cdot, x_0) [\text{Im}(m_{+, \alpha}(i, x_0))]^{-1/2}$$

satisfies the analogues of (A.10), (A.11). In addition, $\psi_{+, \alpha}(\cdot, x, x_0)$ is the right half-line Weyl–Titchmarsh solution (3.10), and $m_{+, \alpha}(\cdot, x_0)$ represents the standard $\mathcal{B}(\mathcal{H})$ -valued right half-line Weyl–Titchmarsh m -function in (3.10) with $\mathcal{B}(\mathcal{H})$ -valued measure $\rho_{+, \alpha}(\cdot, x_0)$ in its Nevanlinna–Herglotz representation (3.17)–(3.19).

This result shows that the entire spectral information for $H_{+, \alpha}$ is also contained in the $\mathcal{B}(\mathcal{H})$ -valued measure $\omega_{+, \alpha}^{Do}(\cdot, x_0)$ (again, including multiplicity properties of the spectrum of $H_{+, \alpha}$). Naturally, the same facts apply to the left half-line $(-\infty, x_0)$.

Turning to the full-line case assuming Hypothesis 4.1, and denoting by H the self-adjoint realization of τ in $L^2(\mathbb{R}; dx; \mathcal{H})$, we now decompose

$$(1.10) \quad L^2(\mathbb{R}; dx; \mathcal{H}) = L^2((-\infty, x_0); dx; \mathcal{H}) \oplus L^2((x_0, \infty); dx; \mathcal{H}),$$

and introduce the orthogonal projections P_{\pm, x_0} of $L^2(\mathbb{R}; dx; \mathcal{H})$ onto the left/right subspaces $L^2((x_0, \pm\infty); dx; \mathcal{H})$. Thus, we introduce the 2×2 block operator representation,

$$(1.11) \quad (H - zI)^{-1} = \begin{pmatrix} P_{-, x_0}(H - zI)^{-1}P_{-, x_0} & P_{-, x_0}(H - zI)^{-1}P_{+, x_0} \\ P_{+, x_0}(H - zI)^{-1}P_{-, x_0} & P_{+, x_0}(H - zI)^{-1}P_{+, x_0} \end{pmatrix},$$

and introduce with respect to the decomposition (1.10), the minimal operator H_{\min}

in $L^2(\mathbb{R}; dx; \mathcal{H})$ via

$$(1.12) \quad H_{\min} := H_{-, \min} \oplus H_{+, \min}, \quad H_{\min}^* = H_{-, \min}^* \oplus H_{+, \min}^*,$$

$$\mathcal{N}_z = \ker(H_{\min}^* - zI) = \ker(H_{-, \min}^* - zI) \oplus \ker(H_{+, \min}^* - zI)$$

$$(1.13) \quad = \mathcal{N}_{-, z} \oplus \mathcal{N}_{+, z}, \quad z \in \mathbb{C} \setminus \mathbb{R},$$

(see the additional comments concerning our choice of minimal operator in Section 6, following (6.36)).

According to (1.3), the full-line Donoghue-type m -function is given by

$$(1.14) \quad M_{H, \mathcal{N}_i}^{Do}(z) = P_{\mathcal{N}_i}(zH + I)(H - zI)^{-1}P_{\mathcal{N}_i}|_{\mathcal{N}_i},$$

$$= \int_{\mathbb{R}} d\Omega_{H, \mathcal{N}_i}^{Do}(\lambda) \left[\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2 + 1} \right], \quad z \in \mathbb{C} \setminus \mathbb{R},$$

where $\Omega_{H, \mathcal{N}_i}^{Do}(\cdot)$ satisfies the analogues of (5.9)–(5.11) (resp., (A.9)–(A.11)).

Combining Corollary 5.8 with the complete non-self-adjointness of H_{\min} proves that the entire spectral information for H , contained in the corresponding family of spectral projections $\{E_H(\lambda)\}_{\lambda \in \mathbb{R}}$ in $L^2(\mathbb{R}; dx; \mathcal{H})$, is already encoded in the $\mathcal{B}(\mathcal{N}_i)$ -valued measure $\Omega_{H, \mathcal{N}_i}^{Do}(\cdot)$ (including multiplicity properties of the spectrum of H).

With respect to the decomposition (1.10), one can represent $M_{H, \mathcal{N}_i}^{Do}(\cdot)$ as the 2×2 block operator,

$$(1.15) \quad M_{H, \mathcal{N}_i}^{Do}(\cdot) = (M_{H, \mathcal{N}_i, \ell, \ell'}^{Do}(\cdot))_{0 \leq \ell, \ell' \leq 1}$$

$$= z \begin{pmatrix} P_{\mathcal{N}_{-, i}} & 0 \\ 0 & P_{\mathcal{N}_{+, i}} \end{pmatrix} + (z^2 + 1) \begin{pmatrix} P_{\mathcal{N}_{-, i}}(H - zI)^{-1}P_{\mathcal{N}_{-, i}} & P_{\mathcal{N}_{-, i}}(H - zI)^{-1}P_{\mathcal{N}_{+, i}} \\ P_{\mathcal{N}_{+, i}}(H - zI)^{-1}P_{\mathcal{N}_{-, i}} & P_{\mathcal{N}_{+, i}}(H - zI)^{-1}P_{\mathcal{N}_{+, i}} \end{pmatrix},$$

employing $P_{\mathcal{N}_{\pm, i}}P_{\pm, x_0} = P_{\mathcal{N}_{\pm, i}}$. Utilizing the fact that

$$(1.16) \quad \left\{ \begin{aligned} \widehat{\Psi}_{-, \alpha, j}(z, \cdot, x_0) &= P_{-, x_0} \psi_{-, \alpha}(z, \cdot, x_0) [-(\operatorname{Im}(z))^{-1} m_{-, \alpha}(z, x_0)]^{-1/2} e_j, \\ \widehat{\Psi}_{+, \alpha, j}(z, \cdot, x_0) &= P_{+, x_0} \psi_{+, \alpha}(z, \cdot, x_0) [(\operatorname{Im}(z))^{-1} m_{+, \alpha}(z, x_0)]^{-1/2} e_j \end{aligned} \right\}_{j \in \mathcal{J}}$$

is an orthonormal basis for $\mathcal{N}_z = \ker(H_{\min}^* - zI)$, $z \in \mathbb{C} \setminus \mathbb{R}$, with $\{e_j\}_{j \in \mathcal{J}}$ an

orthonormal basis for \mathcal{H} , one eventually computes explicitly,

$$\begin{aligned}
 M_{H, \mathcal{N}_i, 0, 0}^{Do}(z) &= \sum_{j, k \in \mathcal{J}} (e_j, M_{\alpha, 0, 0}^{Do}(z, x_0) e_k)_{\mathcal{H}} \\
 &\quad \times (\widehat{\Psi}_{-, a, k}(i, \cdot, x_0), \cdot)_{L^2(\mathbb{R}; dx; \mathcal{H})} \widehat{\Psi}_{-, a, j}(i, \cdot, x_0),
 \end{aligned}
 \tag{1.17}$$

$$\begin{aligned}
 M_{H, \mathcal{N}_i, 0, 1}^{Do}(z) &= \sum_{j, k \in \mathcal{J}} (e_j, M_{\alpha, 0, 1}^{Do}(z, x_0) e_k)_{\mathcal{H}} \\
 &\quad \times (\widehat{\Psi}_{+, a, k}(i, \cdot, x_0), \cdot)_{L^2(\mathbb{R}; dx; \mathcal{H})} \widehat{\Psi}_{-, a, j}(i, \cdot, x_0),
 \end{aligned}
 \tag{1.18}$$

$$\begin{aligned}
 M_{H, \mathcal{N}_i, 1, 0}^{Do}(z) &= \sum_{j, k \in \mathcal{J}} (e_j, M_{\alpha, 1, 0}^{Do}(z, x_0) e_k)_{\mathcal{H}} \\
 &\quad \times (\widehat{\Psi}_{-, a, k}(i, \cdot, x_0), \cdot)_{L^2(\mathbb{R}; dx; \mathcal{H})} \widehat{\Psi}_{+, a, j}(i, \cdot, x_0),
 \end{aligned}
 \tag{1.19}$$

$$\begin{aligned}
 M_{H, \mathcal{N}_i, 1, 1}^{Do}(z) &= \sum_{j, k \in \mathcal{J}} (e_j, M_{\alpha, 1, 1}^{Do}(z, x_0) e_k)_{\mathcal{H}} \\
 &\quad \times (\widehat{\Psi}_{+, a, k}(i, \cdot, x_0), \cdot)_{L^2(\mathbb{R}; dx; \mathcal{H})} \widehat{\Psi}_{+, a, j}(i, \cdot, x_0),
 \end{aligned}
 \tag{1.20}$$

$z \in \mathbb{C} \setminus \mathbb{R}$,

with $M_{\alpha}^{Do}(\cdot, x_0)$ given by

$$\begin{aligned}
 M_{\alpha}^{Do}(z, x_0) &= T_{\alpha}^* M_{\alpha}(z, x_0) T_{\alpha} + E_{\alpha} \\
 &= D_{\alpha} + \int_{\mathbb{R}} d\Omega_{\alpha}^{Do}(\lambda, x_0) \left[\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2 + 1} \right], \quad z \in \mathbb{C} \setminus \mathbb{R}.
 \end{aligned}
 \tag{1.21}$$

Here $D_{\alpha} = \text{Re}(M_{\alpha}^{Do}(i, x_0)) \in \mathcal{B}(\mathcal{H}^2)$, and

$$\Omega_{\alpha}^{Do}(\cdot, x_0) = T_{\alpha}^* \Omega_{\alpha}(\cdot, x_0) T_{\alpha}
 \tag{1.22}$$

satisfies the analogues of (A.10), (A.11). In addition, the 2×2 block operators $T_{\alpha} \in \mathcal{B}(\mathcal{H}^2)$ (with $T_{\alpha}^{-1} \in \mathcal{B}(\mathcal{H}^2)$) and $E_{\alpha} \in \mathcal{B}(\mathcal{H}^2)$ are defined in (6.57) and (6.58), and $M_{\alpha}(\cdot, x_0)$ is the standard $\mathcal{B}(\mathcal{H}^2)$ -valued Weyl–Titchmarsh 2×2 block operator Weyl–Titchmarsh function (4.17)–(4.21) with $\Omega_{\alpha}(\cdot, x_0)$ the $\mathcal{B}(\mathcal{H}^2)$ -valued measure in its Nevanlinna–Herglotz representation (4.22)–(4.24).

This result shows that the entire spectral information for H is also contained in the $\mathcal{B}(\mathcal{H}^2)$ -valued measure $\Omega_{\alpha}^{Do}(\cdot, x_0)$ (again, including multiplicity properties of the spectrum of H).

Remark 1.1. As the first equality in (1.21) shows, $M_{\alpha}^{Do}(z, x_0)$ recovers the traditional Weyl–Titchmarsh operator $M_{\alpha}(z, x_0)$ apart from the boundedly invertible 2×2 block operators T_{α} . The latter is built from the half-line Weyl–Titchmarsh

operators $m_{\pm,\alpha}(z, x_0)$ in a familiar, yet somewhat intriguing, manner (cf. (4.17)–(4.21)),

$$(1.23) \quad M_\alpha(z, x_0) = \begin{pmatrix} W(z)^{-1} & 2^{-1}W(z)^{-1}[m_{-,\alpha}(z, x_0)+m_{+,\alpha}(z, x_0)] \\ 2^{-1}[m_{-,\alpha}(z, x_0)+m_{+,\alpha}(z, x_0)]W(z)^{-1} & m_{\pm,\alpha}(z, x_0)W(z)^{-1}m_{\mp,\alpha}(z, x_0) \end{pmatrix},$$

$z \in \mathbb{C} \setminus \sigma(H),$

abbreviating $W(z) = [m_{-,\alpha}(z, x_0) - m_{+,\alpha}(z, x_0)]$, $z \in \mathbb{C} \setminus \sigma(H)$. In contrast to this construction, combining the Donoghue m -function $M_{H, \mathcal{N}_i}^{Do}(\cdot)$ with the left/right half-line decomposition (1.10), via equation (1.15), directly leads to (1.17)–(1.20), and hence to (1.21), and thus to the $\mathcal{B}(\mathcal{H}^2)$ -valued measure $\Omega_\alpha^{Do}(\cdot, x_0)$ in the Nevanlinna–Herglotz representation of $M_\alpha^{Do}(\cdot, x_0)$, encoding the entire spectral information of H contained in it’s family of spectral projections $E_H(\cdot)$.

Of course, $\Omega_\alpha^{Do}(\cdot, x_0)$ is directly related to the $\mathcal{B}(\mathcal{H}^2)$ -valued Weyl–Titchmarsh measure $\Omega_\alpha(\cdot, x_0)$ in the Nevanlinna–Herglotz representation of $M_\alpha(\cdot, x_0)$ via relation (1.22), but our point is that the simple left/right half-line decomposition (1.10) combined with the Donoghue-type m function (1.14) naturally leads to $\Omega_\alpha^{Do}(\cdot, x_0)$, without employing (1.23). This offers interesting possibilities in the PDE context where \mathbb{R}^n , $n \in \mathbb{N}$, $n \geq 2$, can now be decomposed in various manners, for instance, into the interior and exterior of a given (bounded or unbounded) domain $D \subset \mathbb{R}^n$, a left/right (upper/lower) half-space, etc. In this context we should add that this paper concludes the first part of our program, the treatment of half-line and full-line Schrödinger operators with bounded operator-valued potentials. Part two will aim at certain classes of unbounded operator-valued potentials V , applicable to multi-dimensional Schrödinger operators in $L^2(\mathbb{R}^n; d^n x)$, $n \in \mathbb{N}$, $n \geq 2$, generated by differential expressions of the type $-\Delta + V(\cdot)$. In fact, it was precisely the connection between multi-dimensional Schrödinger operators and one-dimensional Schrödinger operators with unbounded operator-valued potentials which originally motivated our interest in this program. We will return to this circle of ideas elsewhere.

At this point we turn to the content of each section: Section 2 recalls our basic results in [50] on the initial value problem associated with Schrödinger operators with bounded operator-valued potentials. We use this section to introduce some of the basic notation employed subsequently and note that our conditions on $V(\cdot)$ (cf. Hypothesis 2.6) are the most general to date with respect to the local behavior of the potential $V(\cdot)$. Following our detailed treatment in [50], Section 3 introduces maximal and minimal operators associated with the differential expression $\tau = -(d^2/dx^2)I_{\mathcal{H}} + V(\cdot)$ on the interval $(a, b) \subset \mathbb{R}$ (eventually aiming at the case of

a half-line (a, ∞)), and assuming that the left endpoint a is regular for τ and that τ is in the limit-point case at the endpoint b we discuss the family of self-adjoint extensions H_α in $L^2((a, b); dx; \mathcal{H})$ corresponding to boundary conditions of the type

$$(1.24) \quad \sin(\alpha)u'(a) + \cos(\alpha)u(a) = 0,$$

indexed by the self-adjoint operator $\alpha = \alpha^* \in \mathcal{B}(\mathcal{H})$. In addition, we recall elements of Weyl–Titchmarsh theory, the introduction of the operator-valued Weyl–Titchmarsh function $m_\alpha(\cdot) \in \mathcal{B}(\mathcal{H})$ and the Green’s function $G_\alpha(z, \cdot, \cdot) \in \mathcal{B}(\mathcal{H})$ of H_α . In particular, we prove bounded invertibility of $\text{Im}(m_\alpha(\cdot))$ in $\mathcal{B}(\mathcal{H})$ in Theorem 3.3. In Section 4 we recall the analogous results for full-line Schrödinger operators H in $L^2(\mathbb{R}; dx; \mathcal{H})$, employing a 2×2 block operator representation of the associated Weyl–Titchmarsh $M_\alpha(\cdot, x_0)$ -matrix and its $\mathcal{B}(\mathcal{H}^2)$ -valued spectral measure $d\Omega_\alpha(\cdot, x_0)$, decomposing \mathbb{R} into a left and right half-line with respect to the reference point $x_0 \in \mathbb{R}$, $(-\infty, x_0] \cup [x_0, \infty)$. Various basic facts on deficiency subspaces, abstract Donoghue-type m -functions and the bounded invertibility of their imaginary parts, and the notion of completely non-self-adjoint symmetric operators are provided in Section 5. This section also discusses the possibility of a reduction of the spectral family $E_A(\cdot)$ of the self-adjoint operator A in \mathcal{H} to the measure $\Sigma_A(\cdot) = P_{\mathcal{N}}E_A(\cdot)P_{\mathcal{N}}|_{\mathcal{N}}$ in \mathcal{N} (with $P_{\mathcal{N}}$ the orthogonal projection onto a closed linear subspace \mathcal{N} of \mathcal{H}) to the effect that A is unitarily equivalent to the operator of multiplication by the independent variable λ in the space $L^2(\mathbb{R}; d\Sigma_A(\lambda); \mathcal{N})$, yielding a diagonalization of A (see Theorem 5.6). Our final and principal Section 6, establishes complete non-self-adjointness of the minimal operators $H_{\pm, \min}$ in $L^2((x_0, \pm\infty); dx; \mathcal{H})$ (cf. Theorem 6.2), and analyzes in detail the half-line Donoghue-type m -functions $M_{H_{\pm, \min}, \mathcal{N}_{\pm, i}}^{Do}(\cdot, x_0)$ in $\mathcal{N}_{\pm, i}$. In addition, it introduces the derived quantities $m_{\pm, \alpha}^{Do}(\cdot, x_0)$ in \mathcal{H} and subsequently, turns to the full-line Donoghue-type operators $M_{H, \mathcal{N}_i}^{Do}(\cdot)$ in \mathcal{N}_i and $M_\alpha^{Do}(\cdot, x_0)$ in \mathcal{H}^2 . It is then proved that the entire spectral information for H_\pm and H (including multiplicity issues) are encoded in $M_{H_{\pm, \min}, \mathcal{N}_{\pm, i}}^{Do}(\cdot, x_0)$ (equivalently, in $m_{\pm, \alpha}^{Do}(\cdot, x_0)$) and in $M_{H, \mathcal{N}_i}^{Do}(\cdot)$ (equivalently, in $M_\alpha^{Do}(\cdot, x_0)$), respectively. Appendix A collects basic facts on operator-valued Nevanlinna–Herglotz functions. We introduced the background material in Sections 2–4 to make this paper reasonably self-contained.

Finally, we briefly comment on the notation used in this paper: Throughout, \mathcal{H} denotes a separable, complex Hilbert space with inner product and norm denoted by $(\cdot, \cdot)_{\mathcal{H}}$ (linear in the second argument) and $\|\cdot\|_{\mathcal{H}}$, respectively. The identity operator in \mathcal{H} is written as $I_{\mathcal{H}}$. We denote by $\mathcal{B}(\mathcal{H})$ (resp., $\mathcal{B}_\infty(\mathcal{H})$) the Banach space of linear bounded (resp., compact) operators in \mathcal{H} . The domain, range,

kernel (null space), resolvent set, and spectrum of a linear operator will be denoted by $\text{dom}(\cdot)$, $\text{ran}(\cdot)$, $\ker(\cdot)$, $\rho(\cdot)$, and $\sigma(\cdot)$, respectively. The closure of a closable operator S in \mathcal{H} is denoted by \overline{S} . By $\mathfrak{B}(\mathbb{R})$ we denote the collection of Borel subsets of \mathbb{R} .

2 Basics on the initial value problem for Schrödinger operators with operator-valued potentials

In this section we recall the basic results on initial value problems for second-order differential equations of the form $-y'' + Qy = f$ on an arbitrary open interval $(a, b) \subseteq \mathbb{R}$ with a bounded operator-valued coefficient Q , that is, when $Q(x)$ is a bounded operator on a separable, complex Hilbert space \mathcal{H} for a.e. $x \in (a, b)$. We are concerned with two types of situations: in the first one $f(x)$ is an element of the Hilbert space \mathcal{H} for a.e. $x \in (a, b)$, and the solution sought is to take values in \mathcal{H} . In the second situation, $f(x)$ is a bounded operator on \mathcal{H} for a.e. $x \in (a, b)$, as is the proposed solution y .

All results recalled in this section were proved in detail in [50].

We start with some necessary preliminaries: Let $(a, b) \subseteq \mathbb{R}$ be a finite or infinite interval and \mathcal{X} a Banach space. Unless explicitly stated otherwise (such as in the context of operator-valued measures in Nevanlinna–Herglotz representations, cf. Appendix A), integration of \mathcal{X} -valued functions on (a, b) will always be understood in the sense of Bochner (cf., e.g., [10, pp. 6–21], [43, pp. 44–50], [61, pp. 71–86], [79, Ch. III], [104, Sect. V.5] for details). In particular, if $p \geq 1$, the symbol $L^p((a, b); dx; \mathcal{X})$ denotes the set of equivalence classes of strongly measurable \mathcal{X} -valued functions which differ at most on sets of Lebesgue measure zero, such that $\|f(\cdot)\|_{\mathcal{X}}^p \in L^1((a, b); dx)$. The corresponding norm in $L^p((a, b); dx; \mathcal{X})$ is given by $\|f\|_{L^p((a, b); dx; \mathcal{X})} = \left(\int_{(a, b)} dx \|f(x)\|_{\mathcal{X}}^p\right)^{1/p}$, rendering $L^p((a, b); dx; \mathcal{X})$ a Banach space. If \mathcal{H} is a separable Hilbert space, then so is $L^2((a, b); dx; \mathcal{H})$ (see, e.g., [12, Subsects. 4.3.1, 4.3.2], [21, Sect. 7.1]). One recalls that by a result of Pettis [91], if \mathcal{X} is separable, weak measurability of \mathcal{X} -valued functions implies their strong measurability.

Sobolev spaces $W^{n,p}((a, b); dx; \mathcal{X})$ for $n \in \mathbb{N}$ and $p \geq 1$ are defined as follows: $W^{1,p}((a, b); dx; \mathcal{X})$ is the set of all $f \in L^p((a, b); dx; \mathcal{X})$ such that there exists a $g \in L^p((a, b); dx; \mathcal{X})$ and an $x_0 \in (a, b)$ such that

$$(2.1) \quad f(x) = f(x_0) + \int_{x_0}^x dx' g(x') \text{ for a.e. } x \in (a, b).$$

In this case g is the strong derivative of f , $g = f'$. Similarly, $W^{n,p}((a, b); dx; \mathcal{X})$ is the set of all $f \in L^p((a, b); dx; \mathcal{X})$ so that the first n strong derivatives of f are in

$L^p((a, b); dx; \mathcal{X})$. For simplicity of notation we also introduce $W^{0,p}((a, b); dx; \mathcal{X}) = L^p((a, b); dx; \mathcal{X})$. Finally, $W_{loc}^{n,p}((a, b); dx; \mathcal{X})$ is the set of \mathcal{X} -valued functions defined on (a, b) for which the restrictions to any compact interval $[\alpha, \beta] \subset (a, b)$ are in $W^{n,p}((\alpha, \beta); dx; \mathcal{X})$. In particular, this applies to the case $n = 0$ and thus defines $L_{loc}^p((a, b); dx; \mathcal{X})$. If a is finite we may allow $[\alpha, \beta]$ to be a subset of $[a, b)$ and denote the resulting space by $W_{loc}^{n,p}([a, b); dx; \mathcal{X})$ (and again this applies to the case $n = 0$).

Following a frequent practice (cf., e.g., the discussion in [8, Sect. III.1.2]), we will call elements of $W^{1,1}([c, d]; dx; \mathcal{X})$, $[c, d] \subset (a, b)$ (resp., $W_{loc}^{1,1}((a, b); dx; \mathcal{X})$), strongly absolutely continuous \mathcal{X} -valued functions on $[c, d]$ (resp., strongly locally absolutely continuous \mathcal{X} -valued functions on (a, b)), but caution the reader that unless \mathcal{X} possesses the Radon–Nikodym (RN) property, this notion differs from the classical definition of \mathcal{X} -valued absolutely continuous functions (we refer the interested reader to [43, Sect. VII.6] for an extensive list of conditions equivalent to \mathcal{X} having the RN property). Here we just mention that reflexivity of \mathcal{X} implies the RN property.

In the special case where $\mathcal{X} = \mathbb{C}$, we omit \mathcal{X} and just write $L_{loc}^p((a, b); dx)$, as usual.

We emphasize that a strongly continuous operator-valued function $F(x)$, $x \in (a, b)$, always means continuity of $F(\cdot)h$ in \mathcal{H} for all $h \in \mathcal{H}$ (i.e., pointwise continuity of $F(\cdot)$ in \mathcal{H}). The same pointwise conventions will apply to the notions of strongly differentiable and strongly measurable operator-valued functions throughout this manuscript. In particular, and unless explicitly stated otherwise, for operator-valued functions Y , the symbol Y' will be understood in the strong sense; similarly, y' will denote the strong derivative for vector-valued functions y .

Definition 2.1. Let $(a, b) \subseteq \mathbb{R}$ be a finite or infinite interval, and suppose that $Q : (a, b) \rightarrow \mathcal{B}(\mathcal{H})$ is a weakly measurable operator-valued function with $\|Q(\cdot)\|_{\mathcal{B}(\mathcal{H})} \in L_{loc}^1((a, b); dx)$, and that $f \in L_{loc}^1((a, b); dx; \mathcal{H})$. Then the \mathcal{H} -valued function $y : (a, b) \rightarrow \mathcal{H}$ is called a (strong) solution of

$$(2.2) \quad -y'' + Qy = f$$

if $y \in W_{loc}^{2,1}((a, b); dx; \mathcal{H})$ and (2.2) holds a.e. on (a, b) .

One verifies that $Q : (a, b) \rightarrow \mathcal{B}(\mathcal{H})$ satisfies the conditions in Definition 2.1 if and only if Q^* does (a fact that will play a role later on, cf. the paragraph following (2.9)).

Theorem 2.2. Let $(a, b) \subseteq \mathbb{R}$ be a finite or infinite interval and suppose that $V : (a, b) \rightarrow \mathcal{B}(\mathcal{H})$ a weakly measurable operator-valued function with

$\|V(\cdot)\|_{\mathcal{B}(\mathcal{H})} \in L^1_{\text{loc}}((a, b); dx)$. Suppose that $x_0 \in (a, b)$, $z \in \mathbb{C}$, $h_0, h_1 \in \mathcal{H}$, and $f \in L^1_{\text{loc}}((a, b); dx; \mathcal{H})$. Then there is a unique \mathcal{H} -valued solution $y(z, \cdot, x_0) \in W^{2,1}_{\text{loc}}((a, b); dx; \mathcal{H})$ of the initial value problem

$$(2.3) \quad \begin{cases} -y'' + (V - z)y = f \text{ on } (a, b) \setminus E, \\ y(x_0) = h_0, \quad y'(x_0) = h_1, \end{cases}$$

where the exceptional set E is of Lebesgue measure zero and depends only on the representatives chosen for V and f but is independent of z .

Moreover, the following properties hold:

(i) for fixed $x_0, x \in (a, b)$ and $z \in \mathbb{C}$, $y(z, x, x_0)$ depends jointly continuously on $h_0, h_1 \in \mathcal{H}$, and $f \in L^1_{\text{loc}}((a, b); dx; \mathcal{H})$ in the sense that

$$(2.4) \quad \begin{aligned} & \|y(z, x, x_0; h_0, h_1, f) - y(z, x, x_0; \tilde{h}_0, \tilde{h}_1, \tilde{f})\|_{\mathcal{H}} \\ & \leq C(z, V) [\|h_0 - \tilde{h}_0\|_{\mathcal{H}} + \|h_1 - \tilde{h}_1\|_{\mathcal{H}} + \|f - \tilde{f}\|_{L^1([x_0, x]; dx; \mathcal{H})}], \end{aligned}$$

where $C(z, V) > 0$ is a constant, and the dependence of y on the initial data h_0, h_1 and the inhomogeneity f is displayed in (2.4);

(ii) for fixed $x_0 \in (a, b)$ and $z \in \mathbb{C}$, $y(z, x, x_0)$ is strongly continuously differentiable with respect to x on (a, b) ;

(iii) for fixed $x_0 \in (a, b)$ and $z \in \mathbb{C}$, $y'(z, x, x_0)$ is strongly differentiable with respect to x on $(a, b) \setminus E$;

(iv) for fixed $x_0, x \in (a, b)$, $y(z, x, x_0)$ and $y'(z, x, x_0)$ are entire with respect to z .

For classical references on initial value problems we refer, for instance, to [31, Chs. III, VII] and [44, Ch. 10], but we emphasize again that our approach minimizes the smoothness hypotheses on V and f .

Definition 2.3. Let $(a, b) \subseteq \mathbb{R}$ be a finite or infinite interval and assume that $F, Q : (a, b) \rightarrow \mathcal{B}(\mathcal{H})$ are two weakly measurable operator-valued functions such that $\|F(\cdot)\|_{\mathcal{B}(\mathcal{H})}, \|Q(\cdot)\|_{\mathcal{B}(\mathcal{H})} \in L^1_{\text{loc}}((a, b); dx)$. Then the $\mathcal{B}(\mathcal{H})$ -valued function $Y : (a, b) \rightarrow \mathcal{B}(\mathcal{H})$ is called a solution of

$$(2.5) \quad -Y'' + QY = F$$

if $Y(\cdot)h \in W^{2,1}_{\text{loc}}((a, b); dx; \mathcal{H})$ for every $h \in \mathcal{H}$ and $-Y''h + QYh = Fh$ holds a.e. on (a, b) .

Corollary 2.4. Let $(a, b) \subseteq \mathbb{R}$ be a finite or infinite interval, $x_0 \in (a, b)$, $z \in \mathbb{C}$, $Y_0, Y_1 \in \mathcal{B}(\mathcal{H})$, and suppose $F, V : (a, b) \rightarrow \mathcal{B}(\mathcal{H})$ are two weakly measurable operator-valued functions with $\|V(\cdot)\|_{\mathcal{B}(\mathcal{H})}, \|F(\cdot)\|_{\mathcal{B}(\mathcal{H})} \in L^1_{\text{loc}}((a, b); dx)$.

Then there is a unique $\mathcal{B}(\mathcal{H})$ -valued solution $Y(z, \cdot, x_0) : (a, b) \rightarrow \mathcal{B}(\mathcal{H})$ of the initial value problem

$$(2.6) \quad \begin{cases} -Y'' + (V - z)Y = F \text{ on } (a, b) \setminus E, \\ Y(x_0) = Y_0, Y'(x_0) = Y_1. \end{cases}$$

where the exceptional set E is of Lebesgue measure zero and depends only on the representatives chosen for V and F but is independent of z . Moreover, the following properties hold:

- (i) for fixed $x_0 \in (a, b)$ and $z \in \mathbb{C}$, $Y(z, x, x_0)$ is continuously differentiable with respect to x on (a, b) in the $\mathcal{B}(\mathcal{H})$ -norm;
- (ii) for fixed $x_0 \in (a, b)$ and $z \in \mathbb{C}$, $Y'(z, x, x_0)$ is strongly differentiable with respect to x on $(a, b) \setminus E$;
- (iii) for fixed $x_0, x \in (a, b)$, $Y(z, x, x_0)$ and $Y'(z, x, x_0)$ are entire in z in the $\mathcal{B}(\mathcal{H})$ -norm.

Various versions of Theorem 2.2 and Corollary 2.4 exist in the literature under varying assumptions on V and f, F (cf. the discussion in [50] which uses the most general hypotheses to date).

Definition 2.5. Pick $c \in (a, b)$. The endpoint a (resp., b) of the interval (a, b) is called *regular* for the operator-valued differential expression $-(d^2/dx^2) + Q(\cdot)$ if it is finite and if Q is weakly measurable and $\|Q(\cdot)\|_{\mathcal{B}(\mathcal{H})} \in L^1([a, c]; dx)$ (resp., $\|Q(\cdot)\|_{\mathcal{B}(\mathcal{H})} \in L^1([c, b]; dx)$) for some $c \in (a, b)$. Similarly, $-(d^2/dx^2) + Q(\cdot)$ is called *regular at a* (resp., *regular at b*) if a (resp., b) is a regular endpoint for $-(d^2/dx^2) + Q(\cdot)$.

We note that if a (resp., b) is regular for $-(d^2/dx^2) + Q(x)$, one may allow for x_0 to be equal to a (resp., b) in the existence and uniqueness Theorem 2.2.

If f_1, f_2 are strongly continuously differentiable \mathcal{H} -valued functions, we define the Wronskian of f_1 and f_2 by

$$(2.7) \quad W_*(f_1, f_2)(x) = (f_1(x), f_2'(x))_{\mathcal{H}} - (f_1'(x), f_2(x))_{\mathcal{H}}, \quad x \in (a, b).$$

If f_2 is an \mathcal{H} -valued solution of $-y'' + Qy = 0$ and f_1 is an \mathcal{H} -valued solution of $-y'' + Q^*y = 0$, their Wronskian $W_*(f_1, f_2)(x)$ is x -independent, that is,

$$(2.8) \quad \frac{d}{dx} W_*(f_1, f_2)(x) = 0 \text{ for a.e. } x \in (a, b)$$

(in fact, by (2.21), the right-hand side of (2.8) actually vanishes for all $x \in (a, b)$).

We decided to use the symbol $W_*(\cdot, \cdot)$ in (2.7) to indicate its conjugate linear behavior with respect to its first entry.

Similarly, if F_1, F_2 are strongly continuously differentiable $\mathcal{B}(\mathcal{H})$ -valued functions, their Wronskian is defined by

$$(2.9) \quad W(F_1, F_2)(x) = F_1(x)F_2'(x) - F_1'(x)F_2(x), \quad x \in (a, b).$$

Again, if F_2 is a $\mathcal{B}(\mathcal{H})$ -valued solution of $-Y'' + QY = 0$ and F_1 is a $\mathcal{B}(\mathcal{H})$ -valued solution of $-Y'' + YQ = 0$ (the latter is equivalent to $-(Y^*)'' + Q^*Y^* = 0$ and hence can be handled in complete analogy via Theorem 2.2 and Corollary 2.4, replacing Q by Q^*) their Wronskian will be x -independent,

$$(2.10) \quad \frac{d}{dx}W(F_1, F_2)(x) = 0 \text{ for a.e. } x \in (a, b).$$

Our main interest lies in the case where $V(\cdot) = V(\cdot)^* \in \mathcal{B}(\mathcal{H})$ is self-adjoint. Thus, we now introduce the following basic assumption:

Hypothesis 2.6. Let $(a, b) \subseteq \mathbb{R}$, suppose that $V : (a, b) \rightarrow \mathcal{B}(\mathcal{H})$ is a weakly measurable operator-valued function with $\|V(\cdot)\|_{\mathcal{B}(\mathcal{H})} \in L^1_{\text{loc}}((a, b); dx)$, and assume that $V(x) = V(x)^*$ for a.e. $x \in (a, b)$.

Moreover, for the remainder of this paper we assume

$$(2.11) \quad \alpha = \alpha^* \in \mathcal{B}(\mathcal{H}).$$

Assuming Hypothesis 2.6 and (2.11), we introduce the standard fundamental systems of operator-valued solutions of $\tau y = zy$ as follows: Since α is a bounded self-adjoint operator, one may define the self-adjoint operators $A = \sin(\alpha)$ and $B = \cos(\alpha)$ via the spectral theorem. Given such an operator α and a point $x_0 \in (a, b)$ or a regular endpoint for τ , we now define $\theta_\alpha(z, \cdot, x_0), \phi_\alpha(z, \cdot, x_0)$ as those $\mathcal{B}(\mathcal{H})$ -valued solutions of $\tau Y = zY$ (in the sense of Definition 2.3) which satisfy the initial conditions

$$(2.12) \quad \theta_\alpha(z, x_0, x_0) = \phi'_\alpha(z, x_0, x_0) = \cos(\alpha), \quad -\phi_\alpha(z, x_0, x_0) = \theta'_\alpha(z, x_0, x_0) = \sin(\alpha).$$

By Corollary 2.4 (iii), for any fixed $x, x_0 \in (a, b)$, the functions $\theta_\alpha(z, x, x_0), \phi_\alpha(z, x, x_0), \theta_\alpha(\bar{z}, x, x_0)^*$, and $\phi_\alpha(\bar{z}, x, x_0)^*$, as well as their strong x -derivatives are entire with respect to z in the $\mathcal{B}(\mathcal{H})$ -norm.

Since $\theta_\alpha(\bar{z}, \cdot, x_0)^*$ and $\phi_\alpha(\bar{z}, \cdot, x_0)^*$ satisfy the adjoint equation $-Y'' + YV = zY$ and the same initial conditions as θ_α and ϕ_α , respectively, one can show the

following identities (cf. [50]):

$$(2.13) \quad \theta'_\alpha(\bar{z}, x, x_0)^* \theta_\alpha(z, x, x_0) - \theta_\alpha(\bar{z}, x, x_0)^* \theta'_\alpha(z, x, x_0) = 0,$$

$$(2.14) \quad \phi'_\alpha(\bar{z}, x, x_0)^* \phi_\alpha(z, x, x_0) - \phi_\alpha(\bar{z}, x, x_0)^* \phi'_\alpha(z, x, x_0) = 0,$$

$$(2.15) \quad \phi'_\alpha(\bar{z}, x, x_0)^* \theta_\alpha(z, x, x_0) - \phi_\alpha(\bar{z}, x, x_0)^* \theta'_\alpha(z, x, x_0) = I_{\mathcal{H}},$$

$$(2.16) \quad \theta_\alpha(\bar{z}, x, x_0)^* \phi'_\alpha(z, x, x_0) - \theta'_\alpha(\bar{z}, x, x_0)^* \phi_\alpha(z, x, x_0) = I_{\mathcal{H}},$$

as well as,

$$(2.17) \quad \phi_\alpha(z, x, x_0) \theta_\alpha(\bar{z}, x, x_0)^* - \theta_\alpha(z, x, x_0) \phi_\alpha(\bar{z}, x, x_0)^* = 0,$$

$$(2.18) \quad \phi'_\alpha(z, x, x_0) \theta'_\alpha(\bar{z}, x, x_0)^* - \theta'_\alpha(z, x, x_0) \phi'_\alpha(\bar{z}, x, x_0)^* = 0,$$

$$(2.19) \quad \phi'_\alpha(z, x, x_0) \theta_\alpha(\bar{z}, x, x_0)^* - \theta'_\alpha(z, x, x_0) \phi_\alpha(\bar{z}, x, x_0)^* = I_{\mathcal{H}},$$

$$(2.20) \quad \theta_\alpha(z, x, x_0) \phi'_\alpha(\bar{z}, x, x_0)^* - \phi_\alpha(z, x, x_0) \theta'_\alpha(\bar{z}, x, x_0)^* = I_{\mathcal{H}}.$$

Finally, we recall two versions of Green’s formula (resp., Lagrange’s identity).

Lemma 2.7. *Let $(a, b) \subseteq \mathbb{R}$ be a finite or infinite interval, and suppose $[x_1, x_2] \subset (a, b)$.*

(i) *Assume that $f, g \in W_{\text{loc}}^{2,1}((a, b); dx; \mathcal{H})$. Then*

$$(2.21) \quad \int_{x_1}^{x_2} dx [(\tau f)(x), g(x)]_{\mathcal{H}} - (f(x), (\tau g)(x))_{\mathcal{H}} \\ = W_*(f, g)(x_2) - W_*(f, g)(x_1).$$

(ii) *Assume that $F, G : (a, b) \rightarrow \mathcal{B}(\mathcal{H})$ are absolutely continuous operator-valued functions such that F', G' are again differentiable and F'', G'' are weakly measurable. Suppose also that $\|F''\|_{\mathcal{H}}, \|G''\|_{\mathcal{H}} \in L_{\text{loc}}^1((a, b); dx)$. Then*

$$(2.22) \quad \int_{x_1}^{x_2} dx [(\tau F^*)(x)^* G(x) - F(x)(\tau G)(x)] = W(F, G)(x_2) - W(F, G)(x_1).$$

3 Half-line Weyl–Titchmarsh and spectral theory for Schrödinger operators with operator-valued potentials

In this section we recall the basics of Weyl–Titchmarsh and spectral theory for self-adjoint half-line Schrödinger operators H_α in $L^2((a, b); dx; \mathcal{H})$ associated with the operator-valued differential expression $\tau = -(d^2/dx^2)I_{\mathcal{H}} + V(\cdot)$, assuming regularity of the left endpoint a and the limit-point case at the right endpoint b (see Definition 3.1). These results were proved in [50] and [52] and we refer to these sources for details and an extensive bibliography on this topic.

As before, \mathcal{H} denotes a separable Hilbert space and (a, b) denotes a finite or infinite interval. One recalls that $L^2((a, b); dx; \mathcal{H})$ is separable (since \mathcal{H} is) and that

$$(3.1) \quad (f, g)_{L^2((a,b);dx;\mathcal{H})} = \int_a^b dx (f(x), g(x))_{\mathcal{H}}, \quad f, g \in L^2((a, b); dx; \mathcal{H}).$$

Assuming Hypothesis 2.6 throughout this section, we discuss self-adjoint operators in $L^2((a, b); dx; \mathcal{H})$ associated with the operator-valued differential expression $\tau = -(d^2/dx^2)I_{\mathcal{H}} + V(\cdot)$ as suitable restrictions of the *maximal* operator H_{\max} in $L^2((a, b); dx; \mathcal{H})$ defined by

$$(3.2) \quad \begin{aligned} H_{\max} f &= \tau f, \\ f \in \text{dom}(H_{\max}) &= \{g \in L^2((a, b); dx; \mathcal{H}) \mid g \in W_{\text{loc}}^{2,1}((a, b); dx; \mathcal{H}); \\ &\quad \tau g \in L^2((a, b); dx; \mathcal{H})\}. \end{aligned}$$

We also introduce the operator \dot{H}_{\min} in $L^2((a, b); dx; \mathcal{H})$

$$(3.3) \quad \text{dom}(\dot{H}_{\min}) = \{g \in \text{dom}(H_{\max}) \mid \text{supp}(g) \text{ is compact in } (a, b)\},$$

and the *minimal* operator H_{\min} in $L^2((a, b); dx; \mathcal{H})$ associated with τ ,

$$(3.4) \quad H_{\min} = \overline{\dot{H}_{\min}}.$$

One obtains,

$$(3.5) \quad H_{\max} = (\dot{H}_{\min})^*, \quad H_{\max}^* = \overline{\dot{H}_{\min}} = H_{\min}.$$

Moreover, Green’s formula holds, that is, if u and v are in $\text{dom}(H_{\max})$, then

$$(3.6) \quad (H_{\max}u, v)_{L^2((a,b);dx;\mathcal{H})} - (u, H_{\max}v)_{L^2((a,b);dx;\mathcal{H})} = W_*(u, v)(b) - W_*(u, v)(a).$$

Definition 3.1. Assume Hypothesis 2.6. Then the endpoint a (resp., b) is said to be of *limit-point-type* for τ if $W_*(u, v)(a) = 0$ (resp., $W_*(u, v)(b) = 0$) for all $u, v \in \text{dom}(H_{\max})$.

Next, we introduce the subspaces

$$(3.7) \quad \mathcal{D}_z = \{u \in \text{dom}(H_{\max}) \mid H_{\max}u = zu\}, \quad z \in \mathbb{C}.$$

For $z \in \mathbb{C} \setminus \mathbb{R}$, \mathcal{D}_z represent the deficiency subspaces of H_{\min} . Von Neumann’s theory of extensions of symmetric operators implies that

$$(3.8) \quad \text{dom}(H_{\max}) = \text{dom}(H_{\min}) \dot{+} \mathcal{D}_i \dot{+} \mathcal{D}_{-i},$$

where $\dot{+}$ indicates the direct (but not necessarily orthogonal direct) sum in the underlying Hilbert space $L^2((a, b); dx; \mathcal{H})$.

For the remainder of this section we now make the following assumptions:

Hypothesis 3.2. In addition to Hypothesis 2.6 suppose that a is a regular endpoint for τ and b is of limit-point-type for τ .

Given Hypothesis 3.2, it has been shown in [50] that all self-adjoint restrictions, H_α , of H_{\max} , equivalently, all self-adjoint extensions of H_{\min} , are parametrized by $\alpha = \alpha^* \in \mathcal{B}(\mathcal{H})$, with domains given by

$$(3.9) \quad \text{dom}(H_\alpha) = \{u \in \text{dom}(H_{\max}) \mid \sin(\alpha)u'(a) + \cos(\alpha)u(a) = 0\}.$$

Next, we recall that (normalized) $\mathcal{B}(\mathcal{H})$ -valued and square integrable solutions of $\tau Y = zY$, denoted by $\psi_\alpha(z, \cdot, a)$, $z \in \mathbb{C} \setminus \sigma(H_\alpha)$, and traditionally called *Weyl–Titchmarsh* solutions of $\tau Y = zY$, and the $\mathcal{B}(\mathcal{H})$ -valued Weyl–Titchmarsh functions $m_\alpha(z, a)$, have been constructed in [50] to the effect that

$$(3.10) \quad \psi_\alpha(z, x, a) = \theta_\alpha(z, x, a) + \phi_\alpha(z, x, a)m_\alpha(z, a), \quad z \in \mathbb{C} \setminus \sigma(H_\alpha), \quad x \in [a, b].$$

Then $\psi_\alpha(\cdot, x, a)$ is analytic in z on $\mathbb{C} \setminus \mathbb{R}$ for fixed $x \in [a, b)$, and

$$(3.11) \quad \int_a^b dx \|\psi_\alpha(z, x, a)h\|_{\mathcal{H}}^2 < \infty, \quad h \in \mathcal{H}, \quad z \in \mathbb{C} \setminus \sigma(H_\alpha),$$

in particular,

$$(3.12) \quad \psi_\alpha(z, \cdot, a)h \in L^2((a, b); dx; \mathcal{H}), \quad h \in \mathcal{H}, \quad z \in \mathbb{C} \setminus \sigma(H_\alpha),$$

and

$$(3.13) \quad \ker(H_{\max} - zI_{L^2((a,b); dx; \mathcal{H})}) = \{\psi_\alpha(z, \cdot, a)h \mid h \in \mathcal{H}\}. \quad z \in \mathbb{C} \setminus \mathbb{R}.$$

In addition, $m_\alpha(z, a)$ is a $\mathcal{B}(\mathcal{H})$ -valued Nevanlinna–Herglotz function (cf. Definition A.1), and

$$(3.14) \quad m_\alpha(z, a) = m_\alpha(\bar{z}, a)^*, \quad z \in \mathbb{C} \setminus \sigma(H_\alpha).$$

Given $u \in \mathcal{D}_z$, the operator $m_0(z, a)$ assigns Neumann boundary data $u'(a)$ to the Dirichlet boundary data $u(a)$, that is, $m_0(z, a)$ is the (z -dependent) Dirichlet-to-Neumann map.

With the help of Weyl–Titchmarsh solutions one can now describe the resolvent of H_α as follows,

$$(3.15) \quad \begin{aligned} ((H_\alpha - zI_{L^2((a,b); dx; \mathcal{H})})^{-1}u)(x) &= \int_a^b dx' G_\alpha(z, x, x')u(x'), \\ u &\in L^2((a, b); dx; \mathcal{H}), \quad z \in \rho(H_\alpha), \quad x \in [a, b), \end{aligned}$$

with the $\mathcal{B}(\mathcal{H})$ -valued Green’s function $G_a(z, \cdot, \cdot)$ given by

$$(3.16) \quad G_a(z, x, x') = \begin{cases} \phi_a(z, x, a)\psi_a(\bar{z}, x', a)^*, & a \leq x \leq x' < b, \\ \psi_a(z, x, a)\phi_a(\bar{z}, x', a)^*, & a \leq x' \leq x < b, \end{cases} \quad z \in \mathbb{C} \setminus \mathbb{R}.$$

Next, we replace the interval (a, b) by the right half-line (x_0, ∞) and indicate this change with the additional subscript $+$ in $H_{+, \min}, H_{+, \max}, H_{+, a}, \psi_{+, a}(z, \cdot, x_0), m_{+, a}(\cdot, x_0), d\rho_{+, a}(\cdot, x_0), G_{+, a}(z, \cdot, \cdot)$, etc., to distinguish these quantities from the analogous objects on the left half-line $(-\infty, x_0)$ (later indicated with the subscript $-$), which are needed in our subsequent full-line Section 4.

Our aim is to relate the family of spectral projections, $\{E_{H_{+, a}}(\lambda)\}_{\lambda \in \mathbb{R}}$, of the self-adjoint operator $H_{+, a}$ and the $\mathcal{B}(\mathcal{H})$ -valued spectral function $\rho_{+, a}(\lambda, x_0)$, $\lambda \in \mathbb{R}$, which generates the operator-valued measure $d\rho_{+, a}(\cdot, x_0)$ in the Nevanlinna–Herglotz representation (3.17) of $m_{+, a}(\cdot, x_0)$:

$$(3.17) \quad m_{+, a}(z, x_0) = c_{+, a} + \int_{\mathbb{R}} d\rho_{+, a}(\lambda, x_0) \left[\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2 + 1} \right], \quad z \in \mathbb{C} \setminus \sigma(H_{+, a}),$$

where

$$(3.18) \quad c_{+, a} = \operatorname{Re}(m_{+, a}(i, x_0)) \in \mathcal{B}(\mathcal{H}),$$

and $d\rho_{+, a}(\cdot, x_0)$ is a $\mathcal{B}(\mathcal{H})$ -valued measure satisfying

$$(3.19) \quad \int_{\mathbb{R}} d(e, \rho_{+, a}(\lambda, x_0)e)_{\mathcal{H}} (\lambda^2 + 1)^{-1} < \infty, \quad e \in \mathcal{H}.$$

In addition, the Stieltjes inversion formula for the nonnegative $\mathcal{B}(\mathcal{H})$ -valued measure $d\rho_{+, a}(\cdot, x_0)$ reads

$$(3.20) \quad \rho_{+, a}((\lambda_1, \lambda_2], x_0) = \frac{1}{\pi} \lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} \int_{\lambda_1 + \delta}^{\lambda_2 + \delta} d\lambda \operatorname{Im}(m_{+, a}(\lambda + i\varepsilon, x_0)), \quad \lambda_1, \lambda_2 \in \mathbb{R}, \lambda_1 < \lambda_2$$

(cf. Appendix A for details on Nevanlinna–Herglotz functions). We also note that $m_{+, a}(\cdot, x_0)$ and $m_{+, \beta}(\cdot, x_0)$ are related by the following linear fractional transformation,

$$(3.21) \quad m_{+, \beta}(\cdot, x_0) = (C + Dm_{+, a}(\cdot, x_0))(A + Bm_{+, a}(\cdot, x_0))^{-1},$$

where

$$(3.22) \quad \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} \cos(\beta) & \sin(\beta) \\ -\sin(\beta) & \cos(\beta) \end{pmatrix} \begin{pmatrix} \cos(\alpha) & -\sin(\alpha) \\ \sin(\alpha) & \cos(\alpha) \end{pmatrix}.$$

An important consequence of (3.21) and the fact that the m -functions take values in $\mathcal{B}(\mathcal{H})$ is the following invertibility result.

Theorem 3.3. *Assume Hypothesis 3.2, then $[\text{Im}(m_{+, \alpha}(z, x_0))]^{-1} \in \mathcal{B}(\mathcal{H})$ for all $z \in \mathbb{C} \setminus \mathbb{R}$ and $\alpha = \alpha^* \in \mathcal{B}(\mathcal{H})$.*

Proof. Let $z \in \mathbb{C} \setminus \mathbb{R}$ be fixed. We first show that $[\text{Im}(m_{+, 0}(z, x_0))]^{-1} \in \mathcal{B}(\mathcal{H})$. By (3.21),

$$(3.23) \quad m_{+, \beta}(z, x_0) = [\cos(\beta)m_{+, 0}(z, x_0) - \sin(\beta)][\sin(\beta)m_{+, 0}(z, x_0) + \cos(\beta)]^{-1},$$

hence using $\sin^2(\beta) + \cos^2(\beta) = I_{\mathcal{H}}$ and commutativity of $\sin(\beta)$ and $\cos(\beta)$, one gets

$$(3.24) \quad \cos(\beta) - \sin(\beta)m_{+, \beta}(z, x_0) = [\sin(\beta)m_{+, 0}(z, x_0) + \cos(\beta)]^{-1}.$$

Taking $\beta = \beta(z) = \text{arccot}(-\text{Re}(m_{+, 0}(z, x_0))) \in \mathcal{B}(\mathcal{H})$ yields

$$(3.25) \quad \cos(\beta) - \sin(\beta)m_{+, \beta}(z, x_0) = [\sin(\beta)i \text{Im}(m_{+, 0}(z, x_0))]^{-1},$$

and since the left-hand side is in $\mathcal{B}(\mathcal{H})$, also $[\text{Im}(m_{+, 0}(z, x_0))]^{-1} \in \mathcal{B}(\mathcal{H})$.

Next, we show that for any $\alpha = \alpha^* \in \mathcal{B}(\mathcal{H})$, $[\text{Im}(m_{+, \alpha}(z, x_0))]^{-1} \in \mathcal{B}(\mathcal{H})$. Replacing β by α in (3.23) and noting that both $\sin(\alpha)$ and $\cos(\alpha)$ are self-adjoint, one obtains

$$(3.26) \quad m_{+, \alpha}(z, x_0) = [\cos(\alpha)m_{+, 0}(z, x_0) - \sin(\alpha)][\sin(\alpha)m_{+, 0}(z, x_0) + \cos(\alpha)]^{-1},$$

$$m_{+, \alpha}(z, x_0)^* = [m_{+, 0}(z, x_0)^* \sin(\alpha) + \cos(\alpha)]^{-1}[m_{+, 0}(z, x_0)^* \cos(\alpha) - \sin(\alpha)],$$

and consequently

$$(3.27) \quad \begin{aligned} 2i \text{Im}(m_{+, \alpha}(z, x_0)) &= m_{+, \alpha}(z, x_0) - m_{+, \alpha}(z, x_0)^* \\ &= [m_{+, 0}(z, x_0)^* \sin(\alpha) + \cos(\alpha)]^{-1}[2i \text{Im}(m_{+, 0}(z, x_0))] \\ &\quad \times [\sin(\alpha)m_{+, 0}(z, x_0) + \cos(\alpha)]^{-1}. \end{aligned}$$

Since $[\text{Im}(m_{+, 0}(z, x_0))]^{-1} \in \mathcal{B}(\mathcal{H})$, it follows that $[\text{Im}(m_{+, \alpha}(z, x_0))]^{-1} \in \mathcal{B}(\mathcal{H})$. \square

In the following, $C_0^\infty((c, d); \mathcal{H})$, $-\infty \leq c < d \leq \infty$, denotes the usual space of infinitely differentiable \mathcal{H} -valued functions of compact support contained in (c, d) .

Theorem 3.4. *Assume Hypothesis 3.2 and let $f, g \in C_0^\infty((x_0, \infty); \mathcal{H})$, $F \in C(\mathbb{R})$, and $\lambda_1, \lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$. Then,*

$$(3.28) \quad \begin{aligned} &(f, F(H_{+, \alpha})E_{H_{+, \alpha}}((\lambda_1, \lambda_2])g)_{L^2((x_0, \infty); dx; \mathcal{H})} \\ &= (\widehat{f}_{+, \alpha}, M_F M_{\chi_{(\lambda_1, \lambda_2]}} \widehat{g}_{+, \alpha})_{L^2(\mathbb{R}; d\rho_{+, \alpha}(\cdot, x_0); \mathcal{H})}, \end{aligned}$$

where we introduced the notation

$$(3.29) \quad \widehat{u}_{+,a}(\lambda) = \int_{x_0}^{\infty} dx \phi_a(\lambda, x, x_0)^* u(x), \quad \lambda \in \mathbb{R}, \quad u \in C_0^\infty((x_0, \infty); \mathcal{H}),$$

and M_G denotes the maximally defined operator of multiplication by the function $G \in C(\mathbb{R})$ in the Hilbert space $L^2(\mathbb{R}; d\rho_{+,a}; \mathcal{H})$,

$$(3.30) \quad \begin{aligned} (M_G \widehat{u})(\lambda) &= G(\lambda) \widehat{u}(\lambda) \text{ for } \rho_{+,a}\text{-a.e. } \lambda \in \mathbb{R}, \\ \widehat{u} \in \text{dom}(M_G) &= \{ \widehat{v} \in L^2(\mathbb{R}; d\rho_{+,a}(\cdot, x_0); \mathcal{H}) \\ &\quad | G \widehat{v} \in L^2(\mathbb{R}; d\rho_{+,a}(\cdot, x_0); \mathcal{H}) \}. \end{aligned}$$

Here $\rho_{+,a}(\cdot, x_0)$ generates the operator-valued measure in the Nevanlinna–Herglotz representation of the $\mathcal{B}(\mathcal{H})$ -valued Weyl–Titchmarsh function $m_{+,a}(\cdot, x_0) \in \mathcal{B}(\mathcal{H})$ (cf. (3.17)).

For a discussion of the model Hilbert space $L^2(\mathbb{R}; d\Sigma; \mathcal{K})$ for operator-valued measures Σ we refer to [47], [51] and [52, App. B].

In the context of operator-valued potential coefficients of half-line Schrödinger operators we also refer to M. L. Gorbachuk [54], Saitō [99], and Trooshin [101].

The proof of Theorem 3.4 in [52] relies on a version of Stone’s formula in the weak sense (cf., e.g., [46, pp. 1203]):

Lemma 3.5. *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,*

$$(3.31) \quad \begin{aligned} &(f, F(T)E_T((\lambda_1, \lambda_2])g)_{\mathcal{H}} \\ &= \lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} \frac{1}{2\pi i} \int_{\lambda_1 + \delta}^{\lambda_2 + \delta} d\lambda F(\lambda) [(f, (T - (\lambda + i\varepsilon)I_{\mathcal{H}})^{-1}g)_{\mathcal{H}} \\ &\quad - (f, (T - (\lambda - i\varepsilon)I_{\mathcal{H}})^{-1}g)_{\mathcal{H}}]. \end{aligned}$$

One can remove the compact support restrictions on f and g in Theorem 3.4 in the usual way by introducing the map

$$(3.32) \quad \widetilde{U}_{+,a} : \begin{cases} C_0^\infty((x_0, \infty); \mathcal{H}) \rightarrow L^2(\mathbb{R}; d\rho_{+,a}(\cdot, x_0); \mathcal{H}) \\ u \mapsto \widehat{u}_{+,a}(\cdot) = \int_{x_0}^{\infty} dx \phi_a(\cdot, x, x_0)^* u(x). \end{cases}$$

Taking $f = g$, $F = 1$, $\lambda_1 \downarrow -\infty$, and $\lambda_2 \uparrow \infty$ in (3.28) then shows that $\widetilde{U}_{+,a}$ is a densely defined isometry in $L^2((x_0, \infty); dx; \mathcal{H})$, which extends by continuity to an

isometry on $L^2((x_0, \infty); dx; \mathcal{H})$. The latter is denoted by $U_{+, \alpha}$ and given by

$$(3.33) \quad U_{+, \alpha} : \begin{cases} L^2((x_0, \infty); dx; \mathcal{H}) \rightarrow L^2(\mathbb{R}; d\rho_{+, \alpha}(\cdot, x_0); \mathcal{H}) \\ u \mapsto \widehat{u}_{+, \alpha}(\cdot) = \text{s-lim}_{b \uparrow \infty} \int_{x_0}^b dx \phi_\alpha(\cdot, x, x_0)^* u(x), \end{cases}$$

where s-lim refers to the $L^2(\mathbb{R}; d\rho_{+, \alpha}(\cdot, x_0); \mathcal{H})$ -limit. In addition, one can show that the map $U_{+, \alpha}$ in (3.33) is onto and hence that $U_{+, \alpha}$ is unitary (i.e., $U_{+, \alpha}$ and $U_{+, \alpha}^{-1}$ are isometric isomorphisms between the Hilbert spaces $L^2((x_0, \infty); dx; \mathcal{H})$ and $L^2(\mathbb{R}; d\rho_{+, \alpha}(\cdot, x_0); \mathcal{H})$ with

$$(3.34) \quad U_{+, \alpha}^{-1} : \begin{cases} L^2(\mathbb{R}; d\rho_{+, \alpha}; \mathcal{H}) \rightarrow L^2((x_0, \infty); dx; \mathcal{H}) \\ \widehat{u} \mapsto \text{s-lim}_{\mu_1 \downarrow -\infty, \mu_2 \uparrow \infty} \int_{\mu_1}^{\mu_2} \phi_\alpha(\lambda, \cdot, x_0) d\rho_{+, \alpha}(\lambda, x_0) \widehat{u}(\lambda). \end{cases}$$

Here s-lim refers to the $L^2((x_0, \infty); dx; \mathcal{H})$ -limit.

We recall that the essential range of F with respect to a scalar measure μ is defined by

$$(3.35) \quad \text{ess.ran}_\mu(F) = \{z \in \mathbb{C} \mid \text{for all } \varepsilon > 0, \mu(\{\lambda \in \mathbb{R} \mid |F(\lambda) - z| < \varepsilon\}) > 0\},$$

and that $\text{ess.ran}_{\rho_{+, \alpha}}(F)$ for $F \in C(\mathbb{R})$ is then defined to be $\text{ess.ran}_{\nu_{+, \alpha}}(F)$ for any control measure $d\nu_{+, \alpha}$ of the operator-valued measure $d\rho_{+, \alpha}$. Given a complete orthonormal system $\{e_n\}_{n \in \mathcal{J}}$ in \mathcal{H} ($\mathcal{J} \subseteq \mathbb{N}$ an appropriate index set), a convenient control measure for $d\rho_{+, \alpha}$ is given by

$$(3.36) \quad \mu_{+, \alpha}(B) = \sum_{n \in \mathcal{J}} 2^{-n} (e_n, \rho_{+, \alpha}(B, x_0) e_n)_{\mathcal{H}}, \quad B \in \mathfrak{B}(\mathbb{R}).$$

These considerations lead to a variant of the spectral theorem for $H_{+, \alpha}$:

Theorem 3.6. *Assume Hypothesis 3.2 and suppose $F \in C(\mathbb{R})$. Then,*

$$(3.37) \quad U_{+, \alpha} F(H_{+, \alpha}) U_{+, \alpha}^{-1} = M_F I_{\mathcal{H}}$$

in $L^2(\mathbb{R}; d\rho_{+, \alpha}(\cdot, x_0); \mathcal{H})$ (cf. (3.30)). Moreover,

$$(3.38) \quad \sigma(F(H_{+, \alpha})) = \text{ess.ran}_{\rho_{+, \alpha}}(F),$$

$$(3.39) \quad \sigma(H_{+, \alpha}) = \text{supp}(d\rho_{+, \alpha}(\cdot, x_0)),$$

and the multiplicity of the spectrum of $H_{+, \alpha}$ is at most equal to $\dim(\mathcal{H})$.

4 Weyl–Titchmarsh and spectral theory of Schrödinger operators with operator-valued potentials on the real line

In this section we briefly recall the basic spectral theory for full-line Schrödinger operators H in $L^2(\mathbb{R}; dx; \mathcal{H})$, employing a 2×2 block operator representation of the associated Weyl–Titchmarsh matrix and its $\mathcal{B}(\mathcal{H}^2)$ -valued spectral measure, decomposing \mathbb{R} into a left and right half-line with reference point $x_0 \in \mathbb{R}$, $(-\infty, x_0] \cup [x_0, \infty)$.

We make the following basic assumption throughout this section.

Hypothesis 4.1. (i) Assume that

$$(4.1) \quad V \in L^1_{\text{loc}}(\mathbb{R}; dx; \mathcal{H}), \quad V(x) = V(x)^* \text{ for a.e. } x \in \mathbb{R}$$

(ii) Introducing the differential expression τ given by

$$(4.2) \quad \tau = -\frac{d^2}{dx^2} I_{\mathcal{H}} + V(x), \quad x \in \mathbb{R},$$

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 $L^2(\mathbb{R}; dx; \mathcal{H})$ by

$$(4.3)$$

$$Hf = \tau f,$$

$$f \in \text{dom}(H) = \{g \in L^2(\mathbb{R}; dx; \mathcal{H}) \mid g, g' \in W^{2,1}_{\text{loc}}(\mathbb{R}; dx; \mathcal{H}); \tau g \in L^2(\mathbb{R}; dx; \mathcal{H})\}.$$

As in the half-line context we introduce the $\mathcal{B}(\mathcal{H})$ -valued fundamental system of solutions $\phi_\alpha(z, \cdot, x_0)$ and $\theta_\alpha(z, \cdot, x_0)$, $z \in \mathbb{C}$, of

$$(4.4) \quad (\tau\psi)(z, x) = z\psi(z, x), \quad x \in \mathbb{R},$$

with respect to a fixed reference point $x_0 \in \mathbb{R}$, satisfying the initial conditions at the point $x = x_0$,

$$(4.5) \quad \begin{aligned} \phi_\alpha(z, x_0, x_0) &= -\theta'_\alpha(z, x_0, x_0) = -\sin(\alpha), \\ \phi'_\alpha(z, x_0, x_0) &= \theta_\alpha(z, x_0, x_0) = \cos(\alpha), \quad \alpha = \alpha^* \in \mathcal{B}(\mathcal{H}). \end{aligned}$$

Again we note that by Corollary 2.4 (iii), for any fixed $x, x_0 \in \mathbb{R}$, the functions $\theta_\alpha(z, x, x_0)$, $\phi_\alpha(z, x, x_0)$, $\theta_\alpha(\bar{z}, x, x_0)^*$, and $\phi_\alpha(\bar{z}, x, x_0)^*$ as well as their strong x -derivatives are entire with respect to z in the $\mathcal{B}(\mathcal{H})$ -norm. Moreover, by (2.16),

$$(4.6) \quad W(\theta_\alpha(\bar{z}, \cdot, x_0)^*, \phi_\alpha(z, \cdot, x_0))(x) = I_{\mathcal{H}}, \quad z \in \mathbb{C}.$$

Particularly important solutions of (4.4) are the *Weyl–Titchmarsh solutions* $\psi_{\pm,\alpha}(z, \cdot, x_0)$, $z \in \mathbb{C} \setminus \mathbb{R}$, uniquely characterized by

$$(4.7) \quad \begin{aligned} \psi_{\pm,\alpha}(z, \cdot, x_0)h &\in L^2((x_0, \pm\infty); dx; \mathcal{H}), \quad h \in \mathcal{H}, \\ \sin(\alpha)\psi'_{\pm,\alpha}(z, x_0, x_0) + \cos(\alpha)\psi_{\pm,\alpha}(z, x_0, x_0) &= I_{\mathcal{H}}, \quad z \in \mathbb{C} \setminus \sigma(H_{\pm,\alpha}). \end{aligned}$$

The crucial condition in (4.7) 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 $\alpha = \alpha^*$, $\beta = \beta^* \in \mathcal{B}(\mathcal{H})$,

$$(4.8) \quad \psi_{\pm,\alpha}(z, \cdot, x_0) = \psi_{\pm,\beta}(z, \cdot, x_0)C_{\pm}(z, \alpha, \beta, x_0)$$

for some coefficients $C_{\pm}(z, \alpha, \beta, x_0) \in \mathcal{B}(\mathcal{H})$. The normalization in (4.7) shows that $\psi_{\pm,\alpha}(z, \cdot, x_0)$ are of the type

$$(4.9) \quad \psi_{\pm,\alpha}(z, x, x_0) = \theta_{\alpha}(z, x, x_0) + \phi_{\alpha}(z, x, x_0)m_{\pm,\alpha}(z, x_0),$$

$z \in \mathbb{C} \setminus \sigma(H_{\pm,\alpha})$, $x \in \mathbb{R}$, for some coefficients $m_{\pm,\alpha}(z, x_0) \in \mathcal{B}(\mathcal{H})$, the *Weyl–Titchmarsh m -functions* associated with τ , α , and x_0 . In addition, we note that (with $z, z_1, z_2 \in \mathbb{C} \setminus \sigma(H_{\pm,\alpha})$)

$$(4.10) \quad W(\psi_{\pm,\alpha}(\bar{z}_1, x_0, x_0)^*, \psi_{\pm,\alpha}(z_2, x_0, x_0)) = m_{\pm,\alpha}(z_2, x_0) - m_{\pm,\alpha}(z_1, x_0),$$

$$(4.11) \quad \begin{aligned} \frac{d}{dx} W(\psi_{\pm,\alpha}(\bar{z}_1, x, x_0)^*, \psi_{\pm,\alpha}(z_2, x, x_0)) \\ = (z_1 - z_2)\psi_{\pm,\alpha}(\bar{z}_1, x, x_0)^* \psi_{\pm,\alpha}(z_2, x, x_0), \end{aligned}$$

$$(4.12) \quad \begin{aligned} (z_2 - z_1) \int_{x_0}^{\pm\infty} dx \psi_{\pm,\alpha}(\bar{z}_1, x, x_0)^* \psi_{\pm,\alpha}(z_2, x, x_0) \\ = m_{\pm,\alpha}(z_2, x_0) - m_{\pm,\alpha}(z_1, x_0), \end{aligned}$$

$$(4.13) \quad m_{\pm,\alpha}(z, x_0) = m_{\pm,\alpha}(\bar{z}, x_0)^*,$$

$$(4.14) \quad \text{Im}[m_{\pm,\alpha}(z, x_0)] = \text{Im}(z) \int_{x_0}^{\pm\infty} dx \psi_{\pm,\alpha}(z, x, x_0)^* \psi_{\pm,\alpha}(z, x, x_0).$$

In particular, $\pm m_{\pm,\alpha}(\cdot, x_0)$ are operator-valued Nevanlinna–Herglotz functions.

In the following we abbreviate the Wronskian of $\psi_{+,\alpha}(\bar{z}, x, x_0)^*$ and $\psi_{-,\alpha}(z, x, x_0)$ by $W(z)$ (thus, $W(z) = m_{-,\alpha}(z, x_0) - m_{+,\alpha}(z, x_0)$, $z \in \mathbb{C} \setminus \sigma(H)$). The Green’s function $G(z, x, x')$ of the Schrödinger operator H then reads

$$(4.15) \quad G(z, x, x') = \psi_{\mp,\alpha}(z, x, x_0)W(z)^{-1}\psi_{\pm,\alpha}(\bar{z}, x', x_0)^*, \quad x \leq x', \quad z \in \mathbb{C} \setminus \sigma(H).$$

Thus,

$$(4.16) \quad ((H - zI_{L^2(\mathbb{R}; dx; \mathcal{H})})^{-1}f)(x) = \int_{\mathbb{R}} dx' G(z, x, x')f(x'), \quad z \in \mathbb{C} \setminus \sigma(H),$$

$$x \in \mathbb{R}, f \in L^2(\mathbb{R}; dx; \mathcal{H}).$$

Next, we introduce the 2×2 block operator-valued Weyl–Titchmarsh m -function, $M_\alpha(z, x_0) \in \mathcal{B}(\mathcal{H}^2)$,

$$(4.17) \quad M_\alpha(z, x_0) = (M_{\alpha, j, j'}(z, x_0))_{j, j'=0,1}, \quad z \in \mathbb{C} \setminus \sigma(H),$$

$$(4.18) \quad M_{\alpha, 0, 0}(z, x_0) = W(z)^{-1},$$

$$(4.19) \quad M_{\alpha, 0, 1}(z, x_0) = 2^{-1}W(z)^{-1}[m_{-, \alpha}(z, x_0) + m_{+, \alpha}(z, x_0)],$$

$$(4.20) \quad M_{\alpha, 1, 0}(z, x_0) = 2^{-1}[m_{-, \alpha}(z, x_0) + m_{+, \alpha}(z, x_0)]W(z)^{-1},$$

$$(4.21) \quad \begin{aligned} M_{\alpha, 1, 1}(z, x_0) &= m_{+, \alpha}(z, x_0)W(z)^{-1}m_{-, \alpha}(z, x_0) \\ &= m_{-, \alpha}(z, x_0)W(z)^{-1}m_{+, \alpha}(z, x_0). \end{aligned}$$

$M_\alpha(z, x_0)$ is a $\mathcal{B}(\mathcal{H}^2)$ -valued Nevanlinna–Herglotz function with representation

$$(4.22) \quad M_\alpha(z, x_0) = C_\alpha(x_0) + \int_{\mathbb{R}} d\Omega_\alpha(\lambda, x_0) \left[\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2 + 1} \right], \quad z \in \mathbb{C} \setminus \sigma(H),$$

where

$$(4.23) \quad C_\alpha(x_0) = \operatorname{Re}(M_\alpha(i, x_0)) \in \mathcal{B}(\mathcal{H}^2),$$

and $d\Omega_\alpha(\cdot, x_0)$ is a $\mathcal{B}(\mathcal{H}^2)$ -valued measure satisfying

$$(4.24) \quad \int_{\mathbb{R}} (e, d\Omega_\alpha(\lambda, x_0)e)_{\mathcal{H}^2} (\lambda^2 + 1)^{-1} < \infty, \quad e \in \mathcal{H}^2.$$

In addition, the Stieltjes inversion formula for the nonnegative $\mathcal{B}(\mathcal{H}^2)$ -valued measure $d\Omega_\alpha(\cdot, x_0)$ reads

$$(4.25) \quad \Omega_\alpha((\lambda_1, \lambda_2], x_0) = \frac{1}{\pi} \lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} \int_{\lambda_1 + \delta}^{\lambda_2 + \delta} d\lambda \operatorname{Im}(M_\alpha(\lambda + i\varepsilon, x_0)), \quad \lambda_1, \lambda_2 \in \mathbb{R}, \lambda_1 < \lambda_2.$$

In particular, $d\Omega_\alpha(\cdot, x_0)$ is a 2×2 block operator-valued measure with $\mathcal{B}(\mathcal{H})$ -valued entries $d\Omega_{\alpha, \ell, \ell'}(\cdot, x_0)$, $\ell, \ell' = 0, 1$.

Relating the family of spectral projections, $\{E_H(\lambda)\}_{\lambda \in \mathbb{R}}$, of the self-adjoint operator H and the 2×2 operator-valued increasing spectral function $\Omega_\alpha(\lambda, x_0)$, $\lambda \in \mathbb{R}$, which generates the $\mathcal{B}(\mathcal{H}^2)$ -valued measure $d\Omega_\alpha(\cdot, x_0)$ in the Nevanlinna–Herglotz representation (4.22) of $M_\alpha(z, x_0)$, one obtains the following result:

Theorem 4.2. *Let $\alpha = \alpha^* \in \mathcal{B}(\mathcal{H})$, $f, g \in C_0^\infty(\mathbb{R}; \mathcal{H})$, $F \in C(\mathbb{R})$, $x_0 \in \mathbb{R}$, and $\lambda_1, \lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$. Then,*

$$(4.26) \quad (f, F(H)E_H((\lambda_1, \lambda_2]g))_{L^2(\mathbb{R}; dx; \mathcal{H})} = (\widehat{f}_\alpha(\cdot, x_0), M_F M_{\chi_{(\lambda_1, \lambda_2]}} \widehat{g}_\alpha(\cdot, x_0))_{L^2(\mathbb{R}; d\Omega_\alpha(\cdot, x_0); \mathcal{H}^2)}$$

where we introduced the notation

$$(4.27) \quad \begin{aligned} \widehat{u}_{\alpha,0}(\lambda, x_0) &= \int_{\mathbb{R}} dx \theta_\alpha(\lambda, x, x_0)^* u(x), \\ \widehat{u}_{\alpha,1}(\lambda, x_0) &= \int_{\mathbb{R}} dx \phi_\alpha(\lambda, x, x_0)^* u(x), \\ \widehat{u}_\alpha(\lambda, x_0) &= (\widehat{u}_{\alpha,0}(\lambda, x_0), \widehat{u}_{\alpha,1}(\lambda, x_0))^\top, \quad \lambda \in \mathbb{R}, u \in C_0^\infty(\mathbb{R}; \mathcal{H}), \end{aligned}$$

and M_G denotes the maximally defined operator of multiplication by the function $G \in C(\mathbb{R})$ in the Hilbert space $L^2(\mathbb{R}; d\Omega_\alpha(\cdot, x_0); \mathcal{H}^2)$,

$$(4.28) \quad \begin{aligned} (M_G \widehat{u})(\lambda) &= G(\lambda) \widehat{u}(\lambda) = (G(\lambda) \widehat{u}_0(\lambda), G(\lambda) \widehat{u}_1(\lambda))^\top \text{ for } \Omega_\alpha(\cdot, x_0)\text{-a.e. } \lambda \in \mathbb{R}, \\ \widehat{u} \in \text{dom}(M_G) &= \{ \widehat{v} \in L^2(\mathbb{R}; d\Omega_\alpha(\cdot, x_0); \mathcal{H}^2) \mid G \widehat{v} \in L^2(\mathbb{R}; d\Omega_\alpha(\cdot, x_0); \mathcal{H}^2) \}. \end{aligned}$$

As in the half-line case, one can remove the compact support restrictions on f and g in the usual way by considering the map

$$(4.29) \quad \begin{aligned} \widetilde{U}_\alpha(x_0) &: \begin{cases} C_0^\infty(\mathbb{R}) \rightarrow L^2(\mathbb{R}; d\Omega_\alpha(\cdot, x_0); \mathcal{H}^2) \\ u \mapsto \widehat{u}_\alpha(\cdot, x_0) = (\widehat{u}_{\alpha,0}(\lambda, x_0), \widehat{u}_{\alpha,1}(\lambda, x_0))^\top, \end{cases} \\ \widehat{u}_{\alpha,0}(\lambda, x_0) &= \int_{\mathbb{R}} dx \theta_\alpha(\lambda, x, x_0)^* u(x), \\ \widehat{u}_{\alpha,1}(\lambda, x_0) &= \int_{\mathbb{R}} dx \phi_\alpha(\lambda, x, x_0)^* u(x). \end{aligned}$$

Taking $f = g$, $F = 1$, $\lambda_1 \downarrow -\infty$, and $\lambda_2 \uparrow \infty$ in (4.26) then shows that $\widetilde{U}_\alpha(x_0)$ is a densely defined isometry in $L^2(\mathbb{R}; dx; \mathcal{H})$, which extends by continuity to an isometry on $L^2(\mathbb{R}; dx; \mathcal{H})$. The latter is denoted by $U_\alpha(x_0)$ and given by

$$(4.30) \quad \begin{aligned} U_\alpha(x_0) &: \begin{cases} L^2(\mathbb{R}; dx; \mathcal{H}) \rightarrow L^2(\mathbb{R}; d\Omega_\alpha(\cdot, x_0); \mathcal{H}^2) \\ u \mapsto \widehat{u}_\alpha(\cdot, x_0) = (\widehat{u}_{\alpha,0}(\cdot, x_0), \widehat{u}_{\alpha,1}(\cdot, x_0))^\top, \end{cases} \\ \widehat{u}_\alpha(\cdot, x_0) &= \begin{pmatrix} \widehat{u}_{\alpha,0}(\cdot, x_0) \\ \widehat{u}_{\alpha,1}(\cdot, x_0) \end{pmatrix} = \text{s-lim}_{a \downarrow -\infty, b \uparrow \infty} \begin{pmatrix} \int_a^b dx \theta_\alpha(\cdot, x, x_0)^* u(x) \\ \int_a^b dx \phi_\alpha(\cdot, x, x_0)^* u(x) \end{pmatrix}, \end{aligned}$$

where s-lim refers to the $L^2(\mathbb{R}; d\Omega_\alpha(\cdot, x_0); \mathcal{H}^2)$ -limit.

In addition, one can show that the map $U_\alpha(x_0)$ in (4.30) is onto and hence that $U_\alpha(x_0)$ is unitary with

$$(4.31) \quad U_\alpha(x_0)^{-1} : \begin{cases} L^2(\mathbb{R}; d\Omega_\alpha(\cdot, x_0); \mathcal{H}^2) \rightarrow L^2(\mathbb{R}; dx; \mathcal{H}) \\ \widehat{u} \mapsto u_\alpha, \end{cases}$$

$$u_\alpha(\cdot) = \text{s-lim}_{\mu_1 \downarrow -\infty, \mu_2 \uparrow \infty} \int_{\mu_1}^{\mu_2} (\theta_\alpha(\lambda, \cdot, x_0), \phi_\alpha(\lambda, \cdot, x_0)) d\Omega_\alpha(\lambda, x_0) \widehat{u}(\lambda).$$

Here s-lim refers to the $L^2(\mathbb{R}; dx; \mathcal{H})$ -limit.

Again, these considerations lead to a variant of the spectral theorem for H :

Theorem 4.3. *Let $F \in C(\mathbb{R})$ and $x_0 \in \mathbb{R}$. Then,*

$$(4.32) \quad U_\alpha(x_0)F(H)U_\alpha(x_0)^{-1} = M_F$$

in $L^2(\mathbb{R}; d\Omega_\alpha(\cdot, x_0); \mathcal{H}^2)$ (cf. (4.28)). Moreover,

$$(4.33) \quad \sigma(F(H)) = \text{ess.ran}_{\Omega_\alpha}(F),$$

$$(4.34) \quad \sigma(H) = \text{supp}(d\Omega_\alpha(\cdot, x_0)),$$

and the multiplicity of the spectrum of H is at most equal to $2 \dim(\mathcal{H})$.

5 Some facts on deficiency subspaces and abstract Donoghue-type m -functions

Throughout this preparatory section we make the following assumptions.

Hypothesis 5.1. Let \mathcal{K} be a separable, complex Hilbert space, and \dot{A} a densely defined, closed, symmetric operator in \mathcal{K} , with equal deficiency indices (k, k) , $k \in \mathbb{N} \cup \{\infty\}$.

Self-adjoint extensions of \dot{A} in \mathcal{K} will be denoted by A (or by A_α , with α an appropriate operator parameter).

Given Hypothesis 5.1, we will study properties of deficiency spaces of \dot{A} , and introduce operator-valued Donoghue-type m -functions corresponding to A , closely following the treatment in [47]. These results will be applied to Schrödinger operators in the following section.

In the special case $k = 1$, detailed investigation of this type were undertaken by Donoghue [45]. The case $k \in \mathbb{N}$ was discussed in depth in [49] (we also refer to [59] for another comprehensive treatment of this subject). Here we treat the general situation $k \in \mathbb{N} \cup \{\infty\}$, utilizing results in [47], [48].

The deficiency subspaces \mathcal{N}_{z_0} of \dot{A} , $z_0 \in \mathbb{C} \setminus \mathbb{R}$, are given by

$$(5.1) \quad \mathcal{N}_{z_0} = \ker \left((\dot{A})^* - z_0 I_{\mathcal{K}} \right), \quad \dim(\mathcal{N}_{z_0}) = k,$$

and for any self-adjoint extension A of \dot{A} in \mathcal{K} , one has (see also [66, pp. 80–81])

$$(5.2) \quad (A - z_0 I_{\mathcal{K}})(A - z I_{\mathcal{K}})^{-1} \mathcal{N}_{z_0} = \mathcal{N}_z, \quad z, z_0 \in \mathbb{C} \setminus \mathbb{R}.$$

We also note the following result on deficiency spaces.

Lemma 5.2. *Assume Hypothesis 5.1. Suppose $z_0 \in \mathbb{C} \setminus \mathbb{R}$, $h \in \mathcal{K}$, and that A is a self-adjoint extension of \dot{A} . Assume that*

$$(5.3) \quad \text{for all } z \in \mathbb{C} \setminus \mathbb{R}, \quad h \perp \{ (A - z I_{\mathcal{K}})^{-1} \ker \left((\dot{A})^* - z_0 I_{\mathcal{K}} \right) \}.$$

Then,

$$(5.4) \quad \text{for all } z \in \mathbb{C} \setminus \mathbb{R}, \quad h \perp \ker \left((\dot{A})^* - z I_{\mathcal{K}} \right).$$

Proof. Let $f_{z_0} \in \ker \left((\dot{A})^* - z_0 I_{\mathcal{K}} \right)$, then $s\text{-}\lim_{z \rightarrow i\infty} (-z)(A - z I_{\mathcal{K}})^{-1} f_{z_0} = f_{z_0}$ and hence $h \perp f_{z_0}$, that is, $h \perp \ker \left((\dot{A})^* - z_0 I_{\mathcal{K}} \right)$. The latter fact together with (5.3) imply (5.4) due to (5.2). □

Next, given a self-adjoint extension A of \dot{A} in \mathcal{K} and a closed, linear subspace \mathcal{N} of \mathcal{K} , $\mathcal{N} \subseteq \mathcal{K}$, the Donoghue-type m -operator $M_{A,\mathcal{N}}^{Do}(z) \in \mathcal{B}(\mathcal{N})$ associated with the pair (A, \mathcal{N}) is defined by

$$(5.5) \quad \begin{aligned} M_{A,\mathcal{N}}^{Do}(z) &= P_{\mathcal{N}}(zA + I_{\mathcal{K}})(A - z I_{\mathcal{K}})^{-1} P_{\mathcal{N}}|_{\mathcal{N}} \\ &= z I_{\mathcal{N}} + (z^2 + 1) P_{\mathcal{N}}(A - z I_{\mathcal{K}})^{-1} P_{\mathcal{N}}|_{\mathcal{N}}, \quad z \in \mathbb{C} \setminus \mathbb{R}, \end{aligned}$$

with $I_{\mathcal{N}}$ the identity operator in \mathcal{N} and $P_{\mathcal{N}}$ the orthogonal projection in \mathcal{K} onto \mathcal{N} . In our principal Section 6, we will exclusively focus on the particular case $\mathcal{N} = \mathcal{N}_i = \ker \left((\dot{A})^* - i I_{\mathcal{K}} \right)$.

We turn to the Nevanlinna–Herglotz property of $M_{A,\mathcal{N}}^{Do}(\cdot)$ next:

Theorem 5.3. *Assume Hypothesis 5.1. Let A be a self-adjoint extension of \dot{A} with associated orthogonal family of spectral projections $\{E_A(\lambda)\}_{\lambda \in \mathbb{R}}$, and \mathcal{N} a closed subspace of \mathcal{K} . Then the Donoghue-type m -operator $M_{A,\mathcal{N}}^{Do}(z)$ is analytic for $z \in \mathbb{C} \setminus \mathbb{R}$ and*

$$(5.6) \quad [\text{Im}(z)]^{-1} \text{Im} \left(M_{A,\mathcal{N}}^{Do}(z) \right) \geq 2 \left[(|z|^2 + 1) + \left[(|z|^2 - 1)^2 + 4(\text{Re}(z))^2 \right]^{1/2} \right]^{-1} I_{\mathcal{N}}, \quad z \in \mathbb{C} \setminus \mathbb{R}.$$

In particular,

$$(5.7) \quad [\operatorname{Im} (M_{A,\mathcal{N}}^{Do}(z))]^{-1} \in \mathcal{B}(\mathcal{N}), \quad z \in \mathbb{C} \setminus \mathbb{R},$$

and $M_{A,\mathcal{N}}^{Do}(\cdot)$ is a $\mathcal{B}(\mathcal{N})$ -valued Nevanlinna–Herglotz function that admits the following representation valid in the strong operator topology of \mathcal{N} ,

$$(5.8) \quad M_{A,\mathcal{N}}^{Do}(z) = \int_{\mathbb{R}} d\Omega_{A,\mathcal{N}}^{Do}(\lambda) \left[\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2 + 1} \right], \quad z \in \mathbb{C} \setminus \mathbb{R},$$

where (see also (A.9)–(A.11))

$$(5.9) \quad \Omega_{A,\mathcal{N}}^{Do}(\lambda) = (\lambda^2 + 1)(P_{\mathcal{N}}E_A(\lambda)P_{\mathcal{N}}|_{\mathcal{N}}),$$

$$(5.10) \quad \int_{\mathbb{R}} d\Omega_{A,\mathcal{N}}^{Do}(\lambda) (1 + \lambda^2)^{-1} = I_{\mathcal{N}},$$

$$(5.11) \quad \int_{\mathbb{R}} d(\xi, \Omega_{A,\mathcal{N}}^{Do}(\lambda)\xi)_{\mathcal{N}} = \infty \text{ for all } \xi \in \mathcal{N} \setminus \{0\}.$$

We just note that inequality (5.6) follows from

$$(5.12) \quad [\operatorname{Im}(z)]^{-1} \operatorname{Im}(M_{A,\mathcal{N}}^{Do}(z)) = P_{\mathcal{N}}(I_{\mathcal{K}} + A^2)^{1/2} ((A - \operatorname{Re}(z)I_{\mathcal{K}})^2 + (\operatorname{Im}(z))^2 I_{\mathcal{K}})^{-1} \\ \times (I_{\mathcal{K}} + A^2)^{1/2} P_{\mathcal{N}}|_{\mathcal{N}}, \quad z \in \mathbb{C} \setminus \mathbb{R},$$

the spectral theorem applied to

$$(I_{\mathcal{K}} + A^2)^{1/2} ((A - \operatorname{Re}(z)I_{\mathcal{K}})^2 + (\operatorname{Im}(z))^2 I_{\mathcal{K}})^{-1} (I_{\mathcal{K}} + A^2)^{1/2},$$

together with

$$(5.13) \quad \inf_{\lambda \in \mathbb{R}} \left(\frac{\lambda^2 + 1}{(\lambda - \operatorname{Re}(z))^2 + (\operatorname{Im}(z))^2} \right) = \inf_{\lambda \in \mathbb{R}} \left(\left| \frac{\lambda - i}{\lambda - z} \right|^2 \right) \\ = \frac{2}{(|z|^2 + 1) + \left[(|z|^2 - 1)^2 + 4(\operatorname{Re}(z))^2 \right]^{1/2}}, \quad z \in \mathbb{C} \setminus \mathbb{R}.$$

Since

$$(5.14) \quad \left[(|z|^2 + 1) + \left[(|z|^2 - 1)^2 + 4(\operatorname{Re}(z))^2 \right]^{1/2} \right] / 2 \\ \leq \left[(|z|^2 + 1) + (|z|^2 - 1) + 2|\operatorname{Re}(z)| \right] / 2 \\ = \max(1, |z|^2) + |\operatorname{Re}(z)|, \quad z \in \mathbb{C} \setminus \mathbb{R},$$

the lower bound (5.6) improves the one for $[\operatorname{Im}(z)]^{-1} \operatorname{Im} (M_{A,\mathcal{N}}^{Do}(z))$ recorded in [47] and [48] if $\operatorname{Re}(z) \neq 0^1$.

¹We note that [47] and [48] contain a typographical error in this context in the sense that $\operatorname{Im}(z)$ must be replaced by $[\operatorname{Im}(z)]^{-1}$ in (4.16) of [47] and (40) of [48].

Operators of the type $M_{A, \mathcal{N}}^{Do}(\cdot)$ and some of its variants have attracted considerable attention in the literature. They appear to go back to Krein [65] (see also [67]), Saakjan [98], and independently, Donoghue [45]. There appears to have been no connection between Donoghue and M. Krein’s school in this context. The interested reader can find a variety of additional results, for instance, in [7], [9], [13], [14]–[16], [24]–[29], [35]–[41], [47]–[49], [60], [68], [69], [70], [72], [73], [76], [77], [78], [81], [90], [93], [94], [97], and the references therein. We also add that a model operator approach for the pair (\dot{A}, A) on the basis of the operator-valued measure $\Omega_{A, \mathcal{N}_i}$ has been developed in detail in [47].

In addition, we mention the following well-known fact (cf., e.g., [47, Lemma 4.5], [66, pp. 80–81]):

Lemma 5.4. *Assume Hypothesis 5.1. Then \mathcal{K} decomposes into the direct orthogonal sum*

$$(5.15) \quad \mathcal{K} = \mathcal{K}_0 \oplus \mathcal{K}_0^\perp, \quad \ker((\dot{A})^* - zI_{\mathcal{K}}) \subset \mathcal{K}_0, \quad z \in \mathbb{C} \setminus \mathbb{R},$$

$$(5.16) \quad \mathcal{K}_0^\perp = \bigcap_{z \in \mathbb{C} \setminus \mathbb{R}} \ker((\dot{A})^* - zI_{\mathcal{K}})^\perp = \bigcap_{z \in \mathbb{C} \setminus \mathbb{R}} \text{ran}(\dot{A} - zI_{\mathcal{K}}),$$

where \mathcal{K}_0 and \mathcal{K}_0^\perp are invariant subspaces for all self-adjoint extensions A of \dot{A} in \mathcal{K} , that is,

$$(5.17) \quad (A - zI_{\mathcal{K}})^{-1}\mathcal{K}_0 \subseteq \mathcal{K}_0, \quad (A - zI_{\mathcal{K}})^{-1}\mathcal{K}_0^\perp \subseteq \mathcal{K}_0^\perp, \quad z \in \mathbb{C} \setminus \mathbb{R}.$$

In addition,

$$(5.18) \quad \mathcal{K}_0 = \overline{\text{lin. span}\{(A - zI_{\mathcal{K}})^{-1}u_+ \mid u_+ \in \mathcal{N}_i, z \in \mathbb{C} \setminus \mathbb{R}\}}.$$

Moreover, all self-adjoint extensions of \dot{A} coincide on \mathcal{K}_0^\perp , that is, if A_α denotes an arbitrary self-adjoint extension of \dot{A} , then

$$(5.19) \quad A_\alpha = A_{0,\alpha} \oplus A_0^\perp \text{ in } \mathcal{K} = \mathcal{K}_0 \oplus \mathcal{K}_0^\perp,$$

where

$$(5.20) \quad A_0^\perp \text{ is independent of the chosen } A_\alpha,$$

and $A_{0,\alpha}$ (resp., A_0^\perp) is self-adjoint in \mathcal{K}_0 (resp., \mathcal{K}_0^\perp).

In this context we note that a densely defined closed symmetric operator \dot{A} with deficiency indices (k, k) , $k \in \mathbb{N} \cup \{\infty\}$ is called *completely non-self-adjoint* (equivalently, *simple* or *prime*) in \mathcal{K} if $\mathcal{K}_0^\perp = \{0\}$ in the decomposition (5.15) (cf. [66, pp. 80–81]).

Remark 5.5. In addition to Hypothesis 5.1 assume that \dot{A} is not completely non-self-adjoint in \mathcal{K} . Then in addition to (5.15), (5.19), and (5.20) one obtains

$$(5.21) \quad \dot{A} = \dot{A}_0 \oplus A_0^\perp, \quad \mathcal{N}_i = \mathcal{N}_{0,i} \oplus \{0\}$$

with respect to the decomposition $\mathcal{K} = \mathcal{K}_0 \oplus \mathcal{K}_0^\perp$. In particular, the part A_0^\perp of \dot{A} in \mathcal{K}_0^\perp is self-adjoint. Thus, if $A = A_0 \oplus A_0^\perp$ is a self-adjoint extension of \dot{A} in \mathcal{K} , then

$$(5.22) \quad M_{A, \mathcal{N}_i}^{Do}(z) = M_{A_0, \mathcal{N}_{0,i}}^{Do}(z), \quad z \in \mathbb{C} \setminus \mathbb{R}.$$

This reduces the A -dependent spectral properties of the Donoghue-type operator $M_{A, \mathcal{N}_i}^{Do}(\cdot)$ effectively to those of A_0 . A different manner in which to express this fact would be to note that the subspace \mathcal{K}_0^\perp is “not detectable” by $M_{A, \mathcal{N}_i}^{Do}(\cdot)$ (we refer to [27]) for a systematic investigation of this circle of ideas, particularly, in the context of non-self-adjoint operators).

We are particularly interested in the question under which conditions on \dot{A} , the spectral information for A contained in its family of spectral projections $\{E_A(\lambda)\}_{\lambda \in \mathbb{R}}$ is already encoded in the $\mathcal{B}(\mathcal{N}_i)$ -valued measure $\Omega_{A, \mathcal{N}_i}^{Do}(\cdot)$. In this connection we now mention the following result, denoting by $C_b(\mathbb{R})$ the space of scalar-valued bounded continuous functions on \mathbb{R} :

Theorem 5.6. *Let A be a self-adjoint operator on a separable Hilbert space \mathcal{K} and $\{E_A(\lambda)\}_{\lambda \in \mathbb{R}}$ the family of spectral projections associated with A . Suppose that $\mathcal{N} \subset \mathcal{K}$ is a closed linear subspace such that*

$$(5.23) \quad \overline{\text{lin. span} \{g(A)v \mid g \in C_b(\mathbb{R}), v \in \mathcal{N}\}} = \mathcal{K}.$$

Let $P_{\mathcal{N}}$ be the orthogonal projection in \mathcal{K} onto \mathcal{N} . Then A is unitarily equivalent to the operator of multiplication by the independent variable λ in the space $L^2(\mathbb{R}; d\Sigma_A(\lambda); \mathcal{N})$. Here the operator-valued measure $d\Sigma_A(\cdot)$ is given in terms of the Lebesgue–Stieltjes measure defined by the nondecreasing uniformly bounded family $\Sigma_A(\cdot) = P_{\mathcal{N}}E_A(\cdot)P_{\mathcal{N}}|_{\mathcal{N}}$.

Proof. It suffices to construct a unitary transformation

$$U : \mathcal{K} \rightarrow L^2(\mathbb{R}; d\Sigma_A(\lambda); \mathcal{N})$$

that satisfies $UAu = \lambda Uu$ for all $u \in \mathcal{K}$. First, define U on the set of vectors $\mathcal{S} = \{g(A)v \mid g \in C_b(\mathbb{R}), v \in \mathcal{N}\} \subset \mathcal{K}$ by

$$(5.24) \quad U[g(A)v] = g(\lambda)v, \quad g \in C_b(\mathbb{R}), v \in \mathcal{N},$$

and then extend U by linearity to the span of these vectors, which by assumption is a dense subset of \mathcal{K} . Applying the above definition to the function $\lambda g(\lambda)$ yields $UAu = \lambda Uu$ for all u in \mathcal{S} and hence by linearity also for all u in the dense subset $\text{lin. span}(\mathcal{S})$. In addition, the following simple computation utilizing the spectral theorem for the self-adjoint operator A shows that U is an isometry on \mathcal{S} and hence by linearity also on $\text{lin. span}(\mathcal{S})$,

$$\begin{aligned}
 (f(A)u, g(A)v)_{\mathcal{K}} &= (u, f(A)^*g(A)v)_{\mathcal{K}} = (u, P_{\mathcal{N}}f(A)^*g(A)P_{\mathcal{N}}|_{\mathcal{N}}v)_{\mathcal{N}} \\
 (5.25) \qquad &= \int_{\mathbb{R}} (u, \overline{f(\lambda)}g(\lambda)d\Sigma_A(\lambda)v)_{\mathcal{N}} \\
 &= (f(\cdot)u, g(\cdot)v)_{L^2(\mathbb{R}; d\Sigma_A(\lambda); \mathcal{N})}, \quad f, g \in C_b(\mathbb{R}), \quad u, v \in \mathcal{N}.
 \end{aligned}$$

Thus, U can be extended by continuity to the whole Hilbert space \mathcal{K} . Since the range of U contains the set $\{g(\cdot)v \mid g \in C_b(\mathbb{R}), v \in \mathcal{N}\}$ which is dense in $L^2(\mathbb{R}; d\Sigma_A(\lambda); \mathcal{N})$ (cf. [52, Appendix B]), it follows that U is a unitary transformation. □

Remark 5.7. Since $\{(\lambda - z)^{-1} \mid z \in \mathbb{C} \setminus \mathbb{R}\} \subset C_b(\mathbb{R})$, the condition (5.23) in Theorem 5.6 can be replaced by the following stronger, and frequently encountered, one,

$$(5.26) \qquad \overline{\text{lin. span}\{(A - zI_{\mathcal{K}})^{-1}v \mid z \in \mathbb{C} \setminus \mathbb{R}, v \in \mathcal{N}\}} = \mathcal{K}.$$

Combining Lemma 5.4, Remark 5.5, Theorem 5.6, and Remark 5.7 then yields the following fact:

Corollary 5.8. *Assume Hypothesis 5.1 and suppose that A is a self-adjoint extension of \dot{A} . Let $M_{A, \mathcal{N}_i}^{Do}(\cdot)$ be the Donoghue-type m -operator associated with the pair (A, \mathcal{N}_i) , with $\mathcal{N}_i = \ker((\dot{A})^* - iI_{\mathcal{K}})$, and denote by $\Omega_{A, \mathcal{N}_i}^{Do}(\cdot)$ the $\mathcal{B}(\mathcal{N}_i)$ -valued measure in the Nevanlinna–Herglotz representation of $M_{A, \mathcal{N}_i}^{Do}(\cdot)$ (cf. (5.8)). Then A is unitarily equivalent to the operator of multiplication by the independent variable λ in the space $L^2(\mathbb{R}; (\lambda^2 + 1)^{-1}d\Omega_{A, \mathcal{N}_i}^{Do}(\lambda); \mathcal{N}_i)$, with $\Omega_{A, \mathcal{N}_i}^{Do}(\lambda) = (\lambda^2 + 1)P_{\mathcal{N}_i}E_A(\lambda)P_{\mathcal{N}_i}|_{\mathcal{N}_i}$, $\lambda \in \mathbb{R}$, if and only if \dot{A} is completely non-self-adjoint in \mathcal{K} .*

Proof. If \dot{A} is completely non-self-adjoint in \mathcal{K} , then $\mathcal{K}_0 = \mathcal{K}$, $\mathcal{K}_0^\perp = \{0\}$ in (5.15), together with (5.18), and (5.26) with $\mathcal{N} = \mathcal{N}_i$ yields

$$\Sigma_A(\lambda) = (\lambda^2 + 1)P_{\mathcal{N}_i}E_A(\lambda)P_{\mathcal{N}_i}|_{\mathcal{N}_i} = \Omega_{A, \mathcal{N}_i}^{Do}(\lambda), \quad \lambda \in \mathbb{R},$$

in Theorem 5.6. Conversely, if \dot{A} is not completely non-self-adjoint in \mathcal{K} , then the fact (5.22) shows that $\Omega_{A, \mathcal{N}_i}^{D_o}(\cdot)$ cannot describe the nontrivial self-adjoint operator A_0^\perp in $\mathcal{K}_0^\perp \supsetneq \{0\}$. □

In other words, \dot{A} is completely non-self-adjoint in \mathcal{K} , if and only if the entire spectral information on A contained in its family of spectral projections $E_A(\cdot)$, is already encoded in the $\mathcal{B}(\mathcal{N}_i)$ -valued measure $\Omega_{A, \mathcal{N}_i}^{D_o}(\cdot)$ (including multiplicity properties of the spectrum of A).

6 Donoghue-type m -functions for Schrödinger operators with operator-valued potentials and their connections to Weyl–Titchmarsh m -functions

In our principal section we construct Donoghue-type m -functions for half-line and full-line Schrödinger operators with operator-valued potentials and establish their precise connection with the Weyl–Titchmarsh m -functions discussed in Sections 3 and 4.

To avoid overly lengthy expressions involving resolvent operators, we now simplify our notation a bit and use the symbol I to denote the identity operator in $L^2((x_0, \pm\infty); dx; \mathcal{H})$ and $L^2(\mathbb{R}; dx; \mathcal{H})$.

The principal hypothesis for this section will be the following:

- Hypothesis 6.1.** (i) For half-line Schrödinger operators on $[x_0, \infty)$ we assume Hypothesis 2.6 with $a = x_0$, $b = \infty$ and $\tau = -(d^2/dx^2)I_{\mathcal{H}} + V(x)$ to be in the limit-point case at ∞ .
- (ii) For half-line Schrödinger operators on $(-\infty, x_0]$ we assume Hypothesis 2.6 with $a = -\infty$, $b = x_0$ and $\tau = -(d^2/dx^2)I_{\mathcal{H}} + V(x)$ to be in the limit-point case at $-\infty$.
- (iii) For Schrödinger operators on \mathbb{R} we assume Hypothesis 4.1.

6.1 The half-line case. We start with half-line Schrödinger operators $H_{\pm, \min}$ in $L^2((x_0, \pm\infty); dx; \mathcal{H})$ and note that for $\{e_j\}_{j \in \mathcal{J}}$ a given orthonormal basis in \mathcal{H} ($\mathcal{J} \subseteq \mathbb{N}$ an appropriate index set), and $z \in \mathbb{C} \setminus \mathbb{R}$,

$$(6.1) \quad \{ \psi_{\pm, \alpha}(z, \cdot, x_0) e_j \}_{j \in \mathcal{J}}$$

is a basis in the deficiency subspace

$$\mathcal{N}_{\pm, z} = \ker (H_{\pm, \min}^* - zI).$$

In particular, given $f \in L^2((x_0, \pm\infty); dx; \mathcal{H})$, one has

$$(6.2) \quad f \perp \{ \psi_{\pm, \alpha}(z, \cdot, x_0)e_j \}_{j \in \mathcal{J}},$$

if and only if

$$(6.3) \quad \begin{aligned} 0 &= (\psi_{\pm, \alpha}(z, \cdot, x_0)e_j, f)_{L^2((x_0, \pm\infty); dx; \mathcal{H})} \\ &= \pm \int_{x_0}^{\pm\infty} dx (\psi_{+, \alpha}(z, x, x_0)e_j, f(x))_{\mathcal{H}} \\ &= \pm \int_{x_0}^{\pm\infty} dx (e_j, \psi_{\pm, \alpha}(z, x, x_0)^* f(x))_{\mathcal{H}}, \quad j \in \mathcal{J}, \end{aligned}$$

and since $j \in \mathcal{J}$ is arbitrary,

$$(6.4) \quad \begin{aligned} f \perp \{ \psi_{\pm, \alpha}(z, \cdot, x_0)e_j \}_{j \in \mathcal{J}} \text{ if and only if} \\ \pm \int_{x_0}^{\pm\infty} dx (h, \psi_{\pm, \alpha}(z, x, x_0)^* f(x))_{\mathcal{H}} = 0, \quad h \in \mathcal{H}, \end{aligned}$$

a fact to be exploited below in (6.5).

Next, we prove the following generating property of deficiency spaces of $H_{\pm, \min}$:

Theorem 6.2. *Assume Hypothesis 6.1 (i), respectively, (ii), and suppose that $f \in L^2((x_0, \pm\infty); dx; \mathcal{H})$ satisfies for all $z \in \mathbb{C} \setminus \mathbb{R}$, $f \perp \ker (H_{\pm, \min}^* - zI)$. Then $f = 0$. Equivalently, $H_{\pm, \min}$ are completely non-self-adjoint in $L^2((x_0, \pm\infty); dx; \mathcal{H})$.*

Proof. We focus on the right-half line $[x_0, \infty)$ and recall the $\mathcal{B}(\mathcal{H})$ -valued Green’s function $G_{+, \alpha}(z, \cdot, \cdot)$ in (3.16) of a self-adjoint extension $H_{+, \alpha}$ of $H_{+, \min}$.

Choosing a test vector $\eta \in C_0^\infty((x_0, \infty); \mathcal{H})$, $\lambda_j \in \mathbb{R}$, $j = 1, 2$, $\lambda_1 < \lambda_2$, one computes with the help of Stone’s formula (cf. Lemma 3.5),

$$\begin{aligned}
 & (\eta, E_{H_{+, \alpha}}((\lambda_1, \lambda_2]))f)_{L^2((x_0, \infty); dx; \mathcal{H})} \\
 &= \lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} \frac{1}{2\pi i} \int_{\lambda_1 + \delta}^{\lambda_2 + \delta} d\lambda \left[(\eta, (H_{+, \alpha} - (\lambda + i\varepsilon)I)^{-1}f)_{L^2((x_0, \infty); dx; \mathcal{H})} \right. \\
 &\quad \left. - (\eta, (H_{+, \alpha} - (\lambda - i\varepsilon)I)^{-1}f)_{L^2((x_0, \infty); dx; \mathcal{H})} \right] \\
 &= \lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} \frac{1}{2\pi i} \int_{\lambda_1 + \delta}^{\lambda_2 + \delta} d\lambda \int_{x_0}^{\infty} dx \\
 &\quad \times \left\{ \left[\left(\eta(x), \psi_{+, \alpha}(\lambda + i\varepsilon, x, x_0) \int_{x_0}^x dx' \phi_{\alpha}(\lambda - i\varepsilon, x', x_0)^* f(x') \right)_{\mathcal{H}} \right. \right. \\
 (6.5) \quad &\quad \left. \left. + \underbrace{\int_{x_0}^{\infty} dx' (\phi_{\alpha}(\lambda + i\varepsilon, x, x_0)^* \eta(x), \psi_{+, \alpha}(\lambda - i\varepsilon, x', x_0)^* f(x'))_{\mathcal{H}}}_{=0 \text{ by (6.4)}} \right. \right. \\
 &\quad \left. \left. - \left(\eta(x), \phi_{\alpha}(\lambda + i\varepsilon, x, x_0) \int_{x_0}^x dx' \psi_{+, \alpha}(\lambda - i\varepsilon, x', x_0)^* f(x') \right)_{\mathcal{H}} \right] \right. \\
 &\quad \left. - \left[\left(\eta(x), \psi_{+, \alpha}(\lambda - i\varepsilon, x, x_0) \int_{x_0}^x dx' \phi_{\alpha}(\lambda + i\varepsilon, x', x_0)^* f(x') \right)_{\mathcal{H}} \right. \right. \\
 &\quad \left. \left. + \underbrace{\int_{x_0}^{\infty} dx' (\phi_{\alpha}(\lambda - i\varepsilon, x, x_0)^* \eta(x), \psi_{+, \alpha}(\lambda + i\varepsilon, x', x_0)^* f(x'))_{\mathcal{H}}}_{=0 \text{ by (6.4)}} \right. \right. \\
 &\quad \left. \left. - \left(\eta(x), \phi_{\alpha}(\lambda - i\varepsilon, x, x_0) \int_{x_0}^x dx' \psi_{+, \alpha}(\lambda + i\varepsilon, x', x_0)^* f(x') \right)_{\mathcal{H}} \right] \right\}.
 \end{aligned}$$

Here we twice employed the orthogonality condition (6.4) in the terms with underbraces.

Thus, one finally concludes,

$$\begin{aligned}
 & (\eta, E_{H_{+, \alpha}}((\lambda_1, \lambda_2]))f)_{L^2((x_0, \infty); dx; \mathcal{H})} = \lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} \frac{1}{2\pi i} \int_{\lambda_1 + \delta}^{\lambda_2 + \delta} d\lambda \int_{x_0}^{\infty} dx \int_{x_0}^x dx' \\
 &\quad \times \left[(\eta(x), [\theta_{\alpha}(\lambda + i\varepsilon, x, x_0)\phi_{\alpha}(\lambda - i\varepsilon, x', x_0)^* \right. \\
 (6.6) \quad &\quad \left. - \phi_{\alpha}(\lambda + i\varepsilon, x, x_0)\theta_{\alpha}(\lambda - i\varepsilon, x, x_0)^*]f(x'))_{\mathcal{H}} \right. \\
 &\quad \left. - (\eta(x), [\theta_{\alpha}(\lambda - i\varepsilon, x, x_0)\phi_{\alpha}(\lambda + i\varepsilon, x', x_0)^* \right. \\
 &\quad \left. - \phi_{\alpha}(\lambda - i\varepsilon, x, x_0)\theta_{\alpha}(\lambda + i\varepsilon, x, x_0)^*]f(x'))_{\mathcal{H}} \right] \\
 &\quad = 0.
 \end{aligned}$$

Here we used the fact that η has compact support, rendering all x -integrals over the bounded set $\text{supp}(\eta)$. In addition, we employed the property that for fixed $x \in [x_0, \infty)$, $\phi_{\alpha}(z, x, x_0)$ and $\theta_{\alpha}(z, x, x_0)$ are entire with respect to $z \in \mathbb{C}$, permitting freely the interchange of the ε limit with all integrals and implying the vanishing of the limit $\varepsilon \downarrow 0$ in the last step in (6.6).

Since $\eta \in C_0^\infty((x_0, \infty); \mathcal{H})$ and $\lambda_1, \lambda_2 \in \mathbb{R}$ were arbitrary, (6.6) proves $f = 0$.

The fact that $H_{\pm, \min}$ are completely non-self-adjoint in $L^2((x_0, \pm\infty); dx; \mathcal{H})$ now follows from (5.16). □

We note that Theorem 6.2 in the context of regular (and quasi-regular) half-line differential operators with scalar coefficients has been established by Gilbert [53, Theorem 3]. The corresponding result for $2n \times 2n$ Hamiltonian systems, $n \in \mathbb{N}$, was established in [42, Proposition 7.4], and the case of indefinite Sturm–Liouville operators in the associated Krein space has been treated in [17, Proposition 4.8]. While these proofs exhibit certain similarities with that of Theorem 6.2, it appears that our approach in the case of a regular half-line Schrödinger operator with $\mathcal{B}(\mathcal{H})$ -valued potential is a canonical one.

For future purpose we recall formulas (4.10)–(4.14), and now add some additional results:

Lemma 6.3. *Assume Hypothesis 6.1 (i), respectively, (ii), and let $z \in \mathbb{C} \setminus \mathbb{R}$. Then, for all $h \in \mathcal{H}$, and $\rho_{+, \alpha}(\cdot, x_0)$ -a.e. $\lambda \in \sigma(H_{\pm, \alpha})$,*

$$(6.7) \quad \pm \operatorname{s-lim}_{R \rightarrow \infty} \int_{x_0}^{\pm R} dx \phi_\alpha(\lambda, x, x_0)^* \psi_{\pm, \alpha}(z, x, x_0) h = \pm(\lambda - z)^{-1} h,$$

$$(6.8) \quad \pm \operatorname{s-lim}_{R \rightarrow \infty} \int_{x_0}^{\pm R} dx \theta_\alpha(\lambda, x, x_0)^* \psi_{\pm, \alpha}(z, x, x_0) h = \mp(\lambda - z)^{-1} m_{\pm, \alpha}(z, x_0) h,$$

where s-lim refers to the $L^2(\mathbb{R}; d\rho_{+, \alpha}(\cdot, x_0); \mathcal{H})$ -limit.

Proof. Without loss of generality, we consider the case of $H_{+, \alpha}$ only. Let $u \in C_0^\infty((x_0, \infty); \mathcal{H}) \subset L^2((x_0, \infty); dx; \mathcal{H})$ and $v = (H_{+, \alpha} - zI)^{-1}u$, then by Theorem 3.4, (3.33), and (3.34),

$$(6.9) \quad \begin{aligned} u &= (H_{+, \alpha} - zI)v = \operatorname{s-lim}_{\mu_2 \uparrow \infty, \mu_1 \downarrow -\infty} \int_{\mu_1}^{\mu_2} \phi_\alpha(\lambda, \cdot, x_0) d\rho_{+, \alpha}(\lambda, x_0) \widehat{u}_{+, \alpha}(\lambda) \\ &= \operatorname{s-lim}_{\mu_2 \uparrow \infty, \mu_1 \downarrow -\infty} \int_{\mu_1}^{\mu_2} (\lambda - z)\phi_\alpha(\lambda, \cdot, x_0) d\rho_{+, \alpha}(\lambda, x_0) \widehat{v}_{+, \alpha}(\lambda), \end{aligned}$$

that is,

$$(6.10) \quad \widehat{v}_{+, \alpha}(\lambda) = (\lambda - z)^{-1} \widehat{u}_{+, \alpha}(\lambda) \text{ for } \rho_{+, \alpha}(\cdot, x_0)\text{-a.e. } \lambda \in \sigma(H_{+, \alpha}).$$

Hence,

$$(6.11) \quad \begin{aligned} v &= (H_{+, \alpha} - zI)^{-1}u \\ &= \operatorname{s-lim}_{\mu_2 \uparrow \infty, \mu_1 \downarrow -\infty} \int_{\mu_1}^{\mu_2} \phi_\alpha(\lambda, \cdot, x_0) d\rho_{+, \alpha}(\lambda, x_0) \widehat{u}_{+, \alpha}(\lambda) (\lambda - z)^{-1} \\ &= \int_{x_0}^\infty dx' G_{+, \alpha}(z, \cdot, x') u(x'). \end{aligned}$$

Thus one computes, given unitarity of $U_{+, \alpha}$ (cf. (3.33), (3.34)),

(6.12)

$$\begin{aligned} (h, ((H_{+, \alpha} - zI)^{-1}u)(x))_{\mathcal{H}} &= \int_{x_0}^{\infty} dx' (h, G_{+, \alpha}(z, x, x')u(x'))_{\mathcal{H}} \\ &= \int_{x_0}^{\infty} dx' (G_{+, \alpha}(z, x, x')^*h, u(x'))_{\mathcal{H}} \\ &= \mathop{\text{s-lim}}_{\mu_2 \uparrow \infty, \mu_1 \downarrow -\infty} \int_{\mu_1}^{\mu_2} ((G_{+, \alpha}(\widehat{z}, x, \cdot)^*h)(\lambda), d\rho_{+, \alpha}(\lambda, x_0) \widehat{u}_{+, \alpha}(\lambda))_{\mathcal{H}} \\ &= \mathop{\text{s-lim}}_{\mu_2 \uparrow \infty, \mu_1 \downarrow -\infty} \int_{\mu_1}^{\mu_2} (h, \phi_{\alpha}(\lambda, x, x_0) d\rho_{+, \alpha}(\lambda, x_0) \widehat{u}_{+, \alpha}(\lambda))_{\mathcal{H}} (\lambda - z)^{-1} \\ &= \mathop{\text{s-lim}}_{\mu_2 \uparrow \infty, \mu_1 \downarrow -\infty} \int_{\mu_1}^{\mu_2} ((\lambda - \bar{z})^{-1} \phi_{\alpha}(\lambda, x, x_0)^*h, d\rho_{+, \alpha}(\lambda, x_0) \widehat{u}_{+, \alpha}(\lambda))_{\mathcal{H}}. \end{aligned}$$

Since $u \in C_0^{\infty}((x_0, \infty); \mathcal{H})$ was arbitrary, one concludes that

$$(6.13) \quad \begin{aligned} (G_{+, \alpha}(\widehat{z}, x, \cdot)^*h)(\lambda) &= (\lambda - \bar{z})^{-1} \phi_{\alpha}(\lambda, x, x_0)^*h, \quad h \in \mathcal{H}, z \in \mathbb{C} \setminus \mathbb{R}, \\ &\text{for } \rho_{+, \alpha}(\cdot, x_0)\text{-a.e. } \lambda \in \sigma(H_{+, \alpha}). \end{aligned}$$

In precisely the same manner one derives,

$$(6.14) \quad \begin{aligned} (\partial_x G_{+, \alpha}(\widehat{z}, x, \cdot)^*h)(\lambda) &= (\lambda - \bar{z})^{-1} \phi'_{\alpha}(\lambda, x, x_0)^*h, \quad h \in \mathcal{H}, z \in \mathbb{C} \setminus \mathbb{R}, \\ &\text{for } \rho_{+, \alpha}(\cdot, x_0)\text{-a.e. } \lambda \in \sigma(H_{+, \alpha}). \end{aligned}$$

Taking $x \downarrow x_0$ in (6.13) and (6.14), observing that

$$(6.15) \quad \begin{aligned} G_{+, \alpha}(z, x_0, x') &= \sin(\alpha) \psi_{+, \alpha}(\bar{z}, x', x_0), \\ [\partial_x G_{+, \alpha}(z, x, x')] \Big|_{x=x_0} &= \cos(\alpha) \psi_{+, \alpha}(\bar{z}, x', x_0), \end{aligned}$$

and choosing $h = \sin(\alpha)g$ in (6.13) and $h = \cos(\alpha)g$ in (6.14), $g \in \mathcal{H}$, then yields

$$(6.16) \quad (\psi_{+, \alpha}(\bar{z}, \cdot, x_0) [\widehat{\sin(\alpha)}]^2 g)(\lambda) = (\lambda - \bar{z})^{-1} [\sin(\alpha)]^2 g,$$

$$(6.17) \quad (\psi_{+, \alpha}(\bar{z}, \cdot, x_0) [\widehat{\cos(\alpha)}]^2 g)(\lambda) = (\lambda - \bar{z})^{-1} [\cos(\alpha)]^2 g, \\ g \in \mathcal{H}, z \in \mathbb{C} \setminus \mathbb{R}, \text{ for } \rho_{+, \alpha}(\cdot, x_0)\text{-a.e. } \lambda \in \sigma(H_{+, \alpha}).$$

Adding equations (6.16) and (6.17) yields relation (6.7).

Finally, changing α into $\alpha - (\pi/2)I_{\mathcal{H}}$, and noticing

$$(6.18) \quad \phi_{\alpha - (\pi/2)I_{\mathcal{H}}}(z, \cdot, x_0) = \theta_{\alpha}(z, \cdot, x_0), \quad \theta_{\alpha - (\pi/2)I_{\mathcal{H}}}(z, \cdot, x_0) = -\phi_{\alpha}(z, \cdot, x_0),$$

$$(6.19) \quad m_{+, \alpha - (\pi/2)I_{\mathcal{H}}}(z, x_0) = -[m_{+, \alpha}(z, x_0)]^{-1},$$

$$(6.20) \quad \psi_{+, \alpha - (\pi/2)I_{\mathcal{H}}}(z, \cdot, x_0) = -\psi_{+, \alpha}(z, \cdot, x_0)[m_{+, \alpha}(z, x_0)]^{-1},$$

yields

$$(6.21) \quad \int_{x_0}^{\infty} dx \theta_{\alpha}(\lambda, x, x_0)^* \psi_{\pm, \alpha}(z, x, x_0) \tilde{h} = \mp(\lambda - z)^{-1} m_{\pm, \alpha}(z, x_0) \tilde{h},$$

with $\tilde{h} = -[m_{+, \alpha}(z, x_0)]^{-1} h$, and hence (6.8) since $h \in \mathcal{H}$ was arbitrary. □

By Theorem 3.3

$$(6.22) \quad [\text{Im}(m_{\pm, \alpha}(z, x_0))]^{-1} \in \mathcal{B}(\mathcal{H}), \quad z \in \mathbb{C} \setminus \mathbb{R},$$

therefore,

$$(6.23) \quad \begin{aligned} & (\psi_{\pm, \alpha}(z, \cdot, x_0) [\pm \text{Im}(z)]^{-1} \text{Im}(m_{\pm, \alpha}(z, x_0))]^{-1/2} e_j, \psi_{\pm, \alpha}(z, \cdot, x_0) \\ & \quad \times [\pm \text{Im}(z)]^{-1} \text{Im}(m_{\pm, \alpha}(z, x_0))]^{-1/2} e_k)_{L^2((x_0, \pm\infty); dx; \mathcal{H})} \\ & = ([\pm \text{Im}(m_{\pm, \alpha}(z, x_0))]^{-1/2} e_j, \text{Im}(m_{\pm, \alpha}(z, x_0)) \\ & \quad \times [\pm \text{Im}(m_{\pm, \alpha}(z, x_0))]^{-1/2} e_k)_{\mathcal{H}} \\ & = (e_j, e_k)_{\mathcal{H}} = \delta_{j, k}, \quad j, k \in \mathcal{J}, \quad z \in \mathbb{C} \setminus \mathbb{R}. \end{aligned}$$

Thus, one obtains in addition to (6.1) that

$$(6.24) \quad \{ \Psi_{\pm, \alpha, j}(z, \cdot, x_0) = \psi_{\pm, \alpha}(z, \cdot, x_0) [\pm \text{Im}(z)]^{-1} \text{Im}(m_{\pm, \alpha}(z, x_0))]^{-1/2} e_j \}_{j \in \mathcal{J}}$$

is an orthonormal basis for $\mathcal{N}_{\pm, z} = \ker(H_{\pm, \min}^* - zI)$, $z \in \mathbb{C} \setminus \mathbb{R}$, and hence (cf. the definition of $P_{\mathcal{N}}$ in Section 5)

$$(6.25) \quad P_{\mathcal{N}_{\pm, i}} = \sum_{j \in \mathcal{J}} (\Psi_{\pm, \alpha, j}(i, \cdot, x_0), \cdot)_{L^2((x_0, \pm\infty); dx; \mathcal{H})} \Psi_{\pm, \alpha, j}(i, \cdot, x_0).$$

Consequently (cf. (5.5)), one obtains for the half-line Donoghue-type m -functions,

$$(6.26) \quad \begin{aligned} M_{H_{\pm, \alpha}, \mathcal{N}_{\pm, i}}^{Do}(z, x_0) &= \pm P_{\mathcal{N}_{\pm, i}}(zH_{\pm, \alpha} + I)(H_{\pm, \alpha} - zI)^{-1} P_{\mathcal{N}_{\pm, i}}|_{\mathcal{N}_{\pm, i}}, \\ &= \int_{\mathbb{R}} d\Omega_{H_{\pm, \alpha}, \mathcal{N}_{\pm, i}}^{Do}(\lambda, x_0) \left[\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2 + 1} \right], \quad z \in \mathbb{C} \setminus \mathbb{R}, \end{aligned}$$

where $\Omega_{H_{\pm, \alpha}, \mathcal{N}_{\pm, i}}^{Do}(\cdot, x_0)$ satisfies the analogues of (5.9)–(5.11) (resp., (A.9)–(A.11)).

Next, we explicitly compute $M_{H_{\pm, \alpha}, \mathcal{N}_{\pm, i}}^{Do}(\cdot, x_0)$.

Theorem 6.4. *Assume Hypothesis 6.1 (i), respectively, (ii). Then,*

$$(6.27) \quad \begin{aligned} M_{H_{\pm, \alpha}, \mathcal{N}_{\pm, i}}^{Do}(z, x_0) &= \pm \sum_{j, k \in \mathcal{J}} (e_j, m_{\pm, \alpha}^{Do}(z, x_0) e_k)_{\mathcal{H}} \\ &\quad \times (\Psi_{\pm, \alpha, k}(i, \cdot, x_0), \cdot)_{L^2((x_0, \pm\infty); dx; \mathcal{H})} \Psi_{\pm, \alpha, j}(i, \cdot, x_0)|_{\mathcal{N}_{\pm, i}}, \quad z \in \mathbb{C} \setminus \mathbb{R}, \end{aligned}$$

where the $\mathcal{B}(\mathcal{H})$ -valued Nevanlinna–Herglotz functions $m_{\pm,\alpha}^{Do}(\cdot, x_0)$ are given by

$$(6.28) \quad m_{\pm,\alpha}^{Do}(z, x_0) = \pm[\pm \operatorname{Im}(m_{\pm,\alpha}(i, x_0))]^{-1/2} [m_{\pm,\alpha}(z, x_0) - \operatorname{Re}(m_{\pm,\alpha}(i, x_0))] \\ \times [\pm \operatorname{Im}(m_{\pm,\alpha}(i, x_0))]^{-1/2}$$

$$(6.29) \quad = d_{\pm,\alpha} \pm \int_{\mathbb{R}} d\omega_{\pm,\alpha}^{Do}(\lambda, x_0) \left[\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2 + 1} \right], \quad z \in \mathbb{C} \setminus \mathbb{R}.$$

Here $d_{\pm,\alpha} = \operatorname{Re}(m_{\pm,\alpha}^{Do}(i, x_0)) \in \mathcal{B}(\mathcal{H})$, and

$$(6.30) \quad \omega_{\pm,\alpha}^{Do}(\cdot, x_0) = [\pm \operatorname{Im}(m_{\pm,\alpha}(i, x_0))]^{-1/2} \rho_{\pm,\alpha}(\cdot, x_0) [\pm \operatorname{Im}(m_{\pm,\alpha}(i, x_0))]^{-1/2}$$

satisfy the analogues of (A.10), (A.11).

Proof. We will consider the right half-line $[x_0, \infty)$. To verify (6.27) it suffices to insert (6.25) into (6.26) and then apply (3.28), (3.29) to compute,

$$(6.31) \quad (\Psi_{+, \alpha, j}(i, \cdot, x_0), (zH_{+, \alpha} + I)(H_{+, \alpha} - zI)^{-1} \Psi_{+, \alpha, k}(i, \cdot, x_0))_{L^2((x_0, \infty); dx; \mathcal{H})} \\ = (\widehat{e}_{j, +, \alpha}, (z \cdot + I_{\mathcal{H}})(\cdot - zI_{\mathcal{H}})^{-1} \widehat{e}_{k, +, \alpha})_{L^2(\mathbb{R}; d\rho_{+, \alpha}; \mathcal{H})} \\ = \int_{\mathbb{R}} d(\widehat{e}_{j, +, \alpha}, \rho_{+, \alpha}(\lambda, x_0) \widehat{e}_{k, +, \alpha})_{\mathcal{H}} \frac{z\lambda + 1}{\lambda - z}, \quad j, k \in \mathcal{J},$$

where

$$(6.32) \quad \widehat{e}_{j, +, \alpha}(\lambda) = \int_{x_0}^{\infty} dx \phi_{\alpha}(\lambda, x, x_0)^* \psi_{+, \alpha}(i, x, x_0) [\operatorname{Im}(m_{+, \alpha}(i, x_0))]^{-1/2} e_j \\ = (\lambda - i)^{-1} [\operatorname{Im}(m_{+, \alpha}(i, x_0))]^{-1/2} e_j, \quad j \in \mathcal{J},$$

employing (6.7) (with $z = i$). Thus,

$$(6.33) \quad = \int_{\mathbb{R}} d([\operatorname{Im}(m_{+, \alpha}(i, x_0))]^{-1/2} e_j, \rho_{+, \alpha}(\lambda, x_0) [\operatorname{Im}(m_{+, \alpha}(i, x_0))]^{-1/2} e_k)_{\mathcal{H}} \\ \times \frac{z\lambda + 1}{\lambda - z} \frac{1}{\lambda^2 + 1} \\ = \int_{\mathbb{R}} d([\operatorname{Im}(m_{+, \alpha}(i, x_0))]^{-1/2} e_j, \rho_{+, \alpha}(\lambda, x_0) [\operatorname{Im}(m_{+, \alpha}(i, x_0))]^{-1/2} e_k)_{\mathcal{H}} \\ \times \left[\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2 + 1} \right] \\ = ([\operatorname{Im}(m_{+, \alpha}(i, x_0))]^{-1/2} e_j, [m_{+, \alpha}(z, x_0) - \operatorname{Re}(m_{+, \alpha}(i, x_0))] \\ \times [\operatorname{Im}(m_{+, \alpha}(i, x_0))]^{-1/2} e_k)_{\mathcal{H}},$$

using (3.17), (3.18) in the final step. □

Remark 6.5. Combining Corollary 5.8 and Theorem 6.2 proves that the entire spectral information for $H_{\pm, \alpha}$, contained in the corresponding family of spectral projections $\{E_{H_{\pm, \alpha}}(\lambda)\}_{\lambda \in \mathbb{R}}$ in $L^2((x_0, \pm\infty); dx; \mathcal{H})$, is already encoded in the operator-valued measure $\{\Omega_{H_{\pm, \alpha}, \mathcal{N}_{\pm, i}}^{Do}(\lambda, x_0)\}_{\lambda \in \mathbb{R}}$ in $\mathcal{N}_{\pm, i}$ (including multiplicity properties of the spectrum of $H_{\pm, \alpha}$). By the same token, invoking Theorem 6.4 shows that the entire spectral information for $H_{\pm, \alpha}$ is already contained in $\{\omega_{\pm, \alpha}^{Do}(\lambda, x_0)\}_{\lambda \in \mathbb{R}}$ in \mathcal{H} .

6.2 The full-line case. In the remainder of this section we turn to Schrödinger operators on \mathbb{R} , assuming Hypothesis 4.1. Decomposing

$$(6.34) \quad L^2(\mathbb{R}; dx; \mathcal{H}) = L^2((-\infty, x_0); dx; \mathcal{H}) \oplus L^2((x_0, \infty); dx; \mathcal{H}),$$

and introducing the orthogonal projections P_{\pm, x_0} of $L^2(\mathbb{R}; dx; \mathcal{H})$ onto the left/right subspaces $L^2((x_0, \pm\infty); dx; \mathcal{H})$, we now define a particular minimal operator H_{\min} in $L^2(\mathbb{R}; dx; \mathcal{H})$ via

$$(6.35) \quad H_{\min} := H_{-, \min} \oplus H_{+, \min}, \quad H_{\min}^* = H_{-, \min}^* \oplus H_{+, \min}^*,$$

$$\mathcal{N}_z = \ker(H_{\min}^* - zI) = \ker(H_{-, \min}^* - zI) \oplus \ker(H_{+, \min}^* - zI)$$

$$(6.36) \quad = \mathcal{N}_{-, z} \oplus \mathcal{N}_{+, z}, \quad z \in \mathbb{C} \setminus \mathbb{R}.$$

We note that (6.35) is not the standard minimal operator associated with the differential expression τ on \mathbb{R} . Usually, one introduces

$$(6.37) \quad \widehat{H}_{\min} f = \tau f,$$

$$f \in \text{dom}(\widehat{H}_{\min}) = \{g \in L^2(\mathbb{R}; dx; \mathcal{H}) \mid g \in W_{\text{loc}}^{2,1}(\mathbb{R}; dx; \mathcal{H});$$

$$\text{supp}(g) \text{ compact}; \tau g \in L^2(\mathbb{R}; dx; \mathcal{H})\}.$$

However, due to our limit-point assumption at $\pm\infty$, \widehat{H}_{\min} is essentially self-adjoint and hence (cf. (4.3)),

$$(6.38) \quad \overline{\widehat{H}_{\min}} = H,$$

rendering \widehat{H}_{\min} unsuitable as a minimal operator with nonzero deficiency indices. Consequently, H given by (4.3), as well as the Dirichlet extension, $H_D = H_{-, D} \oplus H_{+, D}$, where $H_{\pm, D} = H_{\pm, 0}$ (i.e., $\alpha = 0$ in (3.9), see also our notational conventions following (3.16)), are particular self-adjoint extensions of H_{\min} in (6.35).

Associated with the operator H in $L^2(\mathbb{R}; dx; \mathcal{H})$ (cf. (4.3)) we now introduce its 2×2 block operator representation via

$$(6.39) \quad (H - zI)^{-1} = \begin{pmatrix} P_{-, x_0}(H - zI)^{-1}P_{-, x_0} & P_{-, x_0}(H - zI)^{-1}P_{+, x_0} \\ P_{+, x_0}(H - zI)^{-1}P_{-, x_0} & P_{+, x_0}(H - zI)^{-1}P_{+, x_0} \end{pmatrix}.$$

Hence (cf. (6.24)),

(6.40)

$$\begin{aligned} \{\widehat{\Psi}_{-,a,j}(z, \cdot, x_0) &= P_{-,x_0} \psi_{-,a}(z, \cdot, x_0) [-(\operatorname{Im}(z))^{-1} \operatorname{Im}(m_{-,a}(z, x_0))]^{-1/2} e_j, \\ \widehat{\Psi}_{+,a,j}(z, \cdot, x_0) &= P_{+,x_0} \psi_{+,a}(z, \cdot, x_0) [(\operatorname{Im}(z))^{-1} \operatorname{Im}(m_{+,a}(z, x_0))]^{-1/2} e_j\}_{j \in \mathcal{J}} \end{aligned}$$

is an orthonormal basis for $\mathcal{N}_z = \ker(H_{\min}^* - zI)$, $z \in \mathbb{C} \setminus \mathbb{R}$, if $\{e_j\}_{j \in \mathcal{J}}$ is an orthonormal basis for \mathcal{H} , and (cf. (6.25))

$$\begin{aligned} P_{\mathcal{N}_i} &= P_{\mathcal{N}_{-,i}} \oplus P_{\mathcal{N}_{+,i}} \\ &= \sum_{j \in \mathcal{J}} \left[(\psi_{-,a}(i, \cdot, x_0) [-\operatorname{Im}(m_{-,a}(i, x_0))]^{-1/2} e_j, \cdot)_{L^2((-\infty, x_0); dx; \mathcal{H})} \right. \\ &\quad \times \psi_{-,a}(i, \cdot, x_0) [-\operatorname{Im}(m_{-,a}(i, x_0))]^{-1/2} e_j \\ &\quad \oplus (\psi_{+,a}(i, \cdot, x_0) [\operatorname{Im}(m_{+,a}(i, x_0))]^{-1/2} e_j, \cdot)_{L^2((x_0, \infty); dx; \mathcal{H})} \\ &\quad \left. \times \psi_{+,a}(i, \cdot, x_0) [\operatorname{Im}(m_{+,a}(i, x_0))]^{-1/2} e_j \right], \end{aligned} \tag{6.41}$$

$$\begin{aligned} &= \sum_{j \in \mathcal{J}} \left[(\widehat{\Psi}_{-,a,j}(i, \cdot, x_0), \cdot)_{L^2((-\infty, x_0); dx; \mathcal{H})} \widehat{\Psi}_{-,a,j}(i, \cdot, x_0) \right. \\ &\quad \left. \oplus (\widehat{\Psi}_{+,a,j}(i, \cdot, x_0), \cdot)_{L^2((x_0, \infty); dx; \mathcal{H})} \widehat{\Psi}_{+,a,j}(i, \cdot, x_0) \right] \end{aligned} \tag{6.42}$$

is the orthogonal projection onto \mathcal{N}_i .

Consequently (cf. (5.5)), one obtains for the full-line Donoghue-type m -function,

$$\begin{aligned} M_{H, \mathcal{N}_i}^{Do}(z) &= P_{\mathcal{N}_i} (zH + I) (H - zI)^{-1} P_{\mathcal{N}_i} |_{\mathcal{N}_i}, \\ &= \int_{\mathbb{R}} d\Omega_{H, \mathcal{N}_i}^{Do}(\lambda) \left[\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2 + 1} \right], \quad z \in \mathbb{C} \setminus \mathbb{R}, \end{aligned} \tag{6.43}$$

where $\Omega_{H, \mathcal{N}_i}^{Do}(\cdot)$ satisfies the analogues of (5.9)–(5.11) (resp., (A.9)–(A.11)). With respect to the decomposition (6.34), one can represent $M_{H, \mathcal{N}_i}^{Do}(\cdot)$ as the 2×2 block operator,

$$\begin{aligned} M_{H, \mathcal{N}_i}^{Do}(\cdot) &= (M_{H, \mathcal{N}_i, \ell, \ell'}^{Do}(\cdot))_{0 \leq \ell, \ell' \leq 1} \\ &= z \begin{pmatrix} P_{\mathcal{N}_{-,i}} & 0 \\ 0 & P_{\mathcal{N}_{+,i}} \end{pmatrix} \\ &\quad + (z^2 + 1) \begin{pmatrix} P_{\mathcal{N}_{-,i}} P_{-,x_0} (H - zI)^{-1} P_{-,x_0} P_{\mathcal{N}_{-,i}} & P_{\mathcal{N}_{-,i}} P_{-,x_0} (H - zI)^{-1} P_{+,x_0} P_{\mathcal{N}_{+,i}} \\ P_{\mathcal{N}_{+,i}} P_{+,x_0} (H - zI)^{-1} P_{-,x_0} P_{\mathcal{N}_{-,i}} & P_{\mathcal{N}_{+,i}} P_{+,x_0} (H - zI)^{-1} P_{+,x_0} P_{\mathcal{N}_{+,i}} \end{pmatrix}, \\ &= z \begin{pmatrix} P_{\mathcal{N}_{-,i}} & 0 \\ 0 & P_{\mathcal{N}_{+,i}} \end{pmatrix} + (z^2 + 1) \begin{pmatrix} P_{\mathcal{N}_{-,i}} (H - zI)^{-1} P_{\mathcal{N}_{-,i}} & P_{\mathcal{N}_{-,i}} (H - zI)^{-1} P_{\mathcal{N}_{+,i}} \\ P_{\mathcal{N}_{+,i}} (H - zI)^{-1} P_{\mathcal{N}_{-,i}} & P_{\mathcal{N}_{+,i}} (H - zI)^{-1} P_{\mathcal{N}_{+,i}} \end{pmatrix}, \end{aligned} \tag{6.44}$$

employing $P_{\mathcal{N}_{\pm,i}}P_{\pm,x_0} = P_{\mathcal{N}_{\pm,i}}$, and hence explicitly obtains,

$$\begin{aligned}
 &M_{H,\mathcal{N}_i,0,0}^{Do}(z) \\
 &= \sum_{j,k \in \mathcal{J}} \left(\widehat{\Psi}_{-,a,j}(i, \cdot, x_0), (zH + I)(H - zI)^{-1} \widehat{\Psi}_{-,a,k}(i, \cdot, x_0) \right)_{L^2(\mathbb{R}; dx; \mathcal{H})} \\
 (6.45) \quad &\quad \times \left(\widehat{\Psi}_{-,a,k}(i, \cdot, x_0), \cdot \right)_{L^2(\mathbb{R}; dx; \mathcal{H})} \widehat{\Psi}_{-,a,j}(i, \cdot, x_0),
 \end{aligned}$$

$$\begin{aligned}
 &M_{H,\mathcal{N}_i,0,1}^{Do}(z) \\
 &= \sum_{j,k \in \mathcal{J}} \left(\widehat{\Psi}_{-,a,j}(i, \cdot, x_0), (zH + I)(H - zI)^{-1} \widehat{\Psi}_{+,a,k}(i, \cdot, x_0) \right)_{L^2(\mathbb{R}; dx; \mathcal{H})} \\
 (6.46) \quad &\quad \times \left(\widehat{\Psi}_{+,a,k}(i, \cdot, x_0), \cdot \right)_{L^2(\mathbb{R}; dx; \mathcal{H})} \widehat{\Psi}_{-,a,j}(i, \cdot, x_0),
 \end{aligned}$$

$$\begin{aligned}
 &M_{H,\mathcal{N}_i,1,0}^{Do}(z) \\
 &= \sum_{j,k \in \mathcal{J}} \left(\widehat{\Psi}_{+,a,j}(i, \cdot, x_0), (zH + I)(H - zI)^{-1} \widehat{\Psi}_{-,a,k}(i, \cdot, x_0) \right)_{L^2(\mathbb{R}; dx; \mathcal{H})} \\
 (6.47) \quad &\quad \times \left(\widehat{\Psi}_{-,a,k}(i, \cdot, x_0), \cdot \right)_{L^2(\mathbb{R}; dx; \mathcal{H})} \widehat{\Psi}_{+,a,j}(i, \cdot, x_0),
 \end{aligned}$$

$$\begin{aligned}
 &M_{H,\mathcal{N}_i,1,1}^{Do}(z) \\
 &= \sum_{j,k \in \mathcal{J}} \left(\widehat{\Psi}_{+,a,j}(i, \cdot, x_0), (zH + I)(H - zI)^{-1} \widehat{\Psi}_{+,a,k}(i, \cdot, x_0) \right)_{L^2(\mathbb{R}; dx; \mathcal{H})} \\
 (6.48) \quad &\quad \times \left(\widehat{\Psi}_{+,a,k}(i, \cdot, x_0), \cdot \right)_{L^2(\mathbb{R}; dx; \mathcal{H})} \widehat{\Psi}_{+,a,j}(i, \cdot, x_0), \\
 &\quad \quad \quad z \in \mathbb{C} \setminus \mathbb{R}.
 \end{aligned}$$

Taking a closer look at equations (6.45)–(6.48) we now state the following preliminary result:

Lemma 6.6. *Assume Hypothesis 4.1. Then,*

$$\begin{aligned}
 &\left(\widehat{\Psi}_{\varepsilon,a,j}(i, \cdot, x_0), (zH + I)(H - zI)^{-1} \widehat{\Psi}_{\varepsilon',a,k}(i, \cdot, x_0) \right)_{L^2(\mathbb{R}; dx; \mathcal{H})} \\
 &= \int_{\mathbb{R}} d(\widehat{e}_{\varepsilon,a,j}(\lambda), \Omega_a(\lambda, x_0) \widehat{e}_{\varepsilon',a,k}(\lambda))_{\mathcal{H}^2} \frac{z\lambda + 1}{\lambda - z} \\
 &= \int_{\mathbb{R}} d(e_{\varepsilon,a,j}(\lambda), \Omega_a(\lambda, x_0) e_{\varepsilon',a,k}(\lambda))_{\mathcal{H}^2} \frac{z\lambda + 1}{(\lambda - z)(\lambda^2 + 1)} \\
 (6.49) \quad &= (e_{\varepsilon,a,j}, [M_a(z, x_0) - \text{Re}(M_a(i, x_0))] e_{\varepsilon',a,k})_{\mathcal{H}^2}, \\
 &\quad \quad \quad \varepsilon, \varepsilon' \in \{+, -\}, j, k \in \mathcal{J}, z \in \mathbb{C} \setminus \mathbb{R},
 \end{aligned}$$

where

$$\begin{aligned} \widehat{e}_{\varepsilon,a,j}(\lambda) &= (\widehat{e}_{\varepsilon,a,j,0}(\lambda), \widehat{e}_{\varepsilon,a,j,1}(\lambda))^\top \\ &= \frac{1}{\lambda - i} e_{\varepsilon,a,j} = \frac{1}{\lambda - i} (e_{\varepsilon,a,j,0}, e_{\varepsilon,a,j,1})^\top \\ &= \frac{1}{\lambda - i} (-\varepsilon m_{\varepsilon,\alpha}(i, x_0) [\varepsilon \operatorname{Im}(m_{\varepsilon,\alpha}(i, x_0))]^{-1/2} e_j, \varepsilon [\varepsilon \operatorname{Im}(m_{\varepsilon,\alpha}(i, x_0))]^{-1/2} e_j)^\top, \end{aligned} \tag{6.50}$$

$$\varepsilon \in \{+, -\}, \quad j \in \mathcal{J}, \quad \lambda \in \mathbb{R}.$$

Proof. The first two equalities in (6.49) follow from (4.26), (4.27) upon introducing $\widehat{e}_{\varepsilon,a,j}(\cdot) = (\widehat{e}_{\varepsilon,a,j,0}(\cdot), \widehat{e}_{\varepsilon,a,j,1}(\cdot))^\top$, where

$$\begin{aligned} \widehat{e}_{\varepsilon,a,j,0}(\lambda) &= \varepsilon \int_{x_0}^{\varepsilon\infty} dx \theta_\alpha(\lambda, x, x_0)^* \psi_{\varepsilon,\alpha}(i, x, x_0) [\varepsilon \operatorname{Im}(m_{\varepsilon,\alpha}(i, x_0))]^{-1/2} e_j \\ &= -\varepsilon (\lambda - i)^{-1} m_{\varepsilon,\alpha}(i, x_0) [\varepsilon \operatorname{Im}(m_{\varepsilon,\alpha}(i, x_0))]^{-1/2} e_j, \end{aligned} \tag{6.51}$$

$$\begin{aligned} \widehat{e}_{\varepsilon,a,j,1}(\lambda) &= \varepsilon \int_{x_0}^{\varepsilon\infty} dx \phi_\alpha(\lambda, x, x_0)^* \psi_{\varepsilon,\alpha}(i, x, x_0) [\varepsilon \operatorname{Im}(m_{\varepsilon,\alpha}(i, x_0))]^{-1/2} e_j \\ &= \varepsilon (\lambda - i)^{-1} [\varepsilon \operatorname{Im}(m_{\varepsilon,\alpha}(i, x_0))]^{-1/2} e_j, \end{aligned} \tag{6.52}$$

$$\varepsilon \in \{+, -\}, \quad j \in \mathcal{J}, \quad \lambda \in \mathbb{R},$$

and we employed (6.8), (6.7) (with $z = i$) to arrive at (6.51), (6.52). The third equality in (6.49) follows from (4.22), (4.23). \square

Next, further reducing the computation (6.49) to scalar products of the type $(e_j, \dots e_k)_{\mathcal{H}}$, $j, k \in \mathcal{J}$, naturally leads to a 2×2 block operator

$$M_\alpha^{Do}(\cdot, x_0) = (M_{\alpha,\ell,\ell'}^{Do}(\cdot, x_0))_{0 \leq \ell, \ell' \leq 1}, \tag{6.53}$$

where

$$\begin{aligned} (e_j, M_{\alpha,0,0}^{Do}(z, x_0) e_k)_{\mathcal{H}} &= (e_{-,a,j}, [M_\alpha(z, x_0) - \operatorname{Re}(M_\alpha(i, x_0))] e_{-,a,k})_{\mathcal{H}^2}, \\ (e_j, M_{\alpha,0,1}^{Do}(z, x_0) e_k)_{\mathcal{H}} &= (e_{-,a,j}, [M_\alpha(z, x_0) - \operatorname{Re}(M_\alpha(i, x_0))] e_{+,a,k})_{\mathcal{H}^2}, \\ (e_j, M_{\alpha,1,0}^{Do}(z, x_0) e_k)_{\mathcal{H}} &= (e_{+,a,j}, [M_\alpha(z, x_0) - \operatorname{Re}(M_\alpha(i, x_0))] e_{-,a,k})_{\mathcal{H}^2}, \\ (e_j, M_{\alpha,1,1}^{Do}(z, x_0) e_k)_{\mathcal{H}} &= (e_{+,a,j}, [M_\alpha(z, x_0) - \operatorname{Re}(M_\alpha(i, x_0))] e_{+,a,k})_{\mathcal{H}^2}, \end{aligned} \tag{6.54}$$

$$j, k \in \mathcal{J}, \quad z \in \mathbb{C} \setminus \mathbb{R}.$$

Theorem 6.7. Assume Hypothesis 4.1. Then $M_\alpha^{Do}(\cdot, x_0)$ is a $\mathcal{B}(\mathcal{H}^2)$ -valued Nevanlinna–Herglotz function given by

$$M_\alpha^{Do}(z, x_0) = T_\alpha^* M_\alpha(z, x_0) T_\alpha + E_\alpha \tag{6.55}$$

$$= \int_{\mathbb{R}} d\Omega_\alpha^{Do}(\lambda, x_0) \left[\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2 + 1} \right], \quad z \in \mathbb{C} \setminus \mathbb{R}, \tag{6.56}$$

where the 2×2 block operators $T_\alpha \in \mathcal{B}(\mathcal{H}^2)$ and $E_\alpha \in \mathcal{B}(\mathcal{H}^2)$ are defined by

$$(6.57) \quad T_\alpha = \begin{pmatrix} m_{-, \alpha}(i, x_0)[- \operatorname{Im}(m_{-, \alpha}(i, x_0))]^{-1/2} & -m_{+, \alpha}(i, x_0)[\operatorname{Im}(m_{+, \alpha}(i, x_0))]^{-1/2} \\ -[- \operatorname{Im}(m_{-, \alpha}(i, x_0))]^{-1/2} & [\operatorname{Im}(m_{+, \alpha}(i, x_0))]^{-1/2} \end{pmatrix},$$

$$E_\alpha = \begin{pmatrix} 0 & E_{\alpha, 0, 1} \\ E_{\alpha, 1, 0} & 0 \end{pmatrix} = E_\alpha^*,$$

$$(6.58) \quad E_{\alpha, 0, 1} = 2^{-1}[- \operatorname{Im}(m_{-, \alpha}(i, x_0))]^{-1/2}[m_{-, \alpha}(-i, x_0) - m_{+, \alpha}(i, x_0)] \\ \times [\operatorname{Im}(m_{+, \alpha}(i, x_0))]^{-1/2},$$

$$E_{\alpha, 1, 0} = 2^{-1}[\operatorname{Im}(m_{+, \alpha}(i, x_0))]^{-1/2}[m_{-, \alpha}(i, x_0) - m_{+, \alpha}(-i, x_0)] \\ \times [- \operatorname{Im}(m_{-, \alpha}(i, x_0))]^{-1/2},$$

and $T_\alpha^{-1} \in \mathcal{B}(\mathcal{H}^2)$, with

$$(6.59) \quad (T_\alpha^{-1})_{0, 0} = [- \operatorname{Im}(m_{-, \alpha}(i, x_0))]^{1/2}[m_{-, \alpha}(i, x_0) - m_{+, \alpha}(i, x_0)]^{-1},$$

$$(6.60) \quad (T_\alpha^{-1})_{0, 1} = [- \operatorname{Im}(m_{-, \alpha}(i, x_0))]^{1/2}[m_{-, \alpha}(i, x_0) - m_{+, \alpha}(i, x_0)]^{-1}m_{+, \alpha}(i, x_0),$$

$$(6.61) \quad (T_\alpha^{-1})_{1, 0} = [\operatorname{Im}(m_{+, \alpha}(i, x_0))]^{1/2}[m_{-, \alpha}(i, x_0) - m_{+, \alpha}(i, x_0)]^{-1},$$

$$(6.62) \quad (T_\alpha^{-1})_{1, 1} = [\operatorname{Im}(m_{+, \alpha}(i, x_0))]^{1/2}[m_{-, \alpha}(i, x_0) - m_{+, \alpha}(i, x_0)]^{-1}m_{-, \alpha}(i, x_0).$$

In addition, $\Omega_\alpha^{Do}(\cdot, x_0) = T_\alpha^* \Omega_\alpha(\cdot, x_0) T_\alpha$ satisfies the analogue of (A.10).

Proof. While (6.56) is clear from (6.55) (one notes that the typical constant term in front of the integral in the representation (6.56) now vanishes as by (6.54), $\operatorname{Re}(M_\alpha^{Do}(i, x_0)) = 0$) and similarly, (6.59)–(6.62) is clear from (6.57), the main burden of proof consists in verifying (6.55), given (6.57), (6.58). This can be achieved after straightforward, yet tedious computations. To illustrate the nature of this computations we just focus on the $(0, 0)$ -entry of the 2×2 block operator (6.55) and consider the term (cf. the first equation in (6.54)), $(e_{-, \alpha, j}, M_\alpha(z, x_0)e_{-, \alpha, k})_{\mathcal{H}^2}$, temporarily suppressing x_0 and α for simplicity:

(6.63)

$$\begin{aligned}
 (e_{-,a,j}, M_\alpha(z, x_0)e_{-,a,k})_{\mathcal{H}^2} &= \left(\begin{pmatrix} m_-(i)[- \operatorname{Im}(m_-(i))]^{-1/2}e_j \\ -[- \operatorname{Im}(m_-(i))]^{-1/2}e_j \end{pmatrix}, \right. \\
 &\quad \left(\begin{array}{cc} [m_-(z)-m_+(z)]^{-1} & 2^{-1}[m_-(z)-m_+(z)]^{-1}[m_-(z)+m_+(z)] \\ 2^{-1}[m_-(z)+m_+(z)][m_-(z)-m_+(z)]^{-1} & m_\mp(z)[m_-(z)-m_+(z)]^{-1}m_\pm(z) \end{array} \right) \\
 &\quad \times \left. \begin{pmatrix} m_-(i)[- \operatorname{Im}(m_-(i))]^{-1/2}e_k \\ -[- \operatorname{Im}(m_-(i))]^{-1/2}e_k \end{pmatrix} \right)_{\mathcal{H}^2} \\
 &= (m_-(i)[- \operatorname{Im}(m_-(i))]^{-1/2}e_j, [m_-(z) - m_+(z)]^{-1} \\
 &\quad \times m_-(i)[- \operatorname{Im}(m_-(i))]^{-1/2}e_k)_{\mathcal{H}^2} \\
 &\quad - 2^{-1}(m_-(i)[- \operatorname{Im}(m_-(i))]^{-1/2}e_j, [m_-(z) - m_+(z)]^{-1}[m_-(z) + m_+(z)] \\
 &\quad \times [- \operatorname{Im}(m_-(i))]^{-1/2}e_k)_{\mathcal{H}^2} \\
 &\quad - 2^{-1}([- \operatorname{Im}(m_-(i))]^{-1/2}e_j, [m_-(z) + m_+(z)][m_-(z) - m_+(z)]^{-1} \\
 &\quad \times m_-(i)[- \operatorname{Im}(m_-(i))]^{-1/2}e_k)_{\mathcal{H}^2} \\
 &\quad + ([- \operatorname{Im}(m_-(i))]^{-1/2}e_j, m_\mp(z)[m_-(z) - m_+(z)]^{-1}m_\pm(z) \\
 &\quad \times [- \operatorname{Im}(m_-(i))]^{-1/2}e_k)_{\mathcal{H}^2} \\
 &= (e_j, [- \operatorname{Im}(m_-(i))]^{-1/2}m_-(i)[m_-(z) - m_+(z)]^{-1} \\
 &\quad \times m_-(i)[- \operatorname{Im}(m_-(i))]^{-1/2}e_k)_{\mathcal{H}^2} \\
 &\quad - 2^{-1}(e_j, [- \operatorname{Im}(m_-(i))]^{-1/2}m_-(i)[m_-(z) - m_+(z)]^{-1}[m_-(z) + m_+(z)] \\
 &\quad \times [- \operatorname{Im}(m_-(i))]^{-1/2}e_k)_{\mathcal{H}^2} \\
 &\quad - 2^{-1}(e_j, [- \operatorname{Im}(m_-(i))]^{-1/2}[m_-(z) + m_+(z)][m_-(z) - m_+(z)]^{-1} \\
 &\quad \times m_-(i)[- \operatorname{Im}(m_-(i))]^{-1/2}e_k)_{\mathcal{H}^2} \\
 &\quad + (e_j, [- \operatorname{Im}(m_-(i))]^{-1/2}m_\mp(z)[m_-(z) - m_+(z)]^{-1}m_\pm(z) \\
 &\quad \times [- \operatorname{Im}(m_-(i))]^{-1/2}e_k)_{\mathcal{H}^2}, \quad z \in \mathbb{C} \setminus \mathbb{R}.
 \end{aligned}$$

Explicitly computing $(e_j, [T_\alpha^* M_\alpha(z, x_0) T_\alpha]_{0,0} e_k)_{\mathcal{H}^2}$, given T_α in (6.57) yields the same expression as in (6.63). Similarly, one verifies that

$$(6.64) \quad (e_{-,a,j}, \operatorname{Re}(M_\alpha(i, x_0))e_{-,a,k})_{\mathcal{H}^2} = 0,$$

verifying the $(0, 0)$ -entry of (6.55). The remaining three entries are verified analogously. □

Combining Lemma 6.6 and Theorem 6.7 then yields the following result:

Theorem 6.8. *Assume Hypothesis 4.1. Then $M_{H, N_i}^{D_0}(\cdot) = (M_{H, N_i, \ell, \ell'}^{D_0}(\cdot))_{0 \leq \ell, \ell' \leq 1}$, explicitly given by (6.43)–(6.48), is of the form,*

$$\begin{aligned}
 M_{H, \mathcal{N}_i, 0, 0}^{Do}(z) &= \sum_{j, k \in \mathcal{J}} (e_j, M_{\alpha, 0, 0}^{Do}(z, x_0) e_k)_{\mathcal{H}} \\
 &\quad \times (\widehat{\Psi}_{-, \alpha, k}(i, \cdot, x_0), \cdot)_{L^2(\mathbb{R}; dx; \mathcal{H})} \widehat{\Psi}_{-, \alpha, j}(i, \cdot, x_0),
 \end{aligned}
 \tag{6.65}$$

$$\begin{aligned}
 M_{H, \mathcal{N}_i, 0, 1}^{Do}(z) &= \sum_{j, k \in \mathcal{J}} (e_j, M_{\alpha, 0, 1}^{Do}(z, x_0) e_k)_{\mathcal{H}} \\
 &\quad \times (\widehat{\Psi}_{+, \alpha, k}(i, \cdot, x_0), \cdot)_{L^2(\mathbb{R}; dx; \mathcal{H})} \widehat{\Psi}_{-, \alpha, j}(i, \cdot, x_0),
 \end{aligned}
 \tag{6.66}$$

$$\begin{aligned}
 M_{H, \mathcal{N}_i, 1, 0}^{Do}(z) &= \sum_{j, k \in \mathcal{J}} (e_j, M_{\alpha, 1, 0}^{Do}(z, x_0) e_k)_{\mathcal{H}} \\
 &\quad \times (\widehat{\Psi}_{-, \alpha, k}(i, \cdot, x_0), \cdot)_{L^2(\mathbb{R}; dx; \mathcal{H})} \widehat{\Psi}_{+, \alpha, j}(i, \cdot, x_0),
 \end{aligned}
 \tag{6.67}$$

$$\begin{aligned}
 M_{H, \mathcal{N}_i, 1, 1}^{Do}(z) &= \sum_{j, k \in \mathcal{J}} (e_j, M_{\alpha, 1, 1}^{Do}(z, x_0) e_k)_{\mathcal{H}} \\
 &\quad \times (\widehat{\Psi}_{+, \alpha, k}(i, \cdot, x_0), \cdot)_{L^2(\mathbb{R}; dx; \mathcal{H})} \widehat{\Psi}_{+, \alpha, j}(i, \cdot, x_0),
 \end{aligned}
 \tag{6.68}$$

$z \in \mathbb{C} \setminus \mathbb{R}$,

with $M_{\alpha}^{Do}(\cdot, x_0)$ given by (6.55)–(6.58).

Remark 6.9. Combining Corollary 5.8 and Theorem 6.8 proves that the entire spectral information for H , contained in the corresponding family of spectral projections $\{E_H(\lambda)\}_{\lambda \in \mathbb{R}}$ in $L^2(\mathbb{R}; dx; \mathcal{H})$, is already encoded in the operator-valued measure $\{\Omega_{H, \mathcal{N}_i}^{Do}(\lambda)\}_{\lambda \in \mathbb{R}}$ in \mathcal{N}_i (including multiplicity properties of the spectrum of H). In addition, invoking Theorem 6.7 shows that for any fixed $\alpha = \alpha^* \in \mathcal{B}(\mathcal{H})$, $x_0 \in \mathbb{R}$, the entire spectral information for H is already contained in $\{\Omega_{\alpha}^{Do}(\lambda, x_0)\}_{\lambda \in \mathbb{R}}$ in \mathcal{H}^2 .

Appendix A Basic facts on bounded operator-valued Nevanlinna–Herglotz functions

We review some basic facts on (bounded) operator-valued Nevanlinna–Herglotz functions (also called Nevanlinna, Pick, R -functions, etc.), frequently employed in the bulk of this paper. For additional details concerning the material in this appendix we refer to [50], [52].

Throughout this appendix, \mathcal{H} is a separable, complex Hilbert space with inner product denoted by $(\cdot, \cdot)_{\mathcal{H}}$, identity operator abbreviated by $I_{\mathcal{H}}$. We also denote $\mathbb{C}_{\pm} = \{z \in \mathbb{C} \mid \pm \operatorname{Im}(z) > 0\}$.

Definition A.1. The map $M : \mathbb{C}_+ \rightarrow \mathcal{B}(\mathcal{H})$ is called a bounded operator-valued Nevanlinna–Herglotz function on \mathcal{H} (in short, a bounded Nevanlinna–Herglotz operator on \mathcal{H}) if M is analytic on \mathbb{C}_+ and $\operatorname{Im}(M(z)) \geq 0$ for all $z \in \mathbb{C}_+$.

Here we follow the standard notation

$$(A.1) \quad \text{Im}(M) = (M - M^*)/(2i), \quad \text{Re}(M) = (M + M^*)/2, \quad M \in \mathcal{B}(\mathcal{H}).$$

Note that M is a bounded Nevanlinna–Herglotz operator if and only if the scalar-valued functions $(u, Mu)_{\mathcal{H}}$ are Nevanlinna–Herglotz for all $u \in \mathcal{H}$.

As in the scalar case one usually extends M to \mathbb{C}_- by reflection, that is, by defining

$$(A.2) \quad M(z) = M(\bar{z})^*, \quad z \in \mathbb{C}_-.$$

Hence M is analytic on $\mathbb{C} \setminus \mathbb{R}$, but $M|_{\mathbb{C}_-}$ and $M|_{\mathbb{C}_+}$, in general, are not analytic continuations of each other.

In contrast to the scalar case, one cannot generally expect strict inequality in $\text{Im}(M(\cdot)) \geq 0$. However, the kernel of $\text{Im}(M(\cdot))$ has the following simple properties recorded in [49, Lemma 5.3] (whose proof was kindly communicated to us by Dirk Buschmann) in the matrix-valued context. Below we indicate that the proof extends to the present infinite-dimensional situation (see also [39, Proposition 1.2 (ii)] for additional results of this kind):

Lemma A.2. *Let $M(\cdot)$ be a $\mathcal{B}(\mathcal{H})$ -valued Nevanlinna–Herglotz function. Then the kernel $\mathcal{H}_0 = \ker(\text{Im}(M(z)))$ is independent of $z \in \mathbb{C} \setminus \mathbb{R}$. Consequently, upon decomposing $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1$, $\mathcal{H}_1 = \mathcal{H}_0^\perp$, $\text{Im}(M(\cdot))$ takes on the form*

$$(A.3) \quad \text{Im}(M(z)) = \begin{pmatrix} 0 & 0 \\ 0 & N_1(z) \end{pmatrix}, \quad z \in \mathbb{C}_+,$$

where $N_1(\cdot) \in \mathcal{B}(\mathcal{H}_1)$ satisfies

$$(A.4) \quad N_1(z) \geq 0, \quad \ker(N_1) = \{0\}, \quad z \in \mathbb{C}_+.$$

Proof. Pick $z_0 \in \mathbb{C} \setminus \mathbb{R}$, and suppose $f_0 \in \ker(\text{Im}(M(z_0)))$. Introducing $m(z) = (f_0, M(z)f_0)_{\mathcal{H}}$, $z \in \mathbb{C} \setminus \mathbb{R}$, $m(\cdot)$ is a scalar Nevanlinna–Herglotz function and $m(z_0) \in \mathbb{R}$. Hence the Nevanlinna–Herglotz function $m(z) - m(z_0)$ has a zero at $z = z_0$, and thus must be a real-valued constant, $m(z) = m(z_0)$, $z \in \mathbb{C} \setminus \mathbb{R}$. Since $(f_0, M(z)^*f_0)_{\mathcal{H}} = \overline{(f_0, M(z)f_0)_{\mathcal{H}}} = \overline{m(z)} = m(z_0) \in \mathbb{R}$, $z \in \mathbb{C} \setminus \mathbb{R}$, one concludes that $(f_0, \text{Im}(M(z))f_0)_{\mathcal{H}} = \pm \| [\pm \text{Im}(M(z))]^{1/2} f_0 \|_{\mathcal{H}}^2 = 0$, $z \in \mathbb{C}_\pm$, that is,

$$(A.5) \quad f_0 \in \ker([\pm \text{Im}(M(z))]^{1/2}) = \ker(\text{Im}(M(z))), \quad z \in \mathbb{C}_\pm,$$

and hence $\ker(M(z_0)) \subseteq \ker(M(z))$, $z \in \mathbb{C} \setminus \mathbb{R}$. Interchanging the role of z_0 and z finally yields $\ker(M(z_0)) = \ker(M(z))$, $z \in \mathbb{C} \setminus \mathbb{R}$. □

Next we recall the definition of a bounded operator-valued measure (see, also [19, p. 319], [75], [92]):

Definition A.3. Let \mathcal{H} be a separable, complex Hilbert space. A map $\Sigma : \mathfrak{B}(\mathbb{R}) \rightarrow \mathfrak{B}(\mathcal{H})$, with $\mathfrak{B}(\mathbb{R})$ the Borel σ -algebra on \mathbb{R} , is called a *bounded, nonnegative, operator-valued measure* if the following conditions (i) and (ii) hold:

- (i) $\Sigma(\emptyset) = 0$ and $0 \leq \Sigma(B) \in \mathfrak{B}(\mathcal{H})$ for all $B \in \mathfrak{B}(\mathbb{R})$;
- (ii) $\Sigma(\cdot)$ is strongly countably additive (i.e., with respect to the strong operator topology in \mathcal{H}), that is,

$$(A.6) \quad \Sigma(B) = \text{s-lim}_{N \rightarrow \infty} \sum_{j=1}^N \Sigma(B_j) \quad \text{whenever } B = \bigcup_{j \in \mathbb{N}} B_j,$$

with $B_k \cap B_\ell = \emptyset$ for $k \neq \ell$, $B_k \in \mathfrak{B}(\mathbb{R})$, $k, \ell \in \mathbb{N}$.

$\Sigma(\cdot)$ is called an (*operator-valued*) *spectral measure* (or an *orthogonal operator-valued measure*) if additionally the following condition (iii) holds:

- (iii) $\Sigma(\cdot)$ is projection-valued (i.e., $\Sigma(B)^2 = \Sigma(B)$, $B \in \mathfrak{B}(\mathbb{R})$) and $\Sigma(\mathbb{R}) = I_{\mathcal{H}}$.

(iv) Let $f \in \mathcal{H}$ and $B \in \mathfrak{B}(\mathbb{R})$. Then the vector-valued measure $\Sigma(\cdot)f$ has *finite variation on B* , denoted by $V(\Sigma f; B)$, if

$$(A.7) \quad V(\Sigma f; B) = \sup \left\{ \sum_{j=1}^N \|\Sigma(B_j)f\|_{\mathcal{H}} \right\} < \infty,$$

where the supremum is taken over all finite sequences $\{B_j\}_{1 \leq j \leq N}$ of pairwise disjoint subsets on \mathbb{R} with $B_j \subseteq B$, $1 \leq j \leq N$. In particular, $\Sigma(\cdot)f$ has *finite total variation* if $V(\Sigma f; \mathbb{R}) < \infty$.

We recall that due to monotonicity considerations, taking the limit in the strong operator topology in (A.6) is equivalent to taking the limit with respect to the weak operator topology in \mathcal{H} .

For relevant material in connection with the following result we refer the reader, for instance, to [1], [5], [6], [11], [19, Sect. VI.5.], [23, Sect. I.4], [29], [30], [32], [37]–[39], [62], [68], [69], [74], [75], [87], [88], [89], [83], [100], [102], and the detailed bibliography in [52].

Theorem A.4. ([6], [23, Sect. I.4], [100].) Let M be a bounded operator-valued Nevanlinna–Herglotz function in \mathcal{H} . Then the following assertions hold:

- (i) For each $f \in \mathcal{H}$, $(f, M(\cdot)f)_{\mathcal{H}}$ is a (scalar) Nevanlinna–Herglotz function.

Suppose that $\{e_j\}_{j \in \mathbb{N}}$ is a complete orthonormal system in \mathcal{H} and that for some subset of \mathbb{R} having positive Lebesgue measure, and for all $j \in \mathbb{N}$, $(e_j, M(\cdot)e_j)_{\mathcal{H}}$ has zero normal limits. Then $M \equiv 0$.

(ii) There exists a bounded, nonnegative $\mathcal{B}(\mathcal{H})$ -valued measure Ω on \mathbb{R} such that the Nevanlinna representation

$$(A.8) \quad M(z) = C + Dz + \int_{\mathbb{R}} d\Omega(\lambda) \left[\frac{1}{\lambda - z} - \frac{\lambda}{\lambda^2 + 1} \right], \quad z \in \mathbb{C}_+,$$

$$(A.9) \quad \tilde{\Omega}((-\infty, \lambda]) = s\text{-}\lim_{\varepsilon \downarrow 0} \int_{-\infty}^{\lambda+\varepsilon} d\Omega(t) (t^2 + 1)^{-1}, \quad \lambda \in \mathbb{R},$$

$$(A.10) \quad \tilde{\Omega}(\mathbb{R}) = \text{Im}(M(i)) - D = \int_{\mathbb{R}} d\Omega(\lambda) (\lambda^2 + 1)^{-1} \in \mathcal{B}(\mathcal{H}),$$

$$(A.11) \quad C = \text{Re}(M(i)), \quad D = s\text{-}\lim_{\eta \uparrow \infty} \frac{1}{i\eta} M(i\eta) \geq 0,$$

holds in the strong sense in \mathcal{H} . Here $\tilde{\Omega}(B) = \int_B (1 + \lambda^2)^{-1} d\Omega(\lambda)$, $B \in \mathcal{B}(\mathbb{R})$.

Let $\lambda_1, \lambda_2 \in \mathbb{R}$, $\lambda_1 < \lambda_2$. Then the Stieltjes inversion formula for Ω reads

$$(A.12) \quad \Omega((\lambda_1, \lambda_2])f = \pi^{-1} s\text{-}\lim_{\delta \downarrow 0} s\text{-}\lim_{\varepsilon \downarrow 0} \int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda \text{Im}(M(\lambda + i\varepsilon))f, \quad f \in \mathcal{H}.$$

(iii) Any isolated poles of M are simple and located on the real axis, the residues at poles being nonpositive bounded operators in $\mathcal{B}(\mathcal{H})$.

For all $\lambda \in \mathbb{R}$,

$$(A.13) \quad s\text{-}\lim_{\varepsilon \downarrow 0} \varepsilon \text{Re}(M(\lambda + i\varepsilon)) = 0,$$

$$(A.14) \quad \Omega(\{\lambda\}) = s\text{-}\lim_{\varepsilon \downarrow 0} \varepsilon \text{Im}(M(\lambda + i\varepsilon)) = -i s\text{-}\lim_{\varepsilon \downarrow 0} \varepsilon M(\lambda + i\varepsilon).$$

(iv) If, in addition, $M(z) \in \mathcal{B}_\infty(\mathcal{H})$, $z \in \mathbb{C}_+$, then the measure Ω in (A.8) is countably additive with respect to the $\mathcal{B}(\mathcal{H})$ -norm, and the Nevanlinna representation (A.8) and the Stieltjes inversion formula (A.12) as well as (A.13), (A.14) hold with the limits taken with respect to the $\|\cdot\|_{\mathcal{B}(\mathcal{H})}$ -norm. (iii) Let $f \in \mathcal{H}$ and assume in addition that $\Omega(\cdot)f$ is of finite total variation. Then for a.e. $\lambda \in \mathbb{R}$, the normal limits $M(\lambda + i0)f$ exist in the strong sense and

$$(A.15) \quad s\text{-}\lim_{\varepsilon \downarrow 0} M(\lambda + i\varepsilon)f = M(\lambda + i0)f = H(\Omega(\cdot)f)(\lambda) + i\pi\Omega'(\lambda)f,$$

where $H(\Omega(\cdot)f)$ denotes the \mathcal{H} -valued Hilbert transform

$$(A.16) \quad H(\Omega(\cdot)f)(\lambda) = \text{p.v.} \int_{-\infty}^{\infty} d\Omega(t)f \frac{1}{t - \lambda} = s\text{-}\lim_{\delta \downarrow 0} \int_{|t-\lambda| \geq \delta} d\Omega(t)f \frac{1}{t - \lambda}.$$

As usual, the normal limits in Theorem A.4 can be replaced by nontangential ones. The nature of the boundary values of $M(\cdot + i0)$ when for some $p > 0$, $M(z) \in \mathcal{B}_p(\mathcal{H})$, $z \in \mathbb{C}_+$, was clarified in detail in [20], [84], [85], [86]. We

also mention that Shmul’yan [100] discusses the Nevanlinna representation (A.8); moreover, certain special classes of Nevanlinna functions, isolated by Kac and Krein [63] in the scalar context, are studied by Brodskii [23, Sect. I.4] and Shmul’yan [100].

Our final result of this appendix offers an elementary proof of bounded invertibility of $\text{Im}(M(z))$ for all $z \in \mathbb{C}_+$ if and only if this property holds for some $z_0 \in \mathbb{C}_+$:

Lemma A.5. *Let M be a bounded operator-valued Nevanlinna–Herglotz function in \mathcal{H} . Then $[\text{Im}(M(z_0))]^{-1} \in \mathcal{B}(\mathcal{H})$ for some $z_0 \in \mathbb{C}_+$ (resp., $z_0 \in \mathbb{C}_-$) if and only if $[\text{Im}(M(z))]^{-1} \in \mathcal{B}(\mathcal{H})$ for all $z \in \mathbb{C}_+$ (resp., $z \in \mathbb{C}_-$).*

Proof. By relation (A.2), it suffices to consider $z_0, z \in \mathbb{C}_+$, and because of Theorem A.4(iii), we can assume that $M(z), z \in \mathbb{C}_+$, has the representation (A.8).

Let $x_0, x \in \mathbb{R}$ and $y_0, y > 0$, then there exists a constant $c \geq 1$ such that

$$(A.17) \quad \sup_{\lambda \in \mathbb{R}} \left(\frac{(\lambda - x)^2 + y^2}{(\lambda - x_0)^2 + y_0^2} \right) \leq c,$$

since the function on the left-hand side is continuous and tends to 1 as $\lambda \rightarrow \pm\infty$. If $[\text{Im}(M(x_0 + iy_0))]^{-1} \in \mathcal{B}(\mathcal{H})$, there exists $\delta > 0$ such that $\text{Im}(M(x_0 + iy_0)) \geq \delta I_{\mathcal{H}}$, and hence, using $c \geq 1, y > 0$, and $\Omega \geq 0$, one obtains

$$(A.18) \quad \begin{aligned} \delta I_{\mathcal{H}} &\leq \text{Im}(M(x_0 + iy_0)) = Dy_0 + \int_{\mathbb{R}} \frac{y_0}{(\lambda - x_0)^2 + y_0^2} d\Omega(\lambda) \\ &\leq \frac{y_0}{y} \left[Dy + c \int_{\mathbb{R}} \frac{y}{(\lambda - x)^2 + y^2} d\Omega(\lambda) \right] \\ &\leq \frac{y_0}{y} \left[cDy + c \int_{\mathbb{R}} \frac{y}{(\lambda - x)^2 + y^2} d\Omega(\lambda) \right] \leq \frac{cy_0}{y} \text{Im}(M(x + iy)). \end{aligned}$$

This completes the proof. □

For a variety of additional spectral results in connection with operator-valued Nevanlinna–Herglotz functions we refer to [22] and [39, Proposition 1.2]. For a systematic treatment of operator-valued Nevanlinna–Herglotz families we refer to [34].

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