SOME APPLICATIONS OF OPERATOR-VALUED HERGLOTZ FUNCTIONS

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Dedicated to Moshe Livsic on the occasion of his 80th birthday

Abstract. We consider operator-valued Herglotz functions and their applications to self-adjoint perturbations of self-adjoint operators and self-adjoint extensions of densely defined closed symmetric operators. Our applications include model operators for both situations, linear fractional transformations for Herglotz operators, results on Friedrichs and Krein extensions, and realization theorems for classes of Herglotz operators. Moreover, we study the concrete case of Schrödinger operators on a half-line and provide two illustrations of Livsic's result [44] on quasi-hermitian extensions in the special case of densely defined symmetric operators with deficiency indices $(1, 1)$.

1. Introduction

The principal purpose of this paper is to extend some of our recent results on matrix-valued Herglotz functions in [30] to the infinite-dimensional context.

Given a complex Hilbert space $\mathcal{K}$, a map $M : \mathbb{C}_+ \to \mathcal{B}(\mathcal{K})$ is called a $\mathcal{K}$-valued Herglotz function (or simply a Herglotz operator) if M is analytic on $\mathbb{C}_+$ and $\operatorname{Im}(M(z)) \geq 0$ for all $z \in \mathbb{C}_+$. (We refer to the end of this introduction for a glossary on the notation used in this paper.) $\mathcal{B}(\mathcal{K})$-valued Herglotz functions admit the celebrated Nevanlinna-Riesz-Herglotz representation studied, for instance, by Brodskii [17], Sect. I.4, Krein and Ovcharenko [40], [41], and Shmulyan [62] in the infinite-dimensional context,

$$M(z) = C + Dz + \int_{\mathbb{R}} d\Omega(\lambda)((\lambda - z)^{-1} - \lambda(1 + \lambda^2)^{-1}), \quad z \in \mathbb{C}_+, \tag{1.1}$$

where,

$$C = C^* \in \mathcal{B}(\mathcal{K}), \quad 0 \leq D \in \mathcal{B}(\mathcal{K}), \tag{1.2}$$

and Ω is a $\mathcal{B}(\mathcal{K})$-valued measure satisfying

$$\int_{\mathbb{R}} d(\xi, \Omega(\lambda)\xi)_{\mathcal{K}} (1 + \lambda^2)^{-1} < \infty \text{ for all } \xi \in \mathcal{K}. \tag{1.3}$$

In this paper we study a subclass of $\mathcal{B}(\mathcal{K})$-valued Herglotz functions where $D = 0$ and the Stieltjes integral in (1.1) is either understood in the norm (cf. Section 3) or the strong operator topology (cf. Section 4) in $\mathcal{K}$. For detailed discussions of

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operator-valued Herglotz functions and their boundary value behavior, see, for instance, [19], [57], Ch. 4, [63], Ch. V, [68]. Throughout this paper we will adhere to the usual convention

$$M(\bar{z}) = M(z)^*, \quad z \in \mathbb{C}_+ \tag{1.4}$$

(see, however, Lemma 4.13).

As discussed in some detail in [30], our notion of Herglotz functions is not without controversy. In fact, the names Pick, Nevanlinna, Nevanlinna-Pick, and R-functions (depending on whether the open upper half-plane $\mathbb{C}_+$ or the open unit disk D are involved, as well as depending on the geographical origin of authors) are also frequently in use. Here we follow a tradition in mathematical physics which appears to favor the terminology of Herglotz functions.

A crucial role in our analysis is played by linear fractional transformations of the type

$$M(z) \longrightarrow M_A(z) = (A_{2,1} + A_{2,2}M(z))(A_{1,1} + A_{1,2}M(z))^{-1}, \quad z \in \mathbb{C}_+, \tag{1.5}$$

where

$$\begin{aligned} &A = \big(A_{p,q}\big)_{1 \le p,q \le 2} \in \mathcal{A}(\mathcal{K} \oplus \mathcal{K}), \\ &\mathcal{A}(\mathcal{K} \oplus \mathcal{K}) = \{A \in \mathcal{B}(\mathcal{K} \oplus \mathcal{K}) \,|\, A^*JA = J\}, \quad J = \begin{pmatrix} 0 & -I_{\mathcal{K}} \\ I_{\mathcal{K}} & 0 \end{pmatrix}. \end{aligned} \tag{1.6}$$

M_A is a Herglotz operator in $\mathcal{K}$ whenever M is one and we refer to Krein and Shmulyan [42] for a detailed study in connection with (1.5), (1.6).

Section 2 provides a detailed study of a model Hilbert space, variants of which are used in Sections 3 and 4. This construction appears to be of independent interest.

In Section 3 we consider self-adjoint perturbations H_L of a self-adjoint (possibly unbounded) operator H_0 in some separable complex Hilbert space $\mathcal{H}$

$$H_L = H_0 + KLK^*, \quad \mathrm{dom}(H_L) = \mathrm{dom}(H_0), \tag{1.7}$$

where $L = L^* \in \mathcal{B}(\mathcal{K})$ and $K \in \mathcal{B}(\mathcal{K}, \mathcal{H})$, with $\mathcal{K}$ another separable complex Hilbert space. We introduce a model operator $\widehat{H}_L$ in $\widehat{\mathcal{H}} = L^2(\mathbb{R}, \mathcal{K}; d\Omega_L)$ for H_L in $\mathcal{H}$, define the Herglotz operator

$$M_L(z) = K^*(H_L - z)^{-1}K = \int_{\mathbb{R}} d\Omega_L(\lambda)(\lambda - z)^{-1}, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{1.8}$$

where

$$\Omega_L(\lambda) = K^*E_L(\lambda)K, \tag{1.9}$$

with $\{E_L(\lambda)\}_{\lambda\in\mathbb{R}}$ the family of orthogonal spectral projections of H_L, and study the pair (H_L, H_0) in terms of $(M_L(z), M_0(z))$ following Donoghue's treatment [25] of rank-one perturbations of H_0. Moreover, we prove a realization theorem for the class of Herglotz operators exemplified by (1.8).

In Section 4 we consider self-adjoint extensions H of a densely defined closed symmetric operator $\dot{H}$ with deficiency indices (k, k), $k \in \mathbb{N} \cup \{\infty\}$ in some separable complex Hilbert space $\mathcal{H}$. We review our recent note [28] on Krein's formula relating self-adjoint extensions of $\dot{H}$ and introduce the corresponding Weyl operators $M_{H,\mathcal{N}}(z)$

$$M_{H,\mathcal{N}}(z) = zI_{\mathcal{N}} + (1 + z^2)P_{\mathcal{N}}(H - z)^{-1}P_{\mathcal{N}}\big|_{\mathcal{N}} \tag{1.10}$$

$$= \int_{\mathbb{R}} d\Omega_{H,\mathcal{N}}(\lambda)((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}), \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{1.11}$$

where $\mathcal{N}$ is a closed linear subspace of the deficiency subspace $\mathcal{N}_+ = \ker(\dot{H}^* - i)$, $P_{\mathcal{N}}$ the orthogonal projection onto $\mathcal{N}$, and

$$\Omega_{H,\mathcal{N}}(\lambda) = (1+\lambda^2)(P_{\mathcal{N}} E_H(\lambda) P_{\mathcal{N}}\big|_{\mathcal{N}}), \tag{1.12}$$

with $\{E_H(\lambda)\}_{\lambda\in\mathbb{R}}$ the family of orthogonal spectral projections of H. Following [28] we study linear fractional transformation of $M_{H,\mathcal{N}_+}(z)$ involving different self-adjoint extensions H of $\dot{H}$. Moreover, following Donoghue [25] in the special case $\dim_{\mathbb{C}}(\mathcal{N}_+) = 1$, we consider a model $(\widehat{\dot{H}}, \widehat{H})$ in $\widehat{\mathcal{H}} = L^2(\mathbb{R}, \mathcal{N}_+; d\Omega_{H,\mathcal{N}_+})$ for the pair $(\dot{H}, H)$ in $\mathcal{H}$, and discuss Friedrichs and Krein extensions of $\dot{H}$ assuming $\dot{H}$ to be bounded from below. We conclude Section 4 with realization theorems for various classes of Weyl operators of the type (1.11).

Section 5 provides concrete applications of the formalism of Section 4 specialized to the case $\dim_{\mathbb{C}}(\mathcal{N}_+) = 1$. We study Schrödinger operators on a half-line and provide two illustrations of Livsic's result [44] on quasi-hermitian extensions in the special case of densely defined closed prime symmetric operators with deficiency indices $(1, 1)$.

Finally, we briefly introduce some of the notation used in this paper. $\mathbb{C}_\pm = \{z \in \mathbb{C} \,|\, \mathrm{Im}(z) \gtrless 0\}$ denote the open upper/lower half-plane, $\bar{z}$ the complex conjugate of $z \in \mathbb{C}$. Complex Hilbert spaces are denoted by $\mathcal{H}$ or $\mathcal{K}$, the scalar product in $\mathcal{H}$ (linear in the second factor) by $(\cdot\,,\cdot)_{\mathcal{H}}$, with $I_{\mathcal{H}}$ the identity operator in $\mathcal{H}$. Direct sums of linear subspaces are indicated by $\dot{+}$, orthogonal direct sums by $\oplus$ (or $\oplus_{\mathcal{H}}$, if necessary). The Banach space of bounded linear operators from $\mathcal{K}$ into $\mathcal{H}$ is denoted by $\mathcal{B}(\mathcal{K}, \mathcal{H})$ (and simply by $\mathcal{B}(\mathcal{H})$ if $\mathcal{K} = \mathcal{H}$). The domain, range, and kernel (null space) of a linear operator T are denoted by $\mathrm{dom}(T)$, $\mathrm{ran}(T)$ and $\ker(T)$, respectively; the resolvent set and spectrum of T by $\rho(T)$ and $\mathrm{spec}(T)$. The adjoint of T is denoted by T^*, $\mathrm{Re}(T) = (T + T^*)/2$ and $\mathrm{Im}(T) = (T - T^*)/(2i)$ (assuming $\mathrm{dom}(T) = \mathrm{dom}(T^*)$) abbreviate the real and imaginary part of T, respectively. The symbol χ_B denotes the characteristic function of $B \subset \mathbb{R}$; Σ denotes the Borel $\sigma-$algebra on $\mathbb{R}$.

2. Construction of a Model Hilbert Space

This section describes in some detail the construction of a model Hilbert space, variants of which will be of crucial importance in Sections 3 and 4. Rather than referring to the theory of direct integrals of Hilbert spaces (see, e.g., [11], Ch. 4, [12], Ch. 7) we briefly develop the necessary machinery from scratch and hint at the construction of related Banach spaces as well.

Let μ denote a $\sigma-$finite Borel measure on $\mathbb{R}$, Σ the Borel $\sigma-$algebra on $\mathbb{R}$, and suppose for each $\lambda \in \mathbb{R}$ we are given a separable complex Hilbert space $\mathcal{K}_\lambda$. Let $\mathcal{S}(\{\mathcal{K}_\lambda\}_{\lambda\in\mathbb{R}})$ be the vector space associated with the product space $\prod_{\lambda\in\mathbb{R}} \mathcal{K}_\lambda$ equipped with the obvious linear structure. Elements f of $\mathcal{S}(\{\mathcal{K}_\lambda\}_{\lambda\in\mathbb{R}})$ are maps

$$\mathbb{R} \ni \lambda \to f = \{f(\lambda) \in \mathcal{K}_\lambda\}_{\lambda\in\mathbb{R}} \in \prod_{\lambda\in\mathbb{R}} \mathcal{K}_\lambda. \tag{2.1}$$

Definition 2.1. A *measurable family of Hilbert spaces* $\mathcal{M}$ modelled on μ and $\{\mathcal{K}_\lambda\}_{\lambda\in\mathbb{R}}$ is a linear subspace $\mathcal{M} \subset \mathcal{S}(\{\mathcal{K}_\lambda\}_{\lambda\in\mathbb{R}})$ such that $f \in \mathcal{M}$ if and only if the map $\mathbb{R} \ni \lambda \to (f(\lambda), g(\lambda))_{\mathcal{K}_\lambda} \in \mathbb{C}$ is $\mu-$measurable for all $g \in \mathcal{M}$.

Moreover, $\mathcal{M}$ is said to be generated by some subset $\mathcal{F}$, $\mathcal{F} \subset \mathcal{M}$, if for every $g \in \mathcal{M}$ we can find a sequence of functions $h_n \in \text{lin.span}\{\chi_B f \in \mathcal{S}(\{\mathcal{K}_\lambda\} \,|\, B \in \Sigma, f \in \mathcal{F}\}$ with $\lim_{n\to\infty} \|g(\lambda) - h_n(\lambda)\|_{\mathcal{K}_\lambda} = 0$ $\mu-$a.e.

The definition of $\mathcal{M}$ was chosen with it's maximality in mind and we refer to Lemma 2.3 and Theorem 2.6 for more details in this respect. An explicit construction of an example of $\mathcal{M}$ will be given in Theorem 2.5.

Remark 2.2. The following properties are proved in a standard manner:
(i) If $f \in \mathcal{M}$, $g \in \mathcal{S}(\{\mathcal{K}_\lambda\}_{\lambda\in\mathbb{R}})$ and $g = f$ $\mu-$a.e. then $g \in \mathcal{M}$.
(ii) If $\{f_n\}_{n\in\mathbb{N}} \in \mathcal{M}$, $g \in \mathcal{S}(\{\mathcal{K}_\lambda\}_{\lambda\in\mathbb{R}})$ and $f_n(\lambda) \to g(\lambda)$ as $n \to \infty$ $\mu-$a.e. (i.e., $\lim_{n\to\infty} \|f_n(\lambda) - g(\lambda)\|_{\mathcal{K}_\lambda} = 0$ $\mu-$a.e.) then $g \in \mathcal{M}$.
(iii) If ϕ is a scalar-valued μ–measurable function and $f \in \mathcal{M}$ then $\phi f \in \mathcal{M}$.
(iv) If $f \in \mathcal{M}$ then $\mathbb{R} \ni \lambda \to \|f(\lambda)\|_{\mathcal{K}_\lambda} \in [0, \infty)$ is μ–measurable.

Let us remark that we shall identify functions in $\mathcal{M}$ which coincide $\mu-$a.e.; thus $\mathcal{M}$ is more precisely a set of equivalence classes of functions.

Lemma 2.3. *Let $\{f_n\}_{n\in\mathbb{N}} \subset \mathcal{S}(\{\mathcal{K}_\lambda\}_{\lambda\in\mathbb{R}})$ such that*
(α) $\mathbb{R} \ni \lambda \to (f_m(\lambda), f_n(\lambda)_{\mathcal{K}_\lambda} \in \mathbb{C}$ is μ–measurable for all $m, n \in \mathbb{N}$.
(β) For $\mu-$a.e. $\lambda \in \mathbb{R}$, $\overline{\text{lin.span}\{f_n(\lambda)\}} = \mathcal{K}_\lambda$.
Then setting

$$\mathcal{M} = \{g \in \mathcal{S}(\{\mathcal{K}_\lambda\}_{\lambda\in\mathbb{R}}) \,|\, (f_n(\lambda), g(\lambda))_{\mathcal{K}_\lambda} \text{ is } \mu\text{–measurable for all } n \in \mathbb{N}\}, \tag{2.2}$$

one infers
(i) $\mathcal{M}$ is a measurable family of Hilbert spaces.
(ii) $\mathcal{M}$ is generated by $\{f_n\}_{n\in\mathbb{N}}$.
(iii) $\mathcal{M}$ is the unique measurable family of Hilbert spaces containing the sequence $\{f_n\}_{n\in\mathbb{N}}$.
(iv) If $\{g_n\}$ is any sequence satisfying (β) then $\mathcal{M}$ is generated by $\{g_n\}$.

Sketch of proof. (i) Without loss of generality, we may assume $\{f_n\}_{n\in\mathbb{N}}$ contains all rational linear combinations, that is, all elements of the type $\sum_{n=1}^N \alpha_n f_n$, with $\alpha_n \in \mathbb{Q}$, $n = 1, \dots, N$, $N \in \mathbb{N}$. For $f \in \mathcal{S}(\{\mathcal{K}_\lambda\}_{\lambda\in\mathbb{R}})$,

$$\|f(\lambda)\|_{\mathcal{K}_\lambda} = \sup_{n\in\mathbb{N}} |(f(\lambda), \chi_{B_n}(\lambda) f_n(\lambda))_{\mathcal{K}_\lambda}|, \tag{2.3}$$

where $B_n = \{\lambda \in \mathbb{R} \,|\, \|f_n(\lambda)\|_{\mathcal{K}_\lambda} \leq 1\}$. Hence, if $f \in \mathcal{M}$ then the map $\mathbb{R} \ni \lambda \to \|f(\lambda)\|_{\mathcal{K}_\lambda} \in [0, \infty)$ is μ–measurable. It then follows easily that $\mathcal{M}$ is a measurable family of Hilbert spaces.
(ii) If $g \in \mathcal{M}$ then

$$\inf_{n\in\mathbb{N}} \|g(\lambda) - f_n(\lambda)\|_{\mathcal{K}_\lambda} = 0 \quad \mu-\text{a.e.} \tag{2.4}$$

It follows that if $\varepsilon(\lambda)$ is any measurable function with $\varepsilon > 0$ on $\mathbb{R}$, then one can find a measurable partition $\{B_n\}_{n\in\mathbb{N}}$ of $\mathbb{R}$ so that

$$\|g(\lambda) - \sum_{n\in\mathbb{N}} \chi_{B_n}(\lambda) f_n(\lambda)\|_{\mathcal{K}_\lambda} \leq \epsilon(\lambda). \tag{2.5}$$

Indeed, for each $\lambda \in \mathbb{R}$ let $N(\lambda)$ be the first n such that

$$\|g(\lambda) - f_{N(\lambda)}(\lambda)\|_{\mathcal{K}_\lambda} < \varepsilon(\lambda). \tag{2.6}$$

Then $\mathbb{R} \ni \lambda \to N(\lambda) \in \mathbb{N}$ is $\mu-$measurable and $B_n = \{\lambda \in \mathbb{R} \,|\, N(\lambda) = n\}$ is the desired partition. This implies (ii).

(iii) If $\mathcal{M}' \subset \mathcal{S}(\{\mathcal{K}_\lambda\}_{\lambda\in\mathbb{R}})$ is a measurable family of Hilbert spaces containing each $\{f_n\}_{n\in\mathbb{N}}$, then $\mathcal{M}' \subseteq \mathcal{M}$. However, $\mathcal{M} \subseteq \mathcal{M}'$ by (ii) then completes the argument.
(iv)This follows immediately from (iii), since we can define $\mathcal{M}'$ in a similar way, that is,

$$\mathcal{M}' = \{h \in \mathcal{S}(\{\mathcal{K}_\lambda\}_{\lambda\in\mathbb{R}}) \,|\, (g_n(\lambda), h(\lambda))_{\mathcal{K}_\lambda} \text{ is } \mu\text{–measurable for all } n \in \mathbb{N}\}, \tag{2.7}$$

and then $\mathcal{M} = \mathcal{M}'$ is clear from (iii). $\square$

Next, let w be a μ–measurable function, $w > 0$ $\mu-$a.e., and consider the space

$$\dot{L}^2(\mathcal{M}; wd\mu) = \{f \in \mathcal{M} \,|\, \int_{\mathbb{R}} w(\lambda)d\mu(\lambda)\|f(\lambda)\|^2_{\mathcal{K}_\lambda} < \infty\} \tag{2.8}$$

with its obvious linear structure. On $\dot{L}^2(\mathcal{M}; wd\mu)$ one defines a semi-inner product $(\cdot,\cdot)_{\dot{L}^2(\mathcal{M};wd\mu)}$ (and hence a semi-norm $\|\cdot\|_{\dot{L}^2(\mathcal{M};wd\mu)}$) by

$$(f, g)_{\dot{L}^2(\mathcal{M};wd\mu)} = \int_{\mathbb{R}} w(\lambda)d\mu(\lambda)(f(\lambda), g(\lambda))_{\mathcal{K}_\lambda}, \quad f, g \in \dot{L}^2(\mathcal{M}; wd\mu). \tag{2.9}$$

That (2.9) defines a semi-inner product immediately follows from the corresponding properties of $(\cdot,\cdot)_{\mathcal{K}_\lambda}$ and the linearity of the integral. Hence $\dot{L}^2(\mathcal{M}; wd\mu)$ represents a pre-Hilbert space and one can complete it in a standard manner as follows. One defines the equivalence relation $\sim$, for elements $f, g \in \dot{L}^2(\mathcal{M}; wd\mu)$ by

$$f \sim g \text{ if and only if } f = g \quad \mu - \text{a.e.} \tag{2.10}$$

and hence introduces the set of equivalence classes of $\dot{L}^2(\mathcal{M}; wd\mu)$ denoted by

$$L^2(\mathcal{M}; wd\mu) = \dot{L}^2(\mathcal{M}; wd\mu)/\sim . \tag{2.11}$$

In particular, introducing the subspace of null functions

$$\begin{aligned} \mathcal{N}(\mathcal{M}; wd\mu) &= \{f \in \dot{L}^2(\mathcal{M}; wd\mu) \,|\, \|f(\lambda)\|_{\mathcal{K}_\lambda} = 0 \text{ for } \mu - \text{a.e. } \lambda \in \mathbb{R}\} \\ &= \{f \in \dot{L}^2(\mathcal{M}; wd\mu) \,|\, \|f\|_{\dot{L}^2(\mathcal{M};wd\mu)} = 0\}, \end{aligned} \tag{2.12}$$

$L^2(\mathcal{M}; wd\mu)$ is precisely the quotient space $\dot{L}^2(\mathcal{M}; wd\mu)/\mathcal{N}(\mathcal{M}; wd\mu)$. Denoting the equivalence class of $f \in \dot{L}^2(\mathcal{M}; wd\mu)$ temporarily by $[f]$, the semi-inner product on $L^2(\mathcal{M}; wd\mu)$

$$([f], [g])_{L^2(\mathcal{M};wd\mu)} = \int_{\mathbb{R}} w(\lambda)d\mu(\lambda)(f(\lambda), g(\lambda))_{\mathcal{K}_\lambda} \tag{2.13}$$

is well-defined (i.e., independent of the chosen representatives of the equivalence classes) and actually an inner product. Thus $L^2(\mathcal{M}; wd\mu)$ is a normed space and by the usual abuse of notation we denote its elements in the following again by f, g, etc. The fundamental fact that $L^2(\mathcal{M}; wd\mu)$ is also complete is discussed next.

Theorem 2.4. *$L^2(\mathcal{M}; wd\mu)$ is complete and hence a Hilbert space.*

Proof. It suffices to prove the following fact: For each $\{f_n\}_{n\in\mathbb{N}} \in L^2(\mathcal{M}; wd\mu)$ with $\sum_{n\in\mathbb{N}} \|f_n\|_{L^2(\mathcal{M};wd\mu)} < \infty$, there is an $f \in L^2(\mathcal{M}; wd\mu)$ such that $\sum_{n\in\mathbb{N}} f_n = f$. Given such a sequence $\{f_n\}_{n\in\mathbb{N}}$ with $\sum_{n\in\mathbb{N}} \|f_n\|_{L^2(\mathcal{M};wd\mu)} = A$ define

$$G(\lambda) = \bigg(\sum_{n\in\mathbb{N}} \|f_n(\lambda)\|_{\mathcal{K}_\lambda}\bigg)^2. \tag{2.14}$$

Then G is $\mu-$measurable. From $\sum_{n=1}^{N} \|f_n\|_{L^2(\mathcal{M};wd\mu)} \leq A$ one computes using Minkowski's inequality,

$$\bigg(\int_{\mathbb{R}} w(\lambda)d\mu(\lambda)\bigg(\sum_{n=1}^{N} \|f_n(\lambda)\|_{\mathcal{K}_\lambda}\bigg)^2\bigg)^{1/2} \leq \sum_{n=1}^{N} \bigg(\int_{\mathbb{R}} w(\lambda)d\mu(\lambda)\|f_n(\lambda)\|^2_{\mathcal{K}_\lambda}\bigg)^{1/2} = \sum_{n=1}^{N} \|f_n\|_{L^2(\mathcal{M};wd\mu)} \leq A, \tag{2.15}$$

that is,

$$\int_{\mathbb{R}} w(\lambda)d\mu(\lambda)\bigg(\sum_{n=1}^{N} \|f_n(\lambda)\|_{\mathcal{K}_\lambda}\bigg)^2 \leq A^2. \tag{2.16}$$

Applying the Monotone Convergence Theorem one then concludes

$$\int_{\mathbb{R}} w(\lambda)d\mu(\lambda)G(\lambda) \leq A^2. \tag{2.17}$$

Thus G is integrable and hence $\mu-$a.e. finite. Consequently, we may define

$$f(\lambda) = \begin{cases} \sum_{n\in\mathbb{N}} f_n(\lambda), & \text{if } \sum_{n\in\mathbb{N}} \|f_n(\lambda)\|_{\mathcal{K}_\lambda} < \infty, \\ 0, & \text{otherwise.} \end{cases} \tag{2.18}$$

Then $\|f(\lambda)\|^2_{\mathcal{K}_\lambda} \leq G(\lambda)$ for $\mu-$a.e. $\lambda \in \mathbb{R}$ and

$$\sum_{n\in\mathbb{N}} f_n(\lambda) = f(\lambda) \quad \mu - \text{a.e.} \tag{2.19}$$

In particular, $f \in L^2(\mathcal{M};wd\mu)$. Finally, since

$$\bigg\|\sum_{n=1}^{N} f_n(\lambda) - f(\lambda)\bigg\|_{\mathcal{K}_\lambda} \to 0 \text{ as } N \to \infty \quad \mu - \text{a.e.} \tag{2.20}$$

and

$$\bigg\|f(\lambda) - \sum_{n=1}^{N} f_n(\lambda)\bigg\|^2_{\mathcal{K}_\lambda} = \bigg\|\sum_{n=N+1}^{\infty} f_n(\lambda)\bigg\|^2_{\mathcal{K}_\lambda} \leq G(\lambda) \quad \mu - \text{a.e.}, \tag{2.21}$$

the Lebesgue Dominated Convergence theorem yields

$$\lim_{N\to\infty} \bigg\|f - \sum_{n=1}^{N} f_n\bigg\|_{L^2(\mathcal{M};wd\mu)} = 0. \tag{2.22}$$

□

Clearly, the analogous construction defines the Banach spaces $L^p(\mathcal{M};wd\mu)$, $p \geq 1$. The case $p = 2$ corresponds precisely to the direct integral of the Hilbert spaces $\mathcal{K}_\lambda$ with respect to the measure $wd\mu$ (see, e.g., [11], Ch. 4, [12], Ch. 7).

Next, suppose $\mathcal{K}$ is a separable complex Hilbert space and $\Omega : \Sigma \to \mathcal{B}(\mathcal{K})$ is a positive measure (i.e., countably additive with respect to the strong operator topology in $\mathcal{K}$). Assume

$$\Omega(\mathbb{R}) = T \geq 0, \quad T \in \mathcal{B}(\mathcal{K}). \tag{2.23}$$

Moreover, let μ be a control measure for Ω, that is,

$$\mu(B) = 0 \text{ if and only if } \Omega(B) = 0 \text{ for all } B \in \Sigma. \tag{2.24}$$

(E.g., $\mu(B) = \sum_{n\in\mathcal{I}} 2^{-n}(e_n, \Omega(B)e_n)_{\mathcal{K}}$, with $\{e_n\}_{n\in\mathcal{I}}$ a complete orthonormal system in $\mathcal{K}$, $\mathcal{I} \subseteq \mathbb{N}$ an appropriate index set.)

Theorem 2.5. *There are separable complex Hilbert spaces $\mathcal{K}_\lambda$, $\lambda \in \mathbb{R}$, a measurable family of Hilbert spaces $\mathcal{M}_\Omega(\mu)$ modelled on μ and $\{\mathcal{K}_\lambda\}_{\lambda\in\mathbb{R}}$, and a bounded linear map $\underline{\Lambda} \in \mathcal{B}(\mathcal{K}, L^2(\mathcal{M}_\Omega(\mu); d\mu))$ so that*
(i) For all $B \in \Sigma$, $\xi, \eta \in \mathcal{K}$,

$$(\xi, \Omega(B)\eta)_{\mathcal{K}} = \int_B d\mu(\lambda)((\underline{\Lambda}\xi)(\lambda), (\underline{\Lambda}\eta)(\lambda))_{\mathcal{K}_\lambda}. \tag{2.25}$$

(ii) $\underline{\Lambda}(\{e_n\}_{n\in\mathcal{I}})$ generates $\mathcal{M}_\Omega(\mu)$, where $\{e_n\}_{n\in\mathcal{I}}$ denotes any sequence of linearly independent elements in $\mathcal{K}$ with the property $\overline{\text{lin.span}\{e_n\}_{n\in\mathcal{I}}} = \mathcal{K}$, $\mathcal{I} \subseteq \mathbb{N}$. In particular, $\underline{\Lambda}(\mathcal{K})$ generates $\mathcal{M}_\Omega(\mu)$.
(iii) For all $\xi \in \mathcal{K}$,

$$\underline{\Lambda}(\Omega(B)\xi) = \chi_B \underline{\Lambda}\xi \quad \mu - a.e. \tag{2.26}$$

Proof. Denote $\mathcal{V} = \text{lin.span}\{e_n\}_{n\in\mathcal{I}}$. By the Radon-Nikodym theorem, there exist μ–measurable $\phi_{m,n}$ such that

$$\int_B d\mu(\lambda)\phi_{m,n}(\lambda) = (e_m, \Omega(B)e_n)_{\mathcal{K}}. \tag{2.27}$$

Next, suppose $v = \sum_{n=1}^N \alpha_n e_n \in \mathcal{V}$, $\alpha_n \in \mathbb{C}$, $n = 1, \dots, N$, $N \in \mathcal{I}$. Then

$$(v, \Omega(B)v)_{\mathcal{K}} = \int_B d\mu(\lambda) \sum_{m,n=1}^N \phi_{m,n}(\lambda)\overline{\alpha_m}\alpha_n. \tag{2.28}$$

By considering only rational linear combinations we can deduce that for μ–a.e. $\lambda \in \mathbb{R}$,

$$\sum_{m,n} \phi_{m,n}(\lambda)\overline{\alpha_m}\alpha_n \geq 0 \text{ for all finite sequences } \{\alpha_n\} \subset \mathbb{C}. \tag{2.29}$$

Hence we can define a semi-inner product $(\cdot,\cdot)_\lambda$ on $\mathcal{V}$ such that

$$(v, w)_\lambda = \sum_{m,n} \phi_{m,n}(\lambda)\overline{\alpha_m}\beta_n \quad \mu - \text{a.e} \tag{2.30}$$

if $v = \sum_n \alpha_n e_n$, $w = \sum_n \beta_n e_n$.
Next, let $\mathcal{K}_\lambda$ be the completion of $\mathcal{V}$ with respect $\|\cdot\|_\lambda$ (or, more precisely the completion of $\mathcal{V}/\mathcal{N}_\lambda$ where $\mathcal{N}_\lambda = \{\xi \in \mathcal{V} \,|\, (\xi,\xi)_\lambda = 0\}$) and consider $\mathcal{S}(\{\mathcal{K}_\lambda\}_{\lambda\in\mathbb{R}})$. Each $v \in \mathcal{V}$ defines an element $\underline{v} = \{\underline{v}(\lambda)\}_{\lambda\in\mathbb{R}} \in \mathcal{S}(\{\mathcal{K}_\lambda\}_{\lambda\in\mathbb{R}})$ by

$$\underline{v}(\lambda) = v \text{ for all } \lambda \in \mathbb{R}. \tag{2.31}$$

Again we identify an element $v \in \mathcal{V}$ with an element in $\mathcal{V}/\mathcal{N}_\lambda \subseteq \mathcal{K}_\lambda$. Applying Lemma 2.3, the collection $\{\underline{e}_n\}_{n\in\mathcal{I}}$ then generates a measurable family of Hilbert spaces $\mathcal{M}_\Omega(\mu)$. If $v \in \mathcal{V}$ then

$$\|\underline{v}\|^2_{L^2(\mathcal{M}_\Omega(\mu);d\mu)} = \int_{\mathbb{R}} d\mu(\lambda)(\underline{v}(\lambda), \underline{v}(\lambda))_\lambda = (v, Tv)_{\mathcal{K}} = \|T^{1/2}v\|^2_{\mathcal{K}}. \tag{2.32}$$

Hence we can define

$$\dot{\underline{\Lambda}} : \mathcal{V} \to L^2(\mathcal{M}_\Omega(\mu); d\mu), \quad v \to \dot{\underline{\Lambda}}v = \underline{v} = \{\underline{v}(\lambda) = v\}_{\lambda\in\mathbb{R}} \tag{2.33}$$

and denote by $\underline{\Lambda} \in \mathcal{B}(\mathcal{K}, L^2(\mathcal{M}_\Omega(\mu); d\mu))$, $\|\underline{\Lambda}\|_{\mathcal{B}(\mathcal{K},L^2(\mathcal{M}_\Omega(\mu);d\mu))} = \|T^{1/2}\|_{\mathcal{B}(\mathcal{K})}$, the closure of $\dot{\underline{\Lambda}}$. Then properties (i)–(iii) hold. □

We now show that this construction is essentially unique.

Theorem 2.6. *Suppose $\mathcal{K}'_\lambda$, $\lambda \in \mathbb{R}$ is a family of separable complex Hilbert spaces, $\mathcal{M}'$ is a measurable family of Hilbert spaces modelled on μ and $\{\mathcal{K}'_\lambda\}$, and $\underline{\Lambda}' \in \mathcal{B}(\mathcal{K}, L^2(\mathcal{M}'; d\mu))$ is a map satisfying (i),(ii), and (iii) of the preceding theorem. Then for μ-a.e. $\lambda \in \mathbb{R}$ there is a unitary operator $U_\lambda : \mathcal{K}_\lambda \to \mathcal{K}'_\lambda$ such that $f = \{f(\lambda)\}_{\lambda\in\mathbb{R}} \in \mathcal{M}_\Omega(\mu)$ if and only if $U_\lambda f(\lambda) \in \mathcal{M}'$ and for all $\xi \in \mathcal{K}$,*

$$(\underline{\Lambda}'\xi)(\lambda) = U_\lambda(\underline{\Lambda}\xi)(\lambda) \quad \mu - a.e. \tag{2.34}$$

Proof. We use the notation of the preceding theorem. We select representatives $f'_n \in \mathcal{M}'$ of $\underline{\Lambda}' e_n$. It follows from condition (i) that for $\mu-$a.e. $\lambda \in \mathbb{R}$ and every $m, n \in \mathcal{I}$ we have

$$(f'_m(\lambda), f'_n(\lambda))_{\mathcal{K}'_\lambda} = (e_m, e_n)_\lambda = (\underline{e}_m(\lambda), \underline{e}_n(\lambda))_{\mathcal{K}_\lambda}. \tag{2.35}$$

Hence we can induce an isometry $U_\lambda : \mathcal{K}_\lambda \to \mathcal{K}'_\lambda$ such that $U_\lambda \underline{e}_n(\lambda) = f'_n(\lambda)$.

It is easy to see that if $v \in \mathcal{V}$ we must have $U_\lambda \underline{v}(\lambda) = (\underline{\Lambda}' v)(\lambda)$ $\mu-$a.e. From the L_2-continuity of both $\underline{\Lambda}$ and $\underline{\Lambda}'$ it follows that for every $\xi \in \mathcal{K}$ we have

$$(\underline{\Lambda}'\xi)(\lambda) = U_\lambda(\underline{\Lambda}\xi)(\lambda) \quad \mu - \text{a.e.} \tag{2.36}$$

We next observe that if $\underline{\Lambda}'(\mathcal{K})$ generates $\mathcal{M}'$ then by a density argument it must also be true that $\{f'_n\}_{n\in\mathcal{I}}$ generates $\mathcal{M}'$. It is then immediate that the linear span of $\{f'_n(\lambda)\}_{n\in\mathcal{I}}$ must be dense for $\mu-$a.e. $\lambda \in \mathbb{R}$. Thus U_λ is actually surjective $\mu-$a.e. and so is unitary.

Finally, if $\xi \in \mathcal{K}$ and $B \in \Sigma$ then $U_\lambda(\chi_B(\lambda)(\underline{\Lambda}\xi)(\lambda)) = \chi_B(\lambda)(\underline{\Lambda}'\xi)(\lambda)$ $\mu-$a.e. Thus it follows by approximation that if $f \in \mathcal{M}_\Omega(\mu)$ then $U_\lambda f(\lambda) \in \mathcal{M}'$. Conversely, a similar argument shows that if $f \in \mathcal{M}'$ then $U_\lambda^{-1} f(\lambda) \in \mathcal{M}_\Omega(\mu)$. ☐

Without going into further details, we note that $\mathcal{M}_\Omega(\mu)$ depends of course on μ. However, a change in μ merely effects a change in density and so $\mathcal{M}_\Omega(\mu)$ can essentially be viewed as $\mu-$independent.

Next, using the notation employed in the proof of Theorem 2.4 we recall

$$\mathcal{V} = \text{lin.span}\{e_n \in \mathcal{K} \,|\, n \in \mathcal{I}\} \tag{2.37}$$

and define

$$\underline{\mathcal{V}}_\Omega = \text{lin.span}\{\chi_B \underline{e}_n \in L^2(\mathcal{M}_\Omega(\mu); d\mu) \,|\, B \in \Sigma,\, n \in \mathcal{I}\}. \tag{2.38}$$

The fact that $\{\underline{e}_n\}_{n\in\mathcal{I}}$ generates $\mathcal{M}_\Omega(\mu)$ implies that $\underline{\mathcal{V}}_\Omega$ is dense in $L^2(\mathcal{M}_\Omega(\mu); d\mu)$, that is,

$$\overline{\underline{\mathcal{V}}_\Omega} = L^2(\mathcal{M}_\Omega(\mu); d\mu). \tag{2.39}$$

The following result will be used in Section 3.

Lemma 2.7. *Suppose $\mathcal{K}$, $\mathcal{H}$ are separable complex Hilbert spaces, $K \in \mathcal{B}(\mathcal{K}, \mathcal{H})$, $\{E(B)\}_{B\in\Sigma}$ is a family of orthogonal projections in $\mathcal{H}$, and assume*

$$\overline{\mathit{lin.span}\{E(B)Ke_n \in \mathcal{H} \,|\, B \in \Sigma,\, n \in \mathcal{I}\}} = \mathcal{H}, \tag{2.40}$$

with $\{e_n\}_{n\in\mathcal{I}}$, $\mathcal{I} \subset \mathbb{N}$ a complete orthonormal system in $\mathcal{K}$. Define

$$\Omega : \Sigma \to \mathcal{B}(\mathcal{K}), \quad \Omega(B) = K^* E(B) K, \tag{2.41}$$

and introduce

$$\dot{U} : \underline{\mathcal{V}}_\Omega \to \mathcal{H},$$

$$\underline{\mathcal{V}}_\Omega \ni \sum_{m=1}^{M}\sum_{n=1}^{N} \alpha_{m,n}\chi_{B_m}\underline{e}_n \to \dot{U}\Big(\sum_{m=1}^{M}\sum_{n=1}^{N} \alpha_{m,n}\chi_{B_m}\underline{e}_n\Big) \tag{2.42}$$
$$= \sum_{m=1}^{M}\sum_{n=1}^{N} \alpha_{m,n}E(B_m)Ke_n \in \mathcal{H},$$
$$\alpha_{m,n} \in \mathbb{C},\ m=1,\dots,M,\ n=1,\dots,N,\ M,N\in\mathcal{I}.$$

Then $\dot{U}$ extends to a unitary operator $U : L^2(\mathcal{M}_\Omega(\mu); d\mu) \to \mathcal{H}$.

Proof. One computes

$$\begin{aligned}
&\Big\|\dot{U}\Big(\sum_{m=1}^{M}\sum_{n=1}^{N} \alpha_{m,n}\chi_{B_m}\underline{e}_n\Big)\Big\|_{\mathcal{H}}^2 \\
&= \sum_{m_1,m_2=1}^{M}\sum_{n_1,n_2=1}^{N} \overline{\alpha_{m_1,n_1}}\alpha_{m_2,n_2}(e_{n_1}, K^*E(B_{m_1}\cap B_{m_2})Ke_{n_2})_{\mathcal{K}} \\
&= \sum_{m_1,m_2=1}^{M}\sum_{n_1,n_2=1}^{N} \overline{\alpha_{m_1,n_1}}\alpha_{m_2,n_2}(e_{n_1}, \Omega(B_{m_1}\cap B_{m_2})e_{n_2})_{\mathcal{K}} \\
&= \sum_{m_1,m_2=1}^{M}\sum_{n_1,n_2}^{N} \overline{\alpha_{m_1,n_1}}\alpha_{m_2,n_2}\int_{B_{m_1}\cap B_{m_2}} d\mu(\lambda)(\underline{e}_{n_1}(\lambda), \underline{e}_{n_2}(\lambda))_{\mathcal{K}_\lambda} \\
&= \Big\|\sum_{m=1}^{M}\sum_{n=1}^{N} \alpha_{m,n}\chi_{B_m}\underline{e}_n\Big\|_{L^2(\mathcal{M}_\Omega(\mu);d\mu)}^2 .
\end{aligned} \tag{2.43}$$

By (2.39), $\dot{U}$ is densely defined and thus extends to an isometry U of $L^2(\mathcal{M}_\Omega(\mu); d\mu)$ into $\mathcal{H}$. In particular, $\operatorname{ran}(U)$ is closed in $\mathcal{H}$. Thus,

$$\operatorname{ran}(U) \supseteq \overline{\text{lin.span}\{E(B)Ke_n \in \mathcal{H} \,|\, B\in\Sigma,\, n\in\mathcal{I}\}} = \mathcal{H} \tag{2.44}$$

by hypothesis (2.41) and hence $U : L^2(\mathcal{M}_\Omega(\mu); d\mu) \to \mathcal{H}$ is a unitary operator. $\square$

In view of our comment following Theorem 2.6, concerning the mild dependence on the control measure μ of $\mathcal{M}_\Omega(\mu)$, we will put more emphasis on the operator-valued measure Ω and hence use the notation $L^2(\mathbb{R}, \mathcal{K}; wd\Omega)$ instead of the more precise $L^2(\mathcal{M}_\Omega(\mu); wd\mu)$ in Section 3.

Finally we adapt Lemma 2.7 to the content of Section 4.

Suppose $\mathcal{N}$ is a separable complex Hilbert space and $\widetilde{\Omega} : \Sigma \to \mathcal{B}(\mathcal{N})$ a positive measure. Assume

$$\widetilde{\Omega}(\mathbb{R}) = \widetilde{T} \geq 0, \quad \widetilde{T} \in \mathcal{B}(\mathcal{N}) \tag{2.45}$$

and let $\tilde{\mu}$ be a control measure for $\widetilde{\Omega}$. Moreover, let $\{u_n\}_{n\in\mathcal{I}}$, $\mathcal{I}\subseteq\mathbb{N}$ be a sequence of linearly independent elements in $\mathcal{N}$ with the property $\overline{\text{lin.span}\{u_n\}_{n\in\mathcal{I}}} = \mathcal{N}$. As discussed in Theorem 2.5, this yields a measurable family of Hilbert spaces $\mathcal{M}_{\widetilde{\Omega}}(\tilde{\mu})$ modelled on $\tilde{\mu}$ and $\{\mathcal{N}_\lambda\}_{\lambda\in\mathbb{R}}$ and a bounded map $\underline{\Lambda} \in \mathcal{B}(\mathcal{N}, L^2(\mathcal{M}_{\widetilde{\Omega}}(\tilde{\mu}); d\tilde{\mu}))$, $\|\underline{\Lambda}\|_{\mathcal{B}(\mathcal{N},L^2(\mathcal{M}_{\widetilde{\Omega}}(\tilde{\mu});d\tilde{\mu}))} = \|\widetilde{T}^{1/2}\|_{\mathcal{B}(\mathcal{N})}$, such that $\underline{\Lambda}(\{u_n\}_{n\in\mathcal{I}})$ generates $\mathcal{M}_{\widetilde{\Omega}}(\tilde{\mu})$ and

$$\underline{\Lambda} : \mathcal{V} \to L^2(\mathcal{M}_{\widetilde{\Omega}}(\tilde{\mu}); d\tilde{\mu}), \quad v \to \underline{\Lambda}v = \underline{v} = \{\underline{v}(\lambda) = v\}_{\lambda\in\mathbb{R}}, \tag{2.46}$$

where

$$\mathcal{V} = \text{lin.span}\{u_n\}_{n\in\mathcal{I}}. \tag{2.47}$$

Each $v \in \mathcal{V}$ defines an element

$$\underline{\underline{v}} = \{\underline{\underline{v}}(\lambda) = (\lambda - i)^{-1}v\}_{\lambda\in\mathbb{R}} \in \mathcal{S}(\{\mathcal{N}_\lambda\}_{\lambda\in\mathbb{R}}) \tag{2.48}$$

and introducing the weight function

$$w_1(\lambda) = 1 + \lambda^2, \quad \lambda \in \mathbb{R} \tag{2.49}$$

and Hilbert space $L^2(\mathcal{M}_{\tilde\Omega}(\tilde\mu); w_1 d\tilde\mu)$ one computes

$$\|\underline{\underline{v}}\|^2_{L^2(\mathcal{M}_{\tilde\Omega}(\tilde\mu);d\tilde\mu)} = \int_{\mathbb{R}} d\tilde\mu(\lambda)\|\underline{\underline{v}}(\lambda)\|^2_{\mathcal{N}_\lambda} = (v, \widetilde{T}v)_{\mathcal{N}} = \|\widetilde{T}^{1/2}v\|^2_{\mathcal{N}}. \tag{2.50}$$

Thus, the linear map

$$\dot{\underline{\underline{\Lambda}}} : \mathcal{V} \to L^2(\mathcal{M}_{\tilde\Omega}(\tilde\mu); w_1 d\tilde\mu), \quad v \to \dot{\underline{\underline{\Lambda}}}v = \underline{\underline{v}} = \{\underline{\underline{v}}(\lambda) = (\lambda - i)^{-1}v\}_{\lambda\in\mathbb{R}} \tag{2.51}$$

extends to $\underline{\underline{\Lambda}} \in \mathcal{B}(\mathcal{N}, L^2(\mathcal{M}_{\tilde\Omega}(\tilde\mu); w_1 d\tilde\mu))$, $\|\underline{\underline{\Lambda}}\|_{\mathcal{B}(\mathcal{N},L^2(\mathcal{M}_{\tilde\Omega}(\tilde\mu);w_1 d\tilde\mu))} = \|\widetilde{T}^{1/2}\|_{\mathcal{B}(\mathcal{N})}$. Introducing

$$\underline{\underline{\mathcal{V}}}_{\tilde\Omega} = \text{lin.span}\{\chi_B \underline{\underline{v}} \in L^2(\mathcal{M}_{\tilde\Omega}(\tilde\mu); w_1 d\tilde\mu) \,|\, B \in \Sigma,\, n \in \mathcal{I}\} \tag{2.52}$$

one infers that $\underline{\underline{\mathcal{V}}}_{\tilde\Omega}$ is dense in $L^2(\mathcal{M}_{\tilde\Omega}(\tilde\mu); w_1 d\tilde\mu)$, that is,

$$\overline{\underline{\underline{\mathcal{V}}}_{\tilde\Omega}} = L^2(\mathcal{M}_{\tilde\Omega}(\tilde\mu); w_1 d\tilde\mu). \tag{2.53}$$

Given these preliminaries we can state the following result.

Lemma 2.8. *Suppose $\mathcal{H}$ is a separable complex Hilbert space, $\mathcal{N}$ a closed linear subspace of $\mathcal{H}$, $P_{\mathcal{N}}$ the orthogonal projection in $\mathcal{H}$ onto $\mathcal{N}$, $\{E(B)\}$, $B \in \Sigma$ a family of orthogonal projections in $\mathcal{H}$, and assume*

$$\overline{\textit{lin.span}\{E(B)u_n \in \mathcal{H} \,|\, B \in \Sigma,\, n \in \mathcal{I}\}} = \mathcal{H}, \tag{2.54}$$

with $\{u_n\}_{n\in\mathcal{I}}$, $\mathcal{I} \subseteq \mathbb{N}$ a complete orthonormal system in $\mathcal{N}$. Define

$$\widetilde\Omega : \Sigma \to \mathcal{B}(\mathcal{N}), \quad \widetilde\Omega(B) = P_{\mathcal{N}} E(B) P_{\mathcal{N}}\big|_{\mathcal{N}}, \tag{2.55}$$

and introduce

$$\begin{aligned} &\dot{\widetilde{U}} : \underline{\underline{\mathcal{V}}}_\Omega \to \mathcal{H}, \\ &\underline{\underline{\mathcal{V}}}_\Omega \ni \sum_{m=1}^{M}\sum_{n=1}^{N} \alpha_{m,n}\chi_{B_m}\underline{\underline{u}}_n \to \dot{\widetilde{U}}\bigg(\sum_{m=1}^{M}\sum_{n=1}^{N} \alpha_{m,n}\chi_{B_m}\underline{\underline{u}}_n\bigg) \\ &\qquad\qquad = \sum_{m=1}^{M}\sum_{n=1}^{N} \alpha_{m,n} E(B_m)u_n \in \mathcal{H}, \\ &\qquad \alpha_{m,n} \in \mathbb{C},\ m = 1, \dots, M,\ n = 1, \dots, N,\ M, N \in \mathcal{I}. \end{aligned} \tag{2.56}$$

Then $\dot{\widetilde{U}}$ extends to a unitary operator $\widetilde{U} : L^2(\mathcal{M}_{\tilde\Omega}(\tilde\mu); w_1 d\mu) \to \mathcal{H}$.

Proof. One computes

$$\bigg\|\dot{\widetilde{U}}\bigg(\sum_{m=1}^{M}\sum_{n=1}^{N} \alpha_{m,n}\chi_{B_m}\underline{\underline{u}}_n\bigg)\bigg\|^2_{\mathcal{H}}$$

$$
\begin{aligned}
&= \sum_{m_1,m_2=1}^{M} \sum_{n_1,n_2=1}^{N} \overline{\alpha_{m_1,n_1}} \alpha_{m_2,n_2} (u_{n_1}, E(B_{m_1} \cap B_{m_2}) u_{n_2})_{\mathcal{N}} \\
&= \sum_{m_1,m_2=1}^{M} \sum_{n_1,n_2=1}^{N} \overline{\alpha_{m_1,n_1}} \alpha_{m_2,n_2} (u_{n_1}, \widetilde{\Omega}(B_{m_1} \cap B_{m_2}) u_{n_2})_{\mathcal{N}} \\
&= \sum_{m_1,m_2=1}^{M} \sum_{n_1,n_2}^{N} \overline{\alpha_{m_1,n_1}} \alpha_{m_2,n_2} \int_{B_{m_1} \cap B_{m_2}} d\tilde{\mu}(\lambda) (\underline{u}_{n_1}(\lambda), \underline{u}_{n_2}(\lambda))_{\mathcal{N}_\lambda} \\
&= \bigg\| \sum_{m=1}^{M} \sum_{n=1}^{N} \alpha_{m,n} \chi_{B_m} \underline{u}_n \bigg\|^2_{L^2(\mathcal{M}_{\tilde{\Omega}}(\tilde{\mu}); w_1 d\tilde{\mu})}. \qquad (2.57)
\end{aligned}
$$

By (2.53), $\dot{\widetilde{U}}$ is densely defined and extends to an isometry $\widetilde{U}$ of $L^2(\mathcal{M}_{\tilde{\Omega}}(\tilde{\mu}); w_1 d\tilde{\mu})$ into $\mathcal{H}$. In particular, $\operatorname{ran}(\widetilde{U})$ is closed in $\mathcal{H}$. Thus,

$$
\operatorname{ran}(\widetilde{U}) \supseteq \overline{\operatorname{lin.span}\{E(B)u_n \in \mathcal{H} \,|\, B \in \Sigma,\, n \in \mathcal{I}\}} = \mathcal{H} \qquad (2.58)
$$

by hypothesis (2.54) and hence $U : L^2(\mathcal{M}_{\tilde{\Omega}}(\tilde{\mu}); w_1 d\tilde{\mu}) \to \mathcal{H}$ is a unitary operator. ☐

Analogous to our comments following Lemma 2.7, in Section 4 we will emphasize the role of $\widetilde{\Omega}$ and hence use the somewhat imprecise notation $L^2(\mathbb{R}, \mathcal{N}; wd\widetilde{\Omega})$, with various weight functions w, as opposed to the precise notation $L^2(\mathcal{M}_{\tilde{\Omega}}(\tilde{\mu}); wd\tilde{\mu})$.

3. On Self-Adjoint Perturbations of Self-Adjoint Operators

In this section we will focus on the following perturbation problem. Assuming

Hypothesis 3.1. *Let $\mathcal{H}$ and $\mathcal{K}$ be separable complex Hilbert spaces, H_0 a self-adjoint (possibly unbounded) operator in $\mathcal{H}$, L a bounded self-adjoint operator in $\mathcal{K}$, and $K : \mathcal{K} \to \mathcal{H}$ a bounded operator,*

we define the self-adjoint operator H_L in $\mathcal{H}$,

$$
H_L = H_0 + KLK^*, \quad \operatorname{dom}(H_L) = \operatorname{dom}(H_0). \qquad (3.1)
$$

Given the perturbation H_L of H_0, we introduce the associated operator-valued Herglotz function in $\mathcal{K}$,

$$
M_L(z) = K^*(H_L - z)^{-1} K, \quad z \in \mathbb{C}\backslash\mathbb{R}, \qquad (3.2)
$$

$$
\frac{1}{\operatorname{Im}(z)} \operatorname{Im}(M_L(z)) = ((H_L - z)^{-1}K)^*(H_L - z)^{-1}K \geq 0, \quad z \in \mathbb{C}\backslash\mathbb{R}, \qquad (3.3)
$$

and study the pair (H_L, H_0) in terms of the corresponding pair $(M_L(z), M_0(z))$. In the special case where $\dim_{\mathbb{C}}(\mathcal{K}) = 1$, this perturbation problem has been studied in detail by Donoghue [25] and later by Simon and Wolf [60] (see also [59]). The case $\dim_{\mathbb{C}}(\mathcal{K}) = n \in \mathbb{N}$, has recently been treated in depth in [30]. In this section we treat the general case $\dim_{\mathbb{C}}(\mathcal{K}) \in \mathbb{N} \cup \{\infty\}$.

Next, let $\{E_0(\lambda)\}_{\lambda \in \mathbb{R}}$ be the family of strongly right-continuous orthogonal spectral projections of H_0 in $\mathcal{H}$ and suppose that $K\mathcal{K} \subseteq \mathcal{H}$ is a generating subspace for H_0, that is, one of the following (equivalent) equations holds in

Hypothesis 3.2.

$$\mathcal{H} = \overline{lin.span\{(H_0 - z)^{-1}Ke_n \in \mathcal{H} \,|\, n \in \mathcal{I},\, z \in \mathbb{C}\backslash\mathbb{R}\}} \tag{3.4a}$$

$$= \overline{lin.span\{E_0(\lambda)Ke_n \in \mathcal{H} \,|\, n \in \mathcal{I},\, \lambda \in \mathbb{R}\}}, \tag{3.4b}$$

where $\{e_n\}_{n\in\mathcal{I}}$, $\mathcal{I} \subseteq \mathbb{N}$ an appropriate index set, represents a complete orthonormal system in $\mathcal{K}$.

Denoting by $\{E_L(\lambda)\}_{\lambda\in\mathbb{R}}$ the family of strongly right-continuous orthogonal spectral projections of H_L in $\mathcal{H}$ one introduces

$$\Omega_L(\lambda) = K^* E_L(\lambda) K, \quad \lambda \in \mathbb{R} \tag{3.5}$$

and hence verifies

$$M_L(z) = K^*(H_L - z)^{-1}K = K^* \int_{\mathbb{R}} dE_L(\lambda)(\lambda - z)^{-1}K$$

$$= \int_{\mathbb{R}} d\Omega_L(\lambda)(\lambda - z)^{-1}, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{3.6}$$

where the operator Stieltjes integral (3.6) converges in the norm of $\mathcal{B}(\mathcal{K})$ (cf. Theorems I.4.2 and I.4.8 in [17]). Since $\text{s-lim}_{z\to i\infty} z(H_L - z)^{-1} = -I_{\mathcal{H}}$, (3.5) implies

$$\Omega_L(\mathbb{R}) = K^*K. \tag{3.7}$$

Moreover, since $\text{s-lim}_{\lambda\downarrow-\infty} E_L(\lambda) = 0$, $\text{s-lim}_{\lambda\uparrow\infty} E_L(\lambda) = I_{\mathcal{H}}$, one infers

$$\operatorname*{s-lim}_{\lambda\downarrow-\infty} \Omega_L(\lambda) = 0, \quad \operatorname*{s-lim}_{\lambda\uparrow\infty} \Omega_L(\lambda) = K^*K \tag{3.8}$$

and $\{\Omega_L(\lambda)\}_{\lambda\in\mathbb{R}} \subset \mathcal{B}(\mathcal{K})$ is a family of uniformly bounded, nonnegative, nondecreasing, strongly right-continuous operators from $\mathcal{K}$ into itself. Let μ_L be a $\sigma-$finite control measure on $\mathbb{R}$ defined, for instance, by

$$\mu_L(\lambda) = \sum_{n\in\mathcal{I}} 2^{-n}(e_n, \Omega_L(\lambda)e_n)_{\mathcal{K}}, \quad \lambda \in \mathbb{R}, \tag{3.9}$$

where $\{e_n\}_{n\in\mathcal{I}}$ denotes a complete orthonormal system in $\mathcal{K}$, and then introduce $L^2(\mathcal{M}_{\Omega_L}(\mu_L); d\mu_L)$ as in Section 3, replacing the pair (Ω, μ) by (Ω_L, μ_L), etc. As noted in Section 2, we will actually use the more suggestive notation $L^2(\mathbb{R}, \mathcal{K}; wd\Omega_L)$ instead of the more precise $L^2(\mathcal{M}_{\Omega_L}(\mu_L); wd\mu_L)$ ($w > 0$ a weight function), for the remainder of this section. Abbreviating $\widehat{\mathcal{H}}_L = L^2(\mathbb{R}, \mathcal{K}; d\Omega_L)$, we introduce the unitary operator $U_L : \widehat{\mathcal{H}}_L \to \mathcal{H}$, as the operator U in Lemma 2.7 and define $\widehat{H}_L$ in $\widehat{\mathcal{H}}_L$ by

$$(\widehat{H}_L \hat{f})(\lambda) = \lambda \hat{f}(\lambda), \quad \hat{f} \in \operatorname{dom}(\widehat{H}_L) = L^2(\mathbb{R}, \mathcal{K}; (1 + \lambda^2)d\Omega_L). \tag{3.10}$$

Theorem 3.3. *Assume Hypotheses* 3.1 *and* 3.2*. Then H_L in $\mathcal{H}$ is unitarily equivalent to $\widehat{H}_L$ in $\widehat{\mathcal{H}}_L$,*

$$H_L = U_L \widehat{H}_L U_L^{-1}. \tag{3.11}$$

The family of strongly right-continuous orthogonal spectral projections $\{\widehat{E}_L(\lambda)\}_{\lambda\in\mathbb{R}}$ of $\widehat{H}_L$ in $\widehat{\mathcal{H}}_L$ is given by

$$(\widehat{E}_L(\lambda)\hat{f})(\nu) = \theta(\lambda - \nu)\hat{f}(\nu) \text{ for } \Omega_L - a.e.\ \nu \in \mathbb{R}, \quad \hat{f} \in \widehat{\mathcal{H}}_L,\ \theta(x) = \begin{cases} 1, & x \geq 0, \\ 0, & x < 0. \end{cases} \tag{3.12}$$

Proof. Consider

$$\underline{e}_n = \{\underline{e}_n(\lambda) = e_n\}_{\lambda\in\mathbb{R}} \in \widehat{\mathcal{H}}_L, \quad n \in \mathcal{I}, \tag{3.13}$$

then

$$U_L\underline{e}_n = \int_{\mathbb{R}} dE_L(\lambda)Ke_n = Ke_n, \quad n \in \mathcal{I} \tag{3.14}$$

and

$$((\widehat{H}_L - z)^{-1}\underline{e}_n)(\lambda) = (\lambda - z)^{-1}\underline{e}_n(\lambda) = (\lambda - z)^{-1}e_n, \quad n \in \mathcal{I},\ z \in \mathbb{C}\backslash\mathbb{R} \tag{3.15}$$

yield

$$U_L(\widehat{H}_L - z)^{-1}\underline{e}_n = \int_{\mathbb{R}} dE_L(\lambda)(\lambda - z)^{-1}Ke_n = (H_L - z)^{-1}Ke_n, \quad n \in \mathcal{I},\, z \in \mathbb{C}\backslash\mathbb{R}. \tag{3.16}$$

Using the resolvent equation for H_L and H_0,

$$\begin{aligned}(H_L - z)^{-1} &= (H_0 - z)^{-1} - (H_L - z)^{-1}KLK^*(H_0 - z)^{-1} && (3.17a)\\ &= (H_0 - z)^{-1} - (H_0 - z)^{-1}KLK^*(H_L - z)^{-1}, \quad z \in \mathbb{C}\backslash\mathbb{R}, && (3.17b)\end{aligned}$$

one verifies

$$\begin{aligned}&(I_{\mathcal{K}} + LK^*(H_0 - z)^{-1}K)(I_{\mathcal{K}} - LK^*(H_L - z)^{-1}K) && (3.18)\\ &= (I_{\mathcal{K}} - LK^*(H_L - z)^{-1}K)(I_{\mathcal{K}} + LK^*(H_0 - z)^{-1}K) = I_{\mathcal{K}}, \quad z \in \mathbb{C}\backslash\mathbb{R} && (3.19)\end{aligned}$$

and

$$(H_L - z)^{-1}K = (H_0 - z)^{-1}K(I_{\mathcal{K}} + LK^*(H_0 - z)^{-1}K)^{-1}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{3.20}$$

Since

$$(I_{\mathcal{K}} + LK^*(H_0 - z)^{-1}K)^{-1} \in \mathcal{B}(\mathcal{K}), \quad z \in \mathbb{C}\backslash\mathbb{R} \tag{3.21}$$

by (3.18), one infers

$$\operatorname{ran}((I_{\mathcal{K}} + LK^*(H_0 - z)^{-1}K)^{-1}) = \mathcal{K}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{3.22}$$

Since by our assumption (3.4), finite linear combinations of $(H_0 - z)^{-1}Ke_n$, $n \in \mathcal{I}$, $z \in \mathbb{C}\backslash\mathbb{R}$ are dense in $\mathcal{H}$, (3.20) and (3.22) then yield the same assertion for $(H_L - z)^{-1}Ke_n$. (I.e., (3.4) is valid with H_0 replaced by any H_L.) Since U_L is unitary by Lemma 2.7, finite linear combinations of vectors of the form $(\widehat{H}_L - z)^{-1}\underline{e}_n$ (cf. (3.16)) are also dense in $\widehat{\mathcal{H}}$. This fact, (3.16), and the first resolvent equation for $\widehat{H}_L$ yield

$$\begin{aligned}&U_L(\widehat{H}_L - z)^{-1}U_L^{-1}U_L(\widehat{H}_L - z')^{-1}\underline{e}_n = U_L(\widehat{H}_L - z)^{-1}U_L^{-1}(H_L - z')^{-1}Ke_n\\ &= (H_L - z)^{-1}(H_L - z')^{-1}Ke_n, \quad n \in \mathcal{I},\ z, z' \in \mathbb{C}\backslash\mathbb{R}. && (3.23)\end{aligned}$$

Since finite linear combinations of $(H_L - z')^{-1}Ke_n$, $n \in \mathcal{I}$ are dense in $\mathcal{H}$ we get

$$U_L(\widehat{H}_L - z)^{-1}U_L^{-1} = (H_L - z)^{-1}, \quad z \in \mathbb{C}\backslash\mathbb{R} \tag{3.24}$$

and hence (3.11). Equation (3.12) is then obvious from (2.26) since $\widehat{H}_L$ is the operator of multiplication by λ in $\widehat{\mathcal{H}}_L$. □

If L_ℓ, $\ell = 1, 2$ are two bounded self-adjoint operators in $\mathcal{K}$ (with $\mathcal{H}, \mathcal{K}, H_0$, and K fixed, i.e., independent of $\ell = 1, 2$) one proves the following result relating $M_{L_1}(z)$ and $M_{L_2}(z)$.

Theorem 3.4. *Assume Hypothesis* 3.1. *Let $z \in \mathbb{C}\backslash\mathbb{R}$ and suppose H_{L_ℓ} and $M_{L_\ell}(z)$ are defined as in* (3.1) *and* (3.2) *with $\mathcal{H}, \mathcal{K}, H_0$ and K independent of $\ell = 1, 2$ and L_ℓ, $\ell = 1, 2$ bounded self-adjoint operators in $\mathcal{K}$. Then*

$$M_{L_2}(z) = M_{L_1}(z)(I_{\mathcal{K}} + (L_2 - L_1)M_{L_1}(z))^{-1} \tag{3.25a}$$

$$= (I_{\mathcal{K}} + M_{L_1}(z)(L_2 - L_1))^{-1} M_{L_1}(z). \tag{3.25b}$$

Proof. Using the resolvent equation for H_{L_2} and H_{L_1},

$$(H_{L_2} - z)^{-1} = (H_{L_1} - z)^{-1} - (H_{L_2} - z)^{-1} K(L_2 - L_1)K^*(H_{L_1} - z)^{-1} \tag{3.26a}$$

$$= (H_{L_1} - z)^{-1} - (H_{L_1} - z)^{-1} K(L_2 - L_1)K^*(H_{L_2} - z)^{-1}, \quad z \in \mathbb{C}\backslash\mathbb{R} \tag{3.26b}$$

and applying K^* on the left and K on the right of both sides of (3.26), results in

$$K^*(H_{L_1} - z)^{-1}K = K^*(H_{L_2} - z)^{-1}K(I + (L_2 - L_1)K^*(H_{L_1} - z)^{-1}K) \tag{3.27a}$$

$$= (I + K^*(H_{L_1} - z)^{-1}K(L_2 - L_1))K^*(H_{L_2} - z)^{-1}K \tag{3.27b}$$

and hence in (3.25). □

A comparison of (3.25) and (1.5), (1.6) then yields

$$A(L_1, L_2) = \begin{pmatrix} I_{\mathcal{K}} & L_2 - L_1 \\ 0 & I_{\mathcal{K}} \end{pmatrix} \in \mathcal{A}(\mathcal{K} \oplus \mathcal{K}) \tag{3.28}$$

for the corresponding matrix A in (1.5), (1.6).

We note that (3.25) also imply

$$(L_2 - L_1)M_{L_2}(z) - I_{\mathcal{K}} = -((L_2 - L_1)M_{L_1}(z) + I_{\mathcal{K}})^{-1}, \tag{3.29a}$$

$$M_{L_2}(z)(L_2 - L_1) - I_{\mathcal{K}} = -(M_{L_1}(z)(L_2 - L_1) + I_{\mathcal{K}})^{-1}. \tag{3.29b}$$

If $K\mathcal{K}$ is not a generating subspace for H_0 (i.e., (3.4) does not hold) then $\mathcal{H}$ decomposes into $\mathcal{H} = \mathcal{H}_{\mathcal{K}} \oplus \mathcal{H}_{\mathcal{K}}^\perp$, with

$$\mathcal{H}_{\mathcal{K}} = \overline{\text{lin.span}\{(H_0 - z)^{-1}Ke_n \in \mathcal{H} \,|\, n \in \mathcal{I},\, z \in \mathbb{C}\backslash\mathbb{R}\}} \tag{3.30a}$$

$$= \overline{\text{lin.span}\{E_0(\lambda)Ke_n \in \mathcal{H} \,|\, n \in \mathcal{I},\, \lambda \in \mathbb{R}\}} \tag{3.30b}$$

and $\mathcal{H}_{\mathcal{K}}$, $\mathcal{H}_{\mathcal{K}}^\perp$ both reducing subspaces for H_L ($\{e_n\}_{n\in\mathcal{I}}$ a complete orthonormal system in $\mathcal{K}$). Moreover, for all $L_\ell \in \mathcal{B}(\mathcal{K})$, $\ell = 1, 2$ self-adjoint,

$$H_{L_1} = H_{L_2} \text{ on } \text{dom}(H_0) \cap \mathcal{H}_{\mathcal{K}}^\perp \tag{3.31}$$

and

$$H_0 = H_{0,\mathcal{K}} \oplus H_{0,\mathcal{K}}^\perp, \quad H_L = H_{L,\mathcal{K}} \oplus H_{0,\mathcal{K}}^\perp, \quad \text{ran}(K) \subseteq \mathcal{H}_{\mathcal{K}}. \tag{3.32}$$

In particular,

$$M_L(z) = K^*(H_L - z)^{-1}K = K^*(H_{L,\mathcal{K}} - z)^{-1}K, \quad z \in \mathbb{C}\backslash\mathbb{R} \tag{3.33}$$

and the L-dependent spectral properties of H_L in $\mathcal{H}$ are effectively reduced to those of $H_{L,\mathcal{K}}$ in $\mathcal{H}_{\mathcal{K}}$.

In connection with our choice of KLK^* as a bounded self-adjoint perturbation of H_0, the following elementary observation might be of interest.

Lemma 3.5. *Let $V \in \mathcal{B}(\mathcal{H})$ be self-adjoint. Then V and $\mathcal{H}$ can be decomposed as*

$$V = K_0 L_0 K_0^* \oplus 0, \quad \mathcal{H} = \overline{\text{ran}(V)} \oplus \ker(V), \tag{3.34}$$

where $K_0 : \mathcal{K} \to \mathcal{H}$, $L_0 = L_0^* \in \mathcal{B}(\mathcal{K})$, and $\mathcal{K} = \overline{\text{ran}(V)}$.

Proof. Since $\overline{\operatorname{ran}(V)} = \ker(V)^\perp$, consider $V_0 = V\big|_{\overline{\operatorname{ran}(V)}} : \mathcal{K} \to \mathcal{K}$, $\mathcal{K} = \overline{\operatorname{ran}(V)}$. Then $V_0 = V_0^* \in \mathcal{B}(\mathcal{K})$ and V_0 admits the spectral representation $V_0 = \int_a^b dF_0(\lambda)\lambda$ for some $a, b \in \mathbb{R}$ and some family of self-adjoint spectral projections $\{F_0(\lambda)\}_{\lambda\in\mathbb{R}}$ of V_0 in $\mathcal{K}$. The decomposition (3.34) then follows upon introducing

$$K_0 = |V_0|^{1/2} = \int_a^b dF_0(\lambda)|\lambda|^{1/2}, \quad L_0 = \operatorname{sgn}(V_0) = \int_a^b dF_0(\lambda)\operatorname{sgn}(\lambda). \tag{3.35}$$

□

In (3.5)–(3.8) we showed that every collection $(H_0, K, L, \mathcal{H}, \mathcal{K})$ gives rise to an operator-valued Herglotz function $M_L(z) = \int_{\mathbb{R}} d\Omega_L(\lambda)(\lambda - z)^{-1}$ with certain properties recorded in (3.7) and (3.8). Conversely, introducing the following class $\mathcal{N}_1(\mathcal{K})$ of $\mathcal{B}(\mathcal{K})$-valued Herglotz functions (we use the symbol $\mathcal{N}_1(\mathcal{K})$ in honor of R. Nevanlinna)

$$\mathcal{N}_1(\mathcal{K}) = \{M \in \mathcal{B}(\mathcal{K}) \text{ Herglotz} \mid M(z) = \int_{\mathbb{R}} d\Omega(\lambda)(\lambda - z)^{-1};\ 0 \le \Omega(\mathbb{R}) \in \mathcal{B}(\mathcal{K})\}, \tag{3.36}$$

we shall show in the remainder of this section that every element M of $\mathcal{N}_1(\mathcal{K})$ can be realized in terms of some collection $(H_0, K, \mathcal{H}, \mathcal{K})$ as in (3.6). (The operator Stieltjes integral in (3.36) converges in the norm of $\mathcal{B}(\mathcal{K})$ by Theorem I.4.2 of [17].) For this purpose we shall use a version of Naimark's dilation theorem [52], [53] as presented in Appendix I of [3] and Appendix I by Brodskii [17].

Theorem 3.6. ([17], App. I, [52].) *Suppose that $\Omega(\lambda)$, $\lambda \in \mathbb{R}$ is a strongly right-continuous nondecreasing function with values in $\mathcal{B}(\mathcal{K})$, $\mathcal{K}$ a complex separable Hilbert space, and assume* $\operatorname{s-lim}_{\lambda\downarrow-\infty}\Omega(\lambda) = 0$. *Then there exists a separable complex Hilbert space $\mathcal{H}$, a $K \in \mathcal{B}(\mathcal{K}, \mathcal{H})$, and an orthogonal family of strongly right-continuous spectral projections $\{E(\lambda)\}_{\lambda\in\mathbb{R}}$ in $\mathcal{H}$ such that* $\operatorname{s-lim}_{\lambda\downarrow-\infty} E(\lambda) = 0$, $\operatorname{s-lim}_{\lambda\uparrow\infty} E(\lambda) = I_{\mathcal{H}}$,

$$\Omega(\lambda) = K^* E(\lambda) K, \quad \lambda \in \mathbb{R}, \tag{3.37}$$

and

$$\overline{\{E(\lambda)K\xi \in \mathcal{H} \mid \xi \in \mathcal{K}, \lambda \in \mathbb{R}\}} = \mathcal{H}. \tag{3.38}$$

Moreover, if for some $\lambda_1, \lambda_2 \in \mathbb{R}$, $\Omega(\lambda_1) = \Omega(\lambda_2)$, then $E(\lambda_1) = E(\lambda_2)$.

The principal realization theorem for Herglotz operators of the type (3.36) then reads as follows

Theorem 3.7. *(i) Any $M \in \mathcal{N}_1(\mathcal{K})$ with associated measure Ω can be realized in the form*

$$M(z) = K^*(H - z)^{-1}K, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{3.39}$$

where H represents a self-adjoint operator in some separable complex Hilbert space $\mathcal{H}$, $K \in \mathcal{B}(\mathcal{K}, \mathcal{H})$, and

$$\Omega(\mathbb{R}) = K^* K. \tag{3.40}$$

(ii) Suppose $M_\ell \in \mathcal{N}_1(\mathcal{K})$ with corresponding measures Ω_ℓ, $\ell = 1, 2$ and $M_1 \ne M_2$. Then M_1 and M_2 can be realized as

$$M_\ell(z) = K^*(H_{L_\ell} - z)^{-1}K, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{3.41}$$

where H_{L_ℓ}, $\ell = 1,2$ are self-adjoint perturbations of one and the same self-adjoint operator H_0 in some separable complex Hilbert space $\mathcal{H}$

$$H_{L_\ell} = H_0 + KL_\ell K^*, \quad \ell = 1,2 \tag{3.42}$$

for some $L_\ell = L_\ell^* \in \mathcal{B}(\mathcal{K})$, $\ell = 1,2$ and some $K \in \mathcal{B}(\mathcal{K},\mathcal{H})$ if and only if the following two conditions hold:

$$\Omega_1(\mathbb{R}) = K^*K = \Omega_2(\mathbb{R}), \tag{3.43}$$

and for all $z \in \mathbb{C}\backslash\mathbb{R}$,

$$M_2(z) = M_1(z)(I_{\mathcal{K}} + (L_2 - L_1)M_1(z))^{-1}. \tag{3.44}$$

Proof. Applying Naimark's dilation theorem, Theorem 3.6, to $\Omega(\lambda)$, $\lambda \in \mathbb{R}$, (assuming $\text{s-lim}_{\lambda\downarrow-\infty}\Omega(\lambda) = 0$ without loss of generality), yields $\Omega(\lambda) = K^*E(\lambda)K$, $\lambda \in \mathbb{R}$ and introducing the self-adjoint operator $H = \int_{\mathbb{R}} dE(\lambda)\lambda$ in $\mathcal{H}$ then proves (3.39). The normalization condition (3.40) then follows as discussed in (3.5)–(3.7). In exactly the same manner one proves the necessity of the normalization (3.43). The necessity of (3.44) was proven in Theorem 3.4. In order to prove sufficiency of (3.43) and (3.44) for (3.41) and (3.42) to hold, we argue as follows. Suppose $\text{s-lim}_{\lambda\downarrow-\infty}\Omega_1(\lambda) = 0$ (otherwise, replace $\Omega_1(\lambda)$ by $\Omega_1(\lambda) - \text{s-lim}_{\nu\downarrow-\infty}\Omega_1(\nu)$) and represent $M_1(z)$ according to part (i) by

$$M_1(z) = K^*(H_1 - z)^{-1}K, \quad z \in \mathbb{C}\backslash\mathbb{R} \tag{3.45}$$

applying Naimark's dilation theorem and Theorem 3.6. Define

$$H_0 = H_1 - KL_1K^*, \quad \text{dom}(H_0) = \text{dom}(H_1) \tag{3.46}$$

for some $L_1 = L_1^* \in \mathcal{B}(\mathcal{K})$. Next, use $L_2 = L_2^* \in \mathcal{B}(\mathcal{K})$ in (3.44) to define

$$H_2 = H_0 + KL_2K^*, \quad \text{dom}(H_2) = \text{dom}(H_0) \tag{3.47}$$

and

$$M_{L_2}(z) = K^*(H_2 - z)^{-1}K. \tag{3.48}$$

By Theorem 3.4,

$$M_{L_2}(z) = M_{L_1}(z)(I_{\mathcal{K}} + (L_2 - L_1)M_1(z))^{-1} = M_2(z), \quad z \in \mathbb{C}\backslash\mathbb{R} \tag{3.49}$$

and the proof is complete. □

For a variety of results related to realization theorems of Herglotz operators we refer, for instance, to [10] and the literature cited therein. Fundamental results on nontangential boundary values of $M_L(z)$ as $z \to x \in \mathbb{R}$, under various conditions on K, can be found in [48]–[51]. Additional results on operators of the type $M_L(z)$ (including cases where K is a suitable unbounded operator) can be found, for instance, in [2], [46], [47] and the references therein.

4. On Self-Adjoint Extensions of Symmetric Operators

In this section we consider self-adjoint extensions H of densely defined closed symmetric operators $\dot{H}$ with deficiency indices (k,k), $k \in \mathbb{N} \cup \{\infty\}$. We revisit Krein's formula relating self-adjoint extensions of $\dot{H}$, introduce the corresponding operator-valued Weyl m-functions and their linear fractional transformations, study a model for the pair $(\dot{H}, H)$, and consider Friedrichs H_F and Krein extensions H_K of $\dot{H}$ in the case where $\dot{H}$ is bounded from below.

In the special case $k = 1$, detailed investigation of this type were undertaken by Donoghue [25]. The case $k \in \mathbb{N}$ was recently discussed in depth in [30] (we also refer to [36] for another comprehensive treatment of this subject). Here we treat the general situation $k \in \mathbb{N} \cup \{\infty\}$ utilizing recent results in [28].

We start with a bit of notation and then recall some pertinent results of [28]. Let $\mathcal{H}$ be a separable complex Hilbert space and $\dot{H} : \mathrm{dom}(\dot{H}) \to \mathcal{H}$, $\overline{\mathrm{dom}(\dot{H})} = \mathcal{H}$ a densely defined closed symmetric linear operator with equal deficiency indices $\mathrm{def}(\dot{H}) = (k, k), k \in \mathbb{N} \cup \{\infty\}$. The deficiency subspaces $\mathcal{N}_\pm$ of $\dot{H}$ are given by

$$\mathcal{N}_\pm = \ker(\dot{H}^* \mp i), \quad \dim_{\mathbb{C}}(\mathcal{N}_\pm) = k \tag{4.1}$$

and for any self-adjoint extension H of $\dot{H}$ in $\mathcal{H}$, the corresponding Cayley transform C_H in $\mathcal{H}$ is defined by

$$C_H = (H + i)(H - i)^{-1}, \tag{4.2}$$

implying

$$C_H \mathcal{N}_- = \mathcal{N}_+. \tag{4.3}$$

Two self-adjoint extensions H_1 and H_2 of $\dot{H}$ are called *relatively prime* (w.r.t. $\dot{H}$) if $\mathrm{dom}(H_1) \cap \mathrm{dom}(H_2) = \mathrm{dom}(\dot{H})$. Associated with H_1 and H_2 we introduce $P_{1,2}(z) \in \mathcal{B}(\mathcal{H})$ by

$$P_{1,2}(z) = (H_1 - z)(H_1 - i)^{-1}((H_2 - z)^{-1} - (H_1 - z)^{-1})(H_1 - z)(H_1 + i)^{-1}, \quad z \in \rho(H_1) \cap \rho(H_2). \tag{4.4}$$

We refer to Lemma 2 of [28] and [58] for a detailed discussion of $P_{1,2}(z)$. Here we only mention the following properties of $P_{1,2}(z)$, $z \in \rho(H_1) \cap \rho(H_2)$,

$$P_{1,2}(z)\big|_{\mathcal{N}_+^\perp} = 0, \quad P_{1,2}(z)\mathcal{N}_+ \subseteq \mathcal{N}_+, \tag{4.5}$$

$$\overline{\mathrm{ran}(P_{1,2}(i))} = \mathcal{N}_+, \quad \mathrm{ran}(P_{1,2}(z)\big|_{\mathcal{N}_+}) \text{ is independent of } z \in \rho(A_1) \cap \rho(A_2), \tag{4.6}$$

$$P_{1,2}(i)\big|_{\mathcal{N}_+} = (i/2)(I - C_{H_2}C_{H_1}^{-1})\big|_{\mathcal{N}_+} = (i/2)(I_{\mathcal{N}_+} + e^{-2i\alpha_{1,2}}) \tag{4.7}$$

for some self-adjoint (possibly unbounded) operator $\alpha_{1,2}$ in $\mathcal{N}_+$.

Next, given a self-adjoint extension H of $\dot{H}$ and a closed linear subspace $\mathcal{N}$ of $\mathcal{N}_+$, $\mathcal{N} \subseteq \mathcal{N}_+$, the Weyl-Titchmarsh operator $M_{H,\mathcal{N}}(z) \in \mathcal{B}(\mathcal{N})$ associated with the pair $(H, \mathcal{N})$ is defined by

$$\begin{aligned} M_{H,\mathcal{N}}(z) &= P_{\mathcal{N}}(zH + I_{\mathcal{H}})(H - z)^{-1}P_{\mathcal{N}}\big|_{\mathcal{N}} \\ &= zI_{\mathcal{N}} + (1 + z^2)P_{\mathcal{N}}(H - z)^{-1}P_{\mathcal{N}}\big|_{\mathcal{N}}, \quad z \in \mathbb{C}\backslash\mathbb{R}, \end{aligned} \tag{4.8}$$

with $I_{\mathcal{N}}$ the identity operator in $\mathcal{N}$ and $P_{\mathcal{N}}$ the orthogonal projection in $\mathcal{H}$ onto $\mathcal{N}$.

One verifies (cf. Lemma 4 in [28]) for H_1 and H_2 relatively prime w.r.t. $\dot{H}$,

$$(P_{1,2}(z)\big|_{\mathcal{N}_+})^{-1} = (P_{1,2}(i)\big|_{\mathcal{N}_+})^{-1} - (z - i)P_{\mathcal{N}_+}(H_1 + i)(H_1 - z)^{-1}P_{\mathcal{N}_+} \tag{4.9a}$$

$$= \tan(\alpha_{1,2}) - M_{H_1,\mathcal{N}_+}(z), \quad z \in \rho(H_1), \tag{4.9b}$$

where

$$C_{H_2}C_{H_1}^{-1}\big|_{\mathcal{N}_+} = -e^{-2i\alpha_{1,2}}. \tag{4.10}$$

Following Saakjan [58] (in a version presented in Theorem 5 and Corollary 6 in [28]), Krein's formula then can be summarized as follows.

Theorem 4.1. ([28], [58].) *Let H_1 and H_2 be self-adjoint extensions of $\dot H$ and $z\in\rho(H_1)\cup\rho(H_2)$. Then*

$$\begin{aligned}(H_2-z)^{-1}&=(H_1-z)^{-1}+(H_1-i)(H_1-z)^{-1}P_{1,2}(z)(H_1+i)(H_1-z)^{-1} &(4.11)\\ &=(H_1-z)^{-1}+(H_1-i)(H_1-z)^{-1}P_{\mathcal{N}_{1,2,+}}\times &(4.12)\\ &\quad\times(\tan(\alpha_{\mathcal{N}_{1,2,+}})-M_{H_1,\mathcal{N}_{1,2,+}}(z))^{-1}P_{\mathcal{N}_{1,2,+}}(H_1+i)(H_1-z)^{-1},\end{aligned}$$

where

$$\mathcal{N}_{1,2,+}=\ker((H_1\big|_{\mathcal{D}(H_1)\cap\mathcal{D}(H_2)})^*-i), \tag{4.13}$$

$$e^{-2i\alpha_{\mathcal{N}_{1,2,+}}}=-C_{H_2}C_{H_1}^{-1}\big|_{\mathcal{N}_{1,2,+}}, \tag{4.14}$$

and

$$P_{1,2}(i)\big|_{\mathcal{N}_{1,2,+}}=(i/2)(I-C_{H_2}C_{H_1}^{-1})\big|_{\mathcal{N}_{1,2,+}}. \tag{4.15}$$

Next we recall that $M_{H,\mathcal{N}}$ and hence $P_{1,2}(z)\big|_{\mathcal{N}_+}$ and $-(P_{1,2}(z)\big|_{\mathcal{N}_+})^{-1}$ (cf. (4.9)), if the latter exists, are operator-valued Herglotz functions.

Theorem 4.2. *Let H be a self-adjoint extension of $\dot H$ with orthogonal family of spectral projections $\{E_H(\lambda)\}_{\lambda\in\mathbb{R}}$, $\mathcal{N}$ a closed subspace of $\mathcal{N}_+$. Then the Weyl-Titchmarch operator $M_{H,\mathcal{N}}(z)$ is analytic for $z\in\mathbb{C}\backslash\mathbb{R}$ and*

$$\mathrm{Im}(z)\mathrm{Im}(M_{H,\mathcal{N}}(z))\geq(\max(1,|z|^2)+|\mathrm{Re}(z)|)^{-1},\quad z\in\mathbb{C}\backslash\mathbb{R}. \tag{4.16}$$

In particular, $M_{H,\mathcal{N}}(z)$ is a $\mathcal{B}(\mathcal{N})$-valued Herglotz function and admits the representation valid in the strong operator topology of $\mathcal{N}$,

$$M_{H,\mathcal{N}}(z)=\int_{\mathbb{R}}d\Omega_{H,\mathcal{N}}(\lambda)((\lambda-z)^{-1}-\lambda(1+\lambda^2)^{-1}),\quad z\in\mathbb{C}\backslash\mathbb{R}, \tag{4.17}$$

where

$$\Omega_{H,\mathcal{N}}(\lambda)=(1+\lambda^2)(P_{\mathcal{N}}E_H(\lambda)P_{\mathcal{N}}\big|_{\mathcal{N}}), \tag{4.18}$$

$$\int_{\mathbb{R}}d\Omega_{H,\mathcal{N}}(\lambda)(1+\lambda^2)^{-1}=I_{\mathcal{N}}, \tag{4.19}$$

$$\int_{\mathbb{R}}d(\xi,\Omega_{H,\mathcal{N}}(\lambda)\xi)_{\mathcal{H}}=\infty\ \textit{for all}\ \xi\in\mathcal{N}\backslash\{0\}. \tag{4.20}$$

Proof. (4.17) has been derived in Lemma 7 of [28], hence we confine ourselves to a few hints. An explicit computation yields

$$\begin{aligned}\mathrm{Im}(z)\mathrm{Im}(M_{H,\mathcal{N}}(z))&=P_{\mathcal{N}}(I_{\mathcal{H}}+H^2)^{1/2}((H-\mathrm{Re}(z))^2+\mathrm{Im}(z))^2)^{-1}\\ &\quad\times(I_{\mathcal{H}}+H^2)^{1/2}P_{\mathcal{N}}\big|_{\mathcal{N}},\quad z\in\mathbb{C}\backslash\mathbb{R}.\end{aligned} \tag{4.21}$$

Together with

$$\frac{1+\lambda^2}{(\lambda-\mathrm{Re}(z))^2+(\mathrm{Im}(z))^2}\geq\frac{1}{\max(1,|z|^2)+|\mathrm{Re}(z)|} \tag{4.22}$$

and the Rayleigh-Ritz argument this yields (4.16). The representation (4.17) and the fact (4.18) follow from (4.8) and $(H-z)^{-1}\xi=\int_{\mathbb{R}}d(E_H(\lambda)\xi)(\lambda-z)^{-1}$, $\xi\in\mathcal{H}$. (4.19) then follows from

$$\begin{aligned}\int_{\mathbb{R}}d(\Omega_{H,\mathcal{N}}(\lambda)\xi)(1+\lambda^2)^{-1}&=\int_{\mathbb{R}}d(P_{\mathcal{N}}E_H(\lambda)\xi)=P_{\mathcal{N}}\int_{\mathbb{R}}d(E_H(\lambda)\xi)\\ &=P_{\mathcal{N}}\xi=\xi\ \text{for all}\ \xi\in\mathcal{N}.\end{aligned} \tag{4.23}$$

Finally,

$$\int_{\mathbb{R}} d(\xi, \Omega_{H,\mathcal{N}}(\lambda)\xi)_{\mathcal{H}} = \int_{\mathbb{R}} d(\xi, E_H(\lambda)\xi)_{\mathcal{H}}(1+\lambda^2) = \infty \text{ for all } \xi \in \mathcal{N}\backslash\{0\} \tag{4.24}$$

since $\mathcal{N} \subseteq \mathcal{N}_+$ and $\mathcal{N}_+ \cap \operatorname{dom}(H) = \{0\}$ by von Neumann's formula

$$\operatorname{dom}(H) = \operatorname{dom}(\dot{H}) \dot{+} \mathcal{N}_+ \dot{+} (-C_H)^{-1}\mathcal{N}_+. \tag{4.25}$$

□

We also recall without proof the principal result of [28], the linear fractional transformation relating the Weyl-Titchmarch operators associated with different self-adjoint extensions of $\dot{H}$.

Theorem 4.3. ([28].) *Let H_1 and H_2 be self-adjoint extensions of $\dot{H}$ and $z \in \rho(H_1) \cap \rho(H_2)$. Then*

$$\begin{aligned} M_{H_2,\mathcal{N}_+}(z) = (P_{1,2}(i)\big|_{\mathcal{N}_+} + (I_{\mathcal{N}_+} + iP_{1,2}(i)\big|_{\mathcal{N}_+})M_{H_1,\mathcal{N}_+}(z)) \times \\ \times ((I_{\mathcal{N}_+} + iP_{1,2}(i)\big|_{\mathcal{N}_+}) - P_{1,2}(i)\big|_{\mathcal{N}_+} M_{H_1,\mathcal{N}_+}(z))^{-1}, \end{aligned} \tag{4.26}$$

where

$$P_{1,2}(i)\big|_{\mathcal{N}_+} = (i/2)(I_{\mathcal{H}} - C_{H_2}C_{H_1}^{-1})\big|_{\mathcal{N}_+}, \tag{4.27}$$

$$I_{\mathcal{N}_+} + iP_{1,2}(i)\big|_{\mathcal{N}_+} = (1/2)(I_{\mathcal{H}} + C_{H_2}C_{H_1}^{-1})\big|_{\mathcal{N}_+}. \tag{4.28}$$

Introducing

$$e^{-2i\alpha_{1,2}} = -C_{H_2}C_{H_1}^{-1}\big|_{\mathcal{N}_+}, \tag{4.29}$$

(4.26) *can be rewritten as*

$$\begin{aligned} M_{H_2,\mathcal{N}_+}(z) = e^{-i\alpha_{1,2}}(\cos(\alpha_{1,2}) + \sin(\alpha_{1,2})M_{H_1,\mathcal{N}_+}(z)) \times \\ \times (\sin(\alpha_{1,2}) - \cos(\alpha_{1,2})M_{H_1,\mathcal{N}_+}(z))^{-1}e^{i\alpha_{1,2}}. \end{aligned} \tag{4.30}$$

A comparison of (4.30) and (1.5), (1.6) then yields

$$A(\alpha_{1,2}) = \begin{pmatrix} e^{-i\alpha_{1,2}}\sin(\alpha_{1,2}) & -e^{-i\alpha_{1,2}}\cos(\alpha_{1,2}) \\ e^{-i\alpha_{1,2}}\cos(\alpha_{1,2}) & e^{-i\alpha_{1,2}}\sin(\alpha_{1,2}) \end{pmatrix} \in \mathcal{A}(\mathcal{K} \oplus \mathcal{K}) \tag{4.31}$$

for the corresponding matrix A in (1.5), (1.6).

Weyl operators of the type $M_{H,\mathcal{N}}(z)$ have attracted considerable attention in the literature. The interested reader can find a variety of additional results, for instance, in [18], [21]–[24], [40], [41], [45], [46], [56].

Next we will prepare some material that eventually will lead to a model for the pair $(\dot{H}, H)$. Let $\mathcal{N}$ be a separable complex Hilbert space, $\{u_n\}_{n\in\mathcal{I}}$, $\mathcal{I} \subseteq \mathbb{N}$ a complete orthonormal system in $\mathcal{N}$, $\{\widetilde{\Omega}(\lambda)\}_{\lambda\in\mathbb{R}}$ a family of strongly right-continuous nondecreasing $\mathcal{B}(\mathcal{N})$-valued functions normalized by

$$\widetilde{\Omega}(\mathbb{R}) = I_{\mathcal{K}}, \tag{4.32}$$

with the property

$$\int_{\mathbb{R}} d(\xi, \widetilde{\Omega}(\lambda)\xi)_{\mathcal{N}}(1+\lambda^2) = \infty \text{ for all } \xi \in \mathcal{N}\backslash\{0\}. \tag{4.33}$$

Introducing the control measure $\tilde{\mu}(B) = \sum_{n\in\mathcal{I}} 2^{-n}(u_n, \widetilde{\Omega}(B)u_n)_{\mathcal{N}}$, $B \in \Sigma$, and $\underline{\Lambda}$ as in Theorem 2.5, we may define $L^p(\mathbb{R}, \mathcal{N}; wd\widetilde{\Omega})$, $p \geq 1$, $w \geq 0$ a weight function, as in Section 2. Of special importance in this section are weight functions of the type $w_r(\lambda) = (1+\lambda^2)^r$, $r \in \mathbb{R}$, $\lambda \in \mathbb{R}$. In particular, introducing

$$\Omega(B) = \int_B (1+\lambda^2) d\tilde{\mu}(\lambda) \frac{d\widetilde{\Omega}}{d\tilde{\mu}}(\lambda), \quad B \in \Sigma, \tag{4.34}$$

we abbreviate $\widehat{\mathcal{H}} = L^2(\mathbb{R}, \mathcal{N}; d\Omega)$ and define the self-adjoint operator $\widehat{H}$ in $\widehat{\mathcal{H}}$,

$$(\widehat{H}\hat{f})(\lambda) = \lambda \hat{f}(\lambda), \quad \hat{f} \in \mathrm{dom}(\widehat{H}) = L^2(\mathbb{R}, \mathcal{N}; (1+\lambda^2)d\Omega), \tag{4.35}$$

with corresponding family of strongly right-continuous orthogonal spectral projections

$$(E_{\hat{H}}(\lambda)\hat{f})(\nu) = \theta(\lambda - \nu)\hat{f}(\nu) \text{ for } \Omega-\text{a.e. } \nu \in \mathbb{R}, \quad \hat{f} \in \widehat{\mathcal{H}}. \tag{4.36}$$

Associated with $\widehat{H}$ we consider the linear operator $\widehat{\dot{H}}$ in $\widehat{\mathcal{H}}$ defined as the following restriction of $\widehat{H}$

$$\begin{aligned} &\mathrm{dom}(\widehat{\dot{H}}) = \{\hat{f} \in \mathrm{dom}(\widehat{H}) \,|\, \int_{\mathbb{R}} (1+\lambda^2) d\tilde{\mu}(\lambda) (\underline{\xi}, \hat{f}(\lambda))_{\mathcal{N}_\lambda} = 0 \text{ for all } \underline{\xi} \in \underline{\Delta}(\mathcal{N})\}, \\ &\widehat{\dot{H}} = \widehat{H}\big|_{\mathrm{dom}(\hat{\dot{H}})}. \end{aligned} \tag{4.37}$$

(The integral in (4.37) is well-defined, see the proof of Theorem 4.4 below.) Here we used the notation introduced in the proof of Theorem 2.5,

$$\underline{\xi} = \underline{\Delta}\xi = \{\underline{\xi}(\lambda) = \xi\}_{\lambda \in \mathbb{R}}. \tag{4.38}$$

Moreover, introducing the scale of Hilbert spaces $\widehat{\mathcal{H}}_{2r} = L^2(\mathbb{R}, \mathcal{N}; (1+\lambda^2)^r d\Omega)$, $r \in \mathbb{R}$, $\widehat{\mathcal{H}}_0 = \widehat{\mathcal{H}}$, we consider the unitary operator R from $\widehat{\mathcal{H}}_2$ to $\widehat{\mathcal{H}}_{-2}$,

$$R : \widehat{\mathcal{H}}_2 \longrightarrow \widehat{\mathcal{H}}_{-2}, \quad \hat{f} \longrightarrow (1+\lambda^2)\hat{f}, \tag{4.39}$$

$$(\hat{f}, \hat{g})_{\hat{\mathcal{H}}_2} = (\hat{f}, R\hat{g})_{\hat{\mathcal{H}}} = (R\hat{f}, \hat{g})_{\hat{\mathcal{H}}} = (R\hat{f}, R\hat{g})_{\hat{\mathcal{H}}_{-2}}, \quad \hat{f}, \hat{g} \in \widehat{\mathcal{H}}_2, \tag{4.40}$$

$$(\hat{u}, \underline{v})_{\hat{\mathcal{H}}_{-2}} = (\hat{u}, R^{-1}\underline{v})_{\hat{\mathcal{H}}_2} = (R^{-1}\hat{u}, \underline{v})_{\hat{\mathcal{H}}} = (R^{-1}\hat{u}, R^{-1}\underline{v})_{\hat{\mathcal{H}}_2}, \quad \hat{u}, \underline{v} \in \widehat{\mathcal{H}}_{-2}. \tag{4.41}$$

In particular,

$$\underline{\underline{\Delta}}(\mathcal{N}) \subset \widehat{\mathcal{H}}, \quad \underline{\Delta}(\mathcal{N}) \subset \widehat{\mathcal{H}}_{-2}, \quad \underline{\xi} \in \underline{\Delta}(\mathcal{N})\backslash\{0\} \Rightarrow \underline{\xi} \notin \widehat{\mathcal{H}} \tag{4.42}$$

(cf. (2.51) and (4.32)–(4.34)).

Theorem 4.4. *The operator* $\widehat{\dot{H}}$ *in* (4.37) *is densely defined symmetric and closed in* $\widehat{\mathcal{H}}$. *Its deficiency indices are given by*

$$\mathrm{def}(\widehat{\dot{\mathrm{H}}}) = (\mathrm{k}, \mathrm{k}), \quad \mathrm{k} = \dim_{\mathbb{C}}(\mathcal{N}) \in \mathbb{N} \cup \{\infty\}, \tag{4.43}$$

and

$$\ker(\widehat{\dot{H}}^* - z) = \overline{\mathit{lin.span}\{\{(\lambda - z)^{-1}e_n\}_{\lambda \in \mathbb{R}} \in \widehat{\mathcal{H}} \,|\, n \in \mathcal{I}\}}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{4.44}$$

Proof. Writing $||\hat{f}(\lambda)||_{\mathcal{N}_\lambda} = (1+\lambda^2)^{-1/2}(1+\lambda^2)^{1/2}||\hat{f}(\lambda)||_{\mathcal{N}_\lambda}$ one infers that $\hat{f} \in L^1(\mathbb{R}, \mathcal{N}; d\Omega)$ for $\hat{f} \in \widehat{\mathcal{H}}_2$. Thus the integral in (4.37) and hence $\mathrm{dom}(\widehat{\dot{H}})$ is well-defined. As a restriction of $\widehat{H}$, $\widehat{\dot{H}}$ is clearly symmetric. By (4.37) and (4.39)–(4.41) one infers

$$\mathrm{dom}(\widehat{H}) = \mathrm{dom}(\widehat{\dot{H}}) = \widehat{\mathcal{H}}_2 \ominus_{\hat{\mathcal{H}}_2} R^{-1}\underline{\Delta}(\mathcal{N}), \tag{4.45}$$

where, in obvious notation, $\ominus_{\hat{\mathcal{H}}_2}$ indicates the orthogonal complement in $\widehat{\mathcal{H}}_2$. Thus $\widehat{\dot{H}}$ has a closed graph.

Next, to prove that $\widehat{\dot{H}}$ is densely defined in $\widehat{\mathcal{H}}$, suppose there is a $\hat{g} \in \widehat{\mathcal{H}}$ such that $\hat{g} \perp \mathrm{dom}(\widehat{\dot{H}})$. Then

$$0 = (\hat{f}, \hat{g})_{\hat{\mathcal{H}}} = (\hat{f}, R^{-1}\hat{g})_{\hat{\mathcal{H}}_2} \text{ for all } \hat{f} \in \mathrm{dom}(\widehat{\dot{H}}) \tag{4.46}$$

and hence $R^{-1}\hat{g} \in R^{-1}\underline{\Lambda}(\mathcal{N})$, that is, there is an $\xi \in \mathcal{N}$ such that $\hat{g} = \underline{\Lambda}\xi$ $\Omega-$a.e. by (4.45). Since $\underline{\Lambda}\xi \in \underline{\Lambda}(\mathcal{N})\backslash\{0\}$ implies $\underline{\Lambda}\xi \notin \widehat{\mathcal{H}}$ by (4.42), $\hat{g} \in \widehat{\mathcal{H}}$ if and only if $\underline{\Lambda}\xi = \hat{g} = 0$. Finally, since $\widehat{H}$ is self-adjoint, $\mathrm{ran}(\widehat{H} - z) = \widehat{\mathcal{H}}$ for all $z \in \mathbb{C}\backslash\mathbb{R}$, and $(\widehat{H} \pm i) : \widehat{\mathcal{H}}_2 \to \widehat{\mathcal{H}}$ is unitary,

$$((\widehat{H} \pm i)\hat{f}, (\widehat{H} \pm i)\hat{g})_{\hat{\mathcal{H}}} = \int_{\mathbb{R}} (1 + \lambda^2)^2 d\tilde{\mu}(\lambda)(\hat{f}(\lambda), \hat{g}(\lambda))_{\mathcal{N}_\lambda} = (\hat{f}, \hat{g})_{\hat{\mathcal{H}}_2}, \quad \hat{f}, \hat{g} \in \widehat{\mathcal{H}}_2. \tag{4.47}$$

Thus (4.45) and (4.46) yield

$$\begin{aligned} \widehat{\mathcal{H}} &= (\widehat{H} \pm i)\widehat{\mathcal{H}}_2 = (\widehat{H} \pm i)(\mathrm{dom}(\widehat{\dot{H}}) \oplus_{\hat{\mathcal{H}}_2} R^{-1}\underline{\Lambda}(\mathcal{N})) \\ &= (\widehat{\dot{H}} \pm i)\mathrm{dom}(\widehat{\dot{H}}) \oplus_{\hat{\mathcal{H}}} \overline{\mathrm{lin.span}\{\{(\lambda \pm i)(1 + \lambda^2)^{-1} u_n\}_{\lambda \in \mathbb{R}} \in \widehat{\mathcal{H}} \,|\, n \in \mathcal{I}\}} \\ &= \mathrm{ran}(\widehat{\dot{H}} \pm i) \oplus_{\hat{\mathcal{H}}} \overline{\mathrm{lin.span}\{\{(\lambda \mp i)^{-1} u_n\}_{\lambda \in \mathbb{R}} \in \widehat{\mathcal{H}} \,|\, n \in \mathcal{I}\}} \end{aligned} \tag{4.48}$$

and hence

$$\ker(\widehat{\dot{H}}^* \mp i) = \overline{\mathrm{lin.span}\{(\{\lambda \mp i)^{-1} u_n\}_{\lambda \in \mathbb{R}} \in \widehat{\mathcal{H}} \,|\, n \in \mathcal{I}\}}. \tag{4.49}$$

Since $(\lambda - z)^{-1}\xi = (\lambda - i)^{-1}\xi + (z - i)(\lambda - z)^{-1}(\lambda - i)^{-1}\xi$, with $\{(\lambda - z)^{-1}(\lambda - i)^{-1}\xi\}_{\lambda \in \mathbb{R}} \in \widehat{\mathcal{H}}_2 = \mathrm{dom}(\widehat{H})$ for all $\xi \in \mathcal{N}$, $z \in \mathbb{C}\backslash\mathbb{R}$, (4.49) yields (4.44). □

Lemma 4.5. *Let $\dot{H}$ be a densely defined linear closed symmetric operator in a separable complex Hilbert space $\mathcal{H}$ with deficiency indices (k, k), $k \in \mathbb{N} \cup \{\infty\}$. Then $\mathcal{H}$ decomposes into the direct orthogonal sum*

$$\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_0^\perp, \quad \ker(\dot{H}^* - i) \subset \mathcal{H}_0, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{4.50}$$

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

$$(H - z)^{-1}\mathcal{H}_0 \subseteq \mathcal{H}_0, \quad (H - z)^{-1}\mathcal{H}_0^\perp \subseteq \mathcal{H}_0^\perp, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{4.51}$$

for all self-adjoint extensions H of $\dot{H}$ in $\mathcal{H}$. Moreover, all self-adjoint extensions $\dot{H}$ coincide on $\mathcal{H}_0^\perp$, that is, if $\{H_\alpha\}_{\alpha \in \mathcal{I}}$ ($\mathcal{I}$ an appropriate index set) denotes the set of all self-adjoint extensions of $\dot{H}$, then

$$H_\alpha = H_{0,\alpha} \oplus H_0^\perp, \quad \alpha \in \mathcal{I} \quad \textit{in} \quad \mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_0^\perp, \tag{4.52}$$

where

$$H_0^\perp \textit{ is independent of } \alpha \in \mathcal{I}. \tag{4.53}$$

Proof. Let H be a fixed self-adjoint extension of $\dot{H}$, denote $\mathcal{N}_\pm = \ker(\dot{H}^* \mp i)$, and define

$$\mathcal{H}_H = \overline{\mathrm{lin.span}\{(H - z)^{-1} u_+ \in \mathcal{H} \,|\, u_+ \in \mathcal{N}_+,\, z \in \mathbb{C}\backslash\mathbb{R}\}}. \tag{4.54}$$

Since $(H-z_1)^{-1}(H-z_2)^{-1} = (z_1-z_2)^{-1}((H-z_1)^{-1}-(H-z_2)^{-1})$, $\mathcal{H}_H$ is invariant with respect to $(H-z)^{-1}$, $(H-z)^{-1}\mathcal{H}_H \subseteq \mathcal{H}_H$, and since $((H-z)^{-1})^* = (H-\bar{z})^{-1}$, also $\mathcal{H}_H^\perp$ is invariant under $(H-z)^{-1}$ for all $z \in \mathbb{C}\backslash\mathbb{R}$. Since $\text{w-lim}_{z\to i\infty}(-z)(H-z)^{-1}f = f$ for all $f \in \mathcal{H}$, one concludes

$$\mathcal{N}_+ \subset \mathcal{H}_H. \tag{4.55}$$

Next, let $v \in \mathcal{H}_H^\perp$. Then also

$$w = (H-z)^{-1}v \in \mathcal{H}_H^\perp, \quad z \in \mathbb{C}\backslash\mathbb{R} \tag{4.56}$$

and

$$(u_+, v)_\mathcal{H} = (u_+, w)_\mathcal{H} = 0, \quad u_+ \in \mathcal{N}_+. \tag{4.57}$$

Since $w \in \operatorname{dom}(H)$

$$w \notin \mathcal{N}_\pm \tag{4.58}$$

(otherwise $\dot{H}^*w = \pm iw$ yields $Hw = \pm iw$ which contradicts the self-adjointness of H). By von Neumann's formulas

$$\operatorname{dom}(\dot{H}^*) = \operatorname{dom}(\dot{H}) \oplus_{\mathcal{H}_+} \mathcal{N}_+ \oplus_{\mathcal{H}_+} \mathcal{N}_-, \tag{4.59}$$

where $\oplus_{\mathcal{H}_+}$ denotes the direct orthogonal sum in the Hilbert space $\mathcal{H}_+$ defined by

$$\mathcal{H}_+ = (\operatorname{dom}(\dot{H}^*), (\cdot,\cdot)_+), \quad (f,g)_+ = (\dot{H}^*f, \dot{H}^*g)_\mathcal{H} + (f,g)_\mathcal{H}, \quad f,g \in \operatorname{dom}(\dot{H}^*). \tag{4.60}$$

Using (4.55), $Hw = zw + v$ (cf. (4.56)), (4.57), and (4.60) one computes

$$\begin{aligned}(u_+, w)_+ &= (\dot{H}^*u_+, \dot{H}^*w)_\mathcal{H} + (u_+, w)_\mathcal{H} = -i(u_+, Hw)_\mathcal{H} + (u_+, w)_\mathcal{H} \\ &= (-iz+1)(u_+, w)_\mathcal{H} - i(u_+, v)_\mathcal{H} = 0.\end{aligned} \tag{4.61}$$

(4.58), (4.59), and (4.61) then prove $w \in \operatorname{dom}(\dot{H})$ and hence

$$Hw = \dot{H}w = zw + v. \tag{4.62}$$

If $\widetilde{H}$ is any other self-adjoint extension of $\dot{H}$, then $w \in \operatorname{dom}(\dot{H})$ also yields

$$\widetilde{H}w = \dot{H}w = zw + v \tag{4.63}$$

and hence

$$w = (H-z)^{-1}v = (\widetilde{H}-z)^{-1}v, \quad v \in \mathcal{H}_H^\perp. \tag{4.64}$$

Thus the resolvents of all self-adjoint extensions of $\dot{H}$ coincide on $\mathcal{H}_H^\perp$. Moreover,

$$((\widetilde{H}-\bar{z})^{-1}u_+, v)_\mathcal{H} = (u_+, (\widetilde{H}-z)^{-1}v)_\mathcal{H} = (u_+, w)_\mathcal{H} = 0 \tag{4.65}$$

yields

$$(\widetilde{H}-z)^{-1}u_+ \perp \mathcal{H}_H^\perp, \quad z \in \mathbb{C}\backslash\mathbb{R} \tag{4.66}$$

and hence $\mathcal{H}_{\tilde{H}} \subseteq \mathcal{H}_H$. By symmetry in H and $\widetilde{H}$, $\mathcal{H}_{\tilde{H}} = \mathcal{H}_H = \mathcal{H}_0$ completing the proof. ☐

In the following we call a densely defined closed symmetric operator $\dot{H}$ with deficiency indices (k,k), $k \in \mathbb{N} \cup \{\infty\}$ *prime* if $\mathcal{H}_0^\perp = \{0\}$ in the decomposition (4.50).

Given these preliminaries we can now discuss a model for the pair $(\dot{H}, H)$.

Theorem 4.6. *Let $\dot{H}$ be a densely defined closed prime symmetric operator in a separable complex Hilbert space $\mathcal{H}$. Assume H to be a self-adjoint extension of $\dot{H}$ in $\mathcal{H}$ with $\{E_H(\lambda)\}_{\lambda\in\mathbb{R}}$ the associated family of strongly right-continuous orthogonal spectral projections of H and define the unitary operator $\widetilde{U} : \widehat{\mathcal{H}} = L^2(\mathbb{R}, \mathcal{N}_+; d\Omega_{H,\mathcal{N}_+}) \to \mathcal{H}$ as the operator $\widetilde{U}$ in Lemma 2.8, where*

$$\Omega_{H,\mathcal{N}_+}(\lambda) = (1+\lambda^2)(P_{\mathcal{N}_+} E_H(\lambda) P_{\mathcal{N}_+}\big|_{\mathcal{N}_+}), \tag{4.67}$$

with $P_{\mathcal{N}_+}$ the orthogonal projection onto $\mathcal{N}_+ = \ker(\dot{H}^* - i)$. Then the pair $(\dot{H}, H)$ is unitarily equivalent to the pair $\widehat{\dot{H}}, \widehat{H})$,

$$\dot{H} = \widetilde{U}\widehat{\dot{H}}\widetilde{U}^{-1}, \quad H = \widetilde{U}\widehat{H}\widetilde{U}^{-1}, \tag{4.68}$$

where $\widehat{H}$ and $\widehat{\dot{H}}$ are defined in (4.32)–(4.37), and Theorem 4.4, and $\mathcal{N}$ is identified with $\mathcal{N}_+$, etc. Moreover,

$$\widetilde{U}\widehat{\mathcal{N}}_+ = \mathcal{N}_+, \tag{4.69}$$

where

$$\widehat{\mathcal{N}}_+ = \overline{lin.span\{\underline{\underline{u}}_{+,n} \in \widehat{\mathcal{H}} \,|\, \underline{\underline{u}}_{+,n}(\lambda) = (\lambda - i)^{-1} u_{+,n},\, \lambda \in \mathbb{R},\, n \in \mathcal{I}\}}, \tag{4.70}$$

with $\{u_{+,n}\}_{n\in\mathcal{I}}$ a complete orthonormal system in $\mathcal{N}_+ = \ker(\dot{H}^* - i)$.

Proof. Consider $\underline{\underline{u}}_{+,n}(\lambda) = (\lambda - i)^{-1} u_{+,n}$, $n \in \mathcal{I}$, then

$$\widetilde{U}\underline{\underline{u}}_{+,n} = \int_{\mathbb{R}} dE_H(\lambda) u_{+,n} = u_{+,n}, \quad n \in \mathcal{I} \tag{4.71}$$

proves (4.69). Moreover,

$$((\widehat{H} - z)^{-1}\underline{\underline{u}}_{+,n})(\lambda) = (\lambda - z)^{-1}(\lambda - i)^{-1} u_{+,n}, \quad n \in \mathcal{I},\, z \in \mathbb{C}\backslash\mathbb{R} \tag{4.72}$$

yields

$$\widetilde{U}(\widehat{H} - z)^{-1}\underline{\underline{u}}_{+,n} = \int_{\mathbb{R}} dE_H(\lambda)(\lambda - z)^{-1} u_{+,n} = (H - z)^{-1} u_{+,n}, \quad n \in \mathcal{I}. \tag{4.73}$$

Since by hypothesis $\dot{H}$ is a prime symmetric operator, finite linear combinations of the right-hand side in (4.73) are dense in $\mathcal{H}$. Since $\widetilde{U}$ is unitary, also finite linear combinations of $(\widehat{H} - z)^{-1}\underline{\underline{u}}_{+,n}$ on the left-hand side of (4.73) are dense in $\widehat{\mathcal{H}}$. Using the first resolvent equation one computes from (4.73)

$$\begin{aligned}\widetilde{U}(\widehat{H} - z)^{-1}\widetilde{U}^{-1}\widetilde{U}(\widehat{H} - z')^{-1}\underline{\underline{u}}_{+,n} &= \widetilde{U}(\widehat{H} - z)^{-1}\widetilde{U}^{-1}(H - z')^{-1} u_{+,n} \\ &= (H - z)^{-1}(H - z')^{-1} u_{+,n}.\end{aligned} \tag{4.74}$$

Since finite linear combinations of the form $(H - z')^{-1} u_{+,n}$ are dense in $\mathcal{H}$ we get

$$\widetilde{U}(\widehat{H} - z)^{-1}\widetilde{U}^{-1} = (H - z)^{-1}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{4.75}$$

(4.69) and (4.75) then yield $\widetilde{U}\widehat{\dot{H}}\widetilde{U}^{-1} = \dot{H}$. ☐

If $\dot{H}$ is a densely defined closed non-prime symmetric operator in $\mathcal{H}$, then in addition to (4.50), (4.52), and (4.53) one obtains

$$\dot{H} = \dot{H}_0 \oplus H_0^{\perp}, \quad \mathcal{N}_+ = \mathcal{N}_{0,+} \oplus \{0\} \tag{4.76}$$

with respect to the decomposition $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_0^\perp$. In particular, the part $H_0^\perp$ of $\dot H$ in $\mathcal{H}_0^\perp$ is self-adjoint. For any closed linear subspace $\mathcal{N}$ of $\mathcal{N}_+$, $\mathcal{N} \subseteq \mathcal{N}_+$, one then infers $\mathcal{N} = \mathcal{N}_0 \oplus \{0\}$, $P_{\mathcal{N}} = P_{\mathcal{N}_0} \oplus 0$ and hence

$$M_{H,\mathcal{N}}(z) = M_{H_0,\mathcal{N}_0}(z), \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{4.77}$$

This reduces the H-dependent spectral properties of the Weyl-Titchmarch operator effectively to that of H_0, where $H = H_0 \oplus H_0^\perp$ is a self-adjoint extension of $\dot H$ in $\mathcal{H}$.

Next we digress a bit to the special case where $\dot H \geq 0$ and characterize Friedrichs and Krein extensions, H_F and H_K, of $\dot H$ in $\mathcal{H}$. Assuming $\dot H$ to be densely defined in $\mathcal{H}$ we recall the definition of H_F and H_K (cf., e.g., [7]),

$$\begin{aligned}
&\mathrm{dom}(H_F^{1/2}) = \{f \in \mathcal{H} \,|\, \text{there is a } \{f_n\}_{n\in\mathbb{N}} \subset \mathrm{dom}(\dot H) \text{ s.t. } \lim_{n\to\infty} \|f_n - f\|_{\mathcal{H}} = 0 \\
&\qquad\qquad \text{and } \lim_{m,n\to\infty} ((f_n - f_m), \dot H(f_n - f_m))_{\mathcal{H}} = 0\}, \\
&H_F = \dot H^*\big|_{\mathrm{dom}(\dot H^*)\cap \mathrm{dom}(H_F^{1/2})},
\end{aligned} \tag{4.78}$$

$$\begin{aligned}
&\mathrm{dom}(H_K) = \{f \in \mathrm{dom}(\dot H^*) \,|\, \text{there is a } \{f_n\}_{n\in\mathbb{N}} \subset \mathrm{dom}(\dot H) \text{ s.t.} \\
&\qquad \lim_{n\to\infty} \|\dot H f_n - \dot H^* f\|_{\mathcal{H}} = 0 \text{ and } \lim_{m,n\to\infty} ((f_n - f_m), \dot H(f_n - f_m))_{\mathcal{H}} = 0\}, \\
&H_K = \dot H^*\big|_{\mathrm{dom}(H_K)}.
\end{aligned} \tag{4.79}$$

Moreover, we recall that

$$\inf \mathrm{spec}(H_F) = \inf\{(g, \dot H g)_{\mathcal{H}} \in \mathbb{R} \,|\, g \in \mathrm{dom}(\dot H), \, \|g\|_{\mathcal{H}} = 1\} \geq 0, \tag{4.80}$$

$$\inf \mathrm{spec}(H_K) = 0, \tag{4.81}$$

and

$$0 \leq (H_F - \mu)^{-1} \leq (\widetilde H - \mu)^{-1} \leq (H_K - \mu)^{-1}, \quad \mu < 0 \tag{4.82}$$

for any nonnegative self-adjoint extension $\widetilde H \geq 0$ of $\dot H$.

Next we discuss a slight refinement of a result of Krein [39] (see also [8], [65], [66]). We will use an efficient summary of Krein's result due to Skau [61] (cf. also [43]), which appears most relevant in our context.

Theorem 4.7. *Let $\dot H \geq 0$ be a densely defined closed nonnegative operator in $\mathcal{H}$ with deficiency subspaces $\mathcal{N}_\pm = \ker(\dot H^* \mp i)$. Suppose H is a self-adjoint extension of $\dot H$ in $\mathcal{H}$ with corresponding family of orthogonal spectral projection $\{E_H(\lambda)\}_{\lambda\in\mathbb{R}}$ and define*

$$\Omega_{H,\mathcal{N}_+}(\lambda) = (1 + \lambda^2)(P_{\mathcal{N}_+} E_H(\lambda) P_{\mathcal{N}_+}\big|_{\mathcal{N}_+}). \tag{4.83}$$

Denote by H_F and H_K the Friedrichs and Krein extension of $\dot H$, respectively. Then (i) $H = H_F$ if and only if $\int_R^\infty d\|E_H(\lambda)u_+\|_{\mathcal{H}}^2 \lambda = \infty$, or equivalently, if and only if $\int_R^\infty d(u_+, \Omega_{H,\mathcal{N}_+}(\lambda)u_+)_{\mathcal{N}_+} \lambda^{-1} = \infty$ for all $R > 0$ and all $u_+ \in \mathcal{N}_+\backslash\{0\}$.
(ii) $H = H_K$ if and only if $\int_0^R d\|E_H(\lambda)u_+\|_{\mathcal{H}}^2 \lambda^{-1} = \infty$, or equivalently, if and only if $\int_0^R d(u_+, \Omega_{H,\mathcal{N}_+}(\lambda)u_+)_{\mathcal{N}_+} \lambda^{-1} = \infty$ for all $R > 0$ and all $u_+ \in \mathcal{N}_+\backslash\{0\}$.
(iii) $H = H_F = H_K$ if and only if $\int_R^\infty d\|E_H(\lambda)u_+\|_{\mathcal{H}}^2 \lambda = \int_0^R d\|E_H(\lambda)u_+\|_{\mathcal{H}}^2 \lambda^{-1} = \infty$, or equivalently, if and only if for all $R > 0$ and all $u_+ \in \mathcal{N}_+ \in \mathcal{N}_+\backslash\{0\}$, $\int_R^\infty d(u_+, \Omega_{H,\mathcal{N}_+}(\lambda)u_+)_{\mathcal{N}_+} \lambda^{-1} = \int_R^\infty d(u_+, \Omega_{H,\mathcal{N}_+}(\lambda)u_+)_{\mathcal{N}_+} \lambda^{-1} = \infty$.

Proof. By Lemma 4.5 and (4.76) we may assume that $\dot H$ is a prime symmetric operator. Moreover, by Theorem 4.6 we may identify $(\dot H, H)$ in $\mathcal{H}$ with the model pair $(\widehat{\dot H}, \widehat H)$ in $\widehat{\mathcal{H}} = L^2(\mathbb{R}, \mathcal{N}_+; d\Omega_{H,\mathcal{N}_+})$. Since by (4.70),

$$\widehat{\mathcal{N}}_+ = \overline{\text{lin.span}\{\underline{\underline{u}}_{+,n} = \{(\lambda - i)^{-1} u_{+,n}\}_{\lambda\in\mathbb{R}} \in \widehat{\mathcal{H}} \,|\, n \in \mathcal{I}\}}, \tag{4.84}$$

statements (i)–(iii) are reduced to those in Krein [39], respectively Skau [61], who use $\ker(\dot H^* + 1)$ instead of $\mathcal{N}_+ = \ker(\dot H^* - i)$, by utilizing the elementary identity $(\lambda+1)^{-1} = (\lambda-i)^{-1} - (1+i)(\lambda+1)^{-1}(\lambda-i)^{-1}$ and the fact that $\{(\lambda+1)^{-1}(\lambda - i)^{-1}u_{+,n}\}_{\lambda\in\mathbb{R}} \in \widehat{\mathcal{H}} = L^2(\mathbb{R}, \mathcal{N}_+; d\Omega_{H,\mathcal{N}_+})$ for all $n \in \mathcal{I}$. □

Corollary 4.8. ([22], [23], [24], [41], [67].)
(i) $H = H_F$ *if and only if* $\lim_{\lambda\downarrow-\infty}(u_+, M_{H,\mathcal{N}_+}(\lambda)u_+)_{\mathcal{N}_+} = -\infty$ *for all* $u_+ \in \mathcal{N}_+\backslash\{0\}$.
(ii) $H = H_K$ *if and only if* $\lim_{\lambda\uparrow 0}(u_+, M_{H,\mathcal{N}_+}(\lambda)u_+)_{\mathcal{N}_+} = \infty$ *for all* $u_+ \in \mathcal{N}_+\backslash\{0\}$.
(iii) $H = H_F = H_K$ *if and only if* $\lim_{\lambda\downarrow-\infty}(u_+, M_{H,\mathcal{N}_+}(\lambda)u_+)_{\mathcal{N}_+} = -\infty$ *and* $\lim_{\lambda\uparrow 0}(u_+, M_{H,\mathcal{N}_+}(\lambda)u_+)_{\mathcal{N}_+} = \infty$ *for all* $u_+ \in \mathcal{N}_+\backslash\{0\}$.

Proof. Since

$$\begin{aligned} M_{H,\mathcal{N}_+}(z) &= zI_{\mathcal{N}_+} + (1+z^2)P_{\mathcal{N}_+}(H-z)^{-1}P_{\mathcal{N}_+}\big|_{\mathcal{N}_+} \\ &= \int_{\mathbb{R}} d\Omega_{H,\mathcal{N}_+}(\lambda)((\lambda-z)^{-1} - \lambda(1+\lambda^2)^{-1}), \quad z \in \mathbb{C}\backslash[0,\infty) \end{aligned} \tag{4.85}$$

by (4.83), it suffices to involve Theorem 4.7 (i)–(iii) and the monotone convergence theorem. □

As a simple illustration we mention the following

Example 4.9. Consider the following operator $\dot H$ in $L^2(\mathbb{R}^n; d^n x)$,

$$\dot H = \overline{-\Delta\big|_{C_0^\infty(\mathbb{R}^n\backslash\{0\})}} \geq 0, \quad n = 2,3. \tag{4.86}$$

Then

$$H_F = H_K = -\Delta, \quad \text{dom}(-\Delta) = H^{2,2}(\mathbb{R}^2) \text{ if } n = 2 \tag{4.87}$$

is the unique nonnegative self-adjoint extension of $\dot H$ in $L^2(\mathbb{R}^2; d^2x)$ and

$$H_F = -\Delta, \quad \text{dom}(-\Delta) = H^{2,2}(\mathbb{R}^3) \text{ if } n = 3, \tag{4.88}$$

$$H_K = Uh_0^N U^{-1} \oplus \bigoplus_{\ell\in\mathbb{N}} Uh_\ell U^{-1} \text{ if } n = 3. \tag{4.89}$$

Here $H^{p,q}(\mathbb{R}^n)$, $p, q \in \mathbb{N}$ denote the usual Sobolev spaces,

$$h_0^N = -\frac{d^2}{dr^2}, \quad r > 0, \tag{4.90}$$

$$\text{dom}(h_0^N) = \{f \in L^2((0,\infty); dr) \,|\, f, f' \in AC([0,R]) \text{ for all } R > 0;\ f'(0_+) = 0; \\ f'' \in L^2((0,\infty); dr)\},$$

$$h_\ell = -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2}, \quad r > 0,\ \ell \in \mathbb{N}, \tag{4.91}$$

$$\text{dom}(h_\ell) = \{f \in L^2((0,\infty); dr) \,|\, f, f' \in AC([0,R]) \text{ for all } R > 0;\ f(0_+) = 0; \\ -f'' + \ell(\ell+1)r^{-2}f \in L^2((0,\infty); dr)\},$$

and U denotes the unitary operator,

$$U : L^2((0,\infty);dr) \to L^2((0,\infty);r^2dr), \quad f(r) \to r^{-1}f(r). \tag{4.92}$$

Equations (4.87)–(4.89) follow from Corollary 4.8 and the facts

$$(u_+, M_{H_F,\mathcal{N}_+}(z)u_+)_{L^2(\mathbb{R}^n;d^nx)} = \begin{cases} -(2/\pi)\ln(z) + 2i, & n = 2, \\ i(2z)^{1/2} + 1, & n = 3, \end{cases} \tag{4.93}$$

and

$$(u_+, M_{H_K,\mathcal{N}_+}(z)u_+)_{L^2(\mathbb{R}^3;d^3x)} = i(2/z)^{1/2} - 1. \tag{4.94}$$

Here

$$\mathcal{N}_+ = \text{lin.span}\{u_+\}, \quad u_+(x) = G_0(i,x,0)/\|G_0(i,\cdot,0)\|_{L^2(\mathbb{R}^n;d^nx)}, \ x \in \mathbb{R}^n\backslash\{0\}, \tag{4.95}$$

where

$$G_0(z,x,y) = \begin{cases} \frac{i}{4}H_0^{(1)}(z^{1/2}|x-y|), & x \neq y, \, n = 2, \\ e^{iz^{1/2}|x-y|}/(4\pi|x-y|), & x \neq y, \, n = 3 \end{cases} \tag{4.96}$$

denotes the Green's function of $-\Delta$ on $H^{2,2}(\mathbb{R}^n)$, $n = 2,3$ (i.e., the integral kernel of the resolvent $(-\Delta - z)^{-1}$) and $H_0^{(1)}(\zeta)$ abbreviates the Hankel function of the first kind and order zero (cf., [1], Sect. 9.1). Equation (4.93) then immediately follows from repeated use of the identity (the first resolvent equation),

$$\int_{\mathbb{R}^n} d^nx' G_0(z_1,x,x')G_0(z_2,x',0) = (z_1 - z_2)^{-1}(G_0(z_1,x,0) - G_0(z_2,x,0)), \qquad x \neq 0, \, z_1 \neq z_2, \, n = 2,3 \tag{4.97}$$

and its limiting case as $x \to 0$. Finally, (4.94) follows from the following arguments. First one notices that $(-(d^2/dr^2) + \nu r^{-2})\big|_{C_0^\infty((0,\infty))}$ is essentially self-adjoint if and only if $\nu \geq 3/4$. Hence it suffices to consider the restriction of $\dot{H}$ to the centrally symmetric subspace of $L^2(\mathbb{R}^3;d^3x)$ corresponding to angular momentum $\ell = 0$. But then it is a well-known fact (cf. Lemma 5.3) that the Dirichlet Donoghue m-function $(u_+, M_{H_F,\mathcal{N}_+}(z)u_+)_{L^2(\mathbb{R}^n;d^nx)}$ corresponding to

$$h_0^D = -\frac{d^2}{dr^2}, \quad r > 0, \tag{4.98}$$
$$\text{dom}(h_0^N) = \{f \in L^2((0,\infty);dr) \,|\, f, f' \in AC([0,R]) \text{ for all } R > 0; \, f(0_+) = 0; \; f'' \in L^2((0,\infty);dr)\},$$

and the Neumann Donoghue m-function $(u_+, M_{H_N,\mathcal{N}_+}(z)u_+)_{L^2(\mathbb{R}^n;d^nx)}$ corresponding to h_0^N in (4.90) are related to each other by (5.29), with $\alpha = \pi/2$, $\beta = \pi/4$, proving (4.94).

Further explicit examples of Krein extensions can be found in [6] and the references therein. All self-adjoint extensions of $\dot{H}$ are described in [5], Section I.1.1 and Ch.1.5. Generalized Friedrichs and Krein extensions in the case where $\dot{H}$ has deficiency indices $(1,1)$ and $\dot{H}$ is not necessarily assumed to be bounded from below, are studied in detail in [32]–[35]. Interesting inverse spectral problems associated with self-adjoint extensions of symmetric operators with gaps were studied in the series of papers [4], [13]–[16].

Finally we discuss some realization theorems for Herglotz operators of the form (4.85). For this purpose introduce the following set of Herglotz operators,

$$\begin{aligned}\mathcal{N}_0(\mathcal{N}) = \{M \in \mathcal{B}(\mathcal{N}) \text{ Herglotz} \,|\, M(z) = \int_{\mathbb{R}} d\Omega(\lambda)((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1});\\ \widetilde{\Omega}(\mathbb{R}) = I_{\mathcal{N}};\ \text{for all } \xi \in \mathcal{N}\backslash\{0\},\ \int_{\mathbb{R}} d(\xi, \Omega(\lambda)\xi)_{\mathcal{N}} = \infty\},\end{aligned} \tag{4.99}$$

$$\begin{aligned}\mathcal{N}_{0,F}(\mathcal{N}) = \{M \in \mathcal{N}_0(\mathcal{N}) \,|\, \text{supp}(\Omega) \subseteq [0,\infty);\ \text{for all } \xi \in \mathcal{N}\backslash\{0\},\\ \int_R^\infty d(\xi, \Omega(\lambda)\xi)_{\mathcal{N}} \lambda^{-1} = \infty \text{ for some } R > 0\},\end{aligned} \tag{4.100}$$

$$\begin{aligned}\mathcal{N}_{0,K}(\mathcal{N}) = \{M \in \mathcal{N}_0(\mathcal{N}) \,|\, \text{supp}(\Omega) \subseteq [0,\infty);\ \text{for all } \xi \in \mathcal{N}\backslash\{0\},\\ \int_0^R d(\xi, \Omega(\lambda)\xi)_{\mathcal{N}} \lambda^{-1} = \infty \text{ for some } R > 0\},\end{aligned} \tag{4.101}$$

$$\begin{aligned}\mathcal{N}_{0,F,K}(\mathcal{N}) &= \{M \in \mathcal{N}_0(\mathcal{N}) \,|\, \text{supp}(\Omega) \subseteq [0,\infty);\ \text{for all } \xi \in \mathcal{N}\backslash\{0\},\\ &\int_R^\infty d(\xi, \Omega(\lambda)\xi)_{\mathcal{N}} \lambda^{-1} = \int_0^R d(\xi, \Omega(\lambda)\xi)_{\mathcal{N}} \lambda^{-1} = \infty \text{ for some } R > 0\}\\ &= \mathcal{N}_{0,F}(\mathcal{N}) \cap \mathcal{N}_{0,K}(\mathcal{N}),\end{aligned} \tag{4.102}$$

where $\mathcal{N}$ is a separable complex Hilbert space, $\text{supp}(\Omega)$ denotes the topological support of Ω, and $\widetilde{\Omega}(\lambda) = (1+\lambda^2)^{-1}\Omega(\lambda)$, $\lambda \in \mathbb{R}$.

Theorem 4.10. *(i) Any $M \in \mathcal{N}_0(\mathcal{N})$ can be realized in the form*

$$M(z) = V^*(zI_{\mathcal{N}_+} + (1+z^2)P_{\mathcal{N}_+}(H - z)^{-1}P_{\mathcal{N}_+}\big|_{\mathcal{N}_+})V, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{4.103}$$

where H denotes a self-adjoint extension of some densely defined closed symmetric operator $\dot{H}$ with deficiency subspaces $\mathcal{N}_\pm$ in some separable Hilbert space $\mathcal{H}$.
(ii) Any $M \in \mathcal{N}_{0,F(resp.K)}(\mathcal{N})$ can be realized in the form

$$M(z) = V^*(zI_{\mathcal{N}_+} + (1+z^2)P_{\mathcal{N}_+}(H_{F(resp.K)} - z)^{-1}P_{\mathcal{N}_+}\big|_{\mathcal{N}_+})V, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{4.104}$$

where $H_{F(resp.K)} \geq 0$ denotes the Friedrichs (respectively, Krein) extension of some densely defined closed symmetric operator $\dot{H}$ with deficiency subspaces $\mathcal{N}_\pm$ in some separable complex Hilbert space $\mathcal{H}$.
(iii) Any $M \in \mathcal{N}_{0,F,K}(\mathcal{N})$ can be realized in the form

$$M(z) = V^*(zI_{\mathcal{N}_+} + (1+z^2)P_{\mathcal{N}_+}(H_{F,K} - z)^{-1}P_{\mathcal{N}_+}\big|_{\mathcal{N}_+})V, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{4.105}$$

where $H_{F,K} \geq 0$ denotes the unique nonnegative self-adjoint extension of some densely defined closed symmetric operator $\dot{H}$ with deficiency subspaces $\mathcal{N}_\pm$ in some separable complex Hilbert space $\mathcal{H}$.

In all cases (i)–(iii), V denotes a unitary operator from $\mathcal{N}$ to $\mathcal{N}_+$.

Proof. (i) Define

$$V : \mathcal{N} \to \widehat{\mathcal{N}}_+, \quad \xi \longrightarrow (\cdot - i)^{-1}\xi \tag{4.106}$$

and use the notation developed for the model pair $(\widehat{\dot{H}}, \widehat{H})$ in (4.32)–(4.37), Theorem 4.4, and Theorem 4.6. Then

$$(V\xi, V\eta)_{\hat{\mathcal{N}}_+} = \int_{\mathbb{R}} d(\xi, \Omega(\lambda)\eta)_{\mathcal{N}}(1+\lambda^2)^{-1} = (\xi, \eta)_{\mathcal{N}}, \quad \xi, \eta \in \mathcal{N} \tag{4.107}$$

shows that V is a linear isometry from $\mathcal{N}$ into $\widehat{\mathcal{H}}_+$,

$$V^*V = I_{\mathcal{N}}, \quad \operatorname{ran}(V^*) = \mathcal{N}. \tag{4.108}$$

By (4.84) (identifying $\mathcal{N}_+$ and $\mathcal{N}$),

$$V^{-1} : \widehat{\mathcal{N}}_+ \to \mathcal{N}, \quad (\cdot - i)^{-1}\xi \longrightarrow \xi \tag{4.109}$$

is also a linear isometry from $\widehat{\mathcal{N}}_+$ into $\mathcal{N}$, implying

$$VV^* = I_{\hat{\mathcal{N}}_+}, \quad \operatorname{ran}(V) = \widehat{\mathcal{N}}_+. \tag{4.110}$$

Thus V is unitary and one computes

$$\begin{aligned}
&(\xi, V^*(zI_{\hat{\mathcal{N}}_+} + (1+z^2)P_{\hat{\mathcal{N}}_+}(\widehat{H} - z)^{-1}P_{\hat{\mathcal{N}}_+}\big|_{\hat{\mathcal{N}}_+})V\eta)_{\mathcal{N}} \\
&= (V\xi, (zI_{\hat{\mathcal{N}}_+} + (1+z^2)P_{\hat{\mathcal{N}}_+}(\widehat{H} - z)^{-1}P_{\hat{\mathcal{N}}_+}\big|_{\hat{\mathcal{N}}_+})V\eta)_{\hat{\mathcal{N}}_+} \\
&= ((\cdot - i)^{-1}\xi, (zI_{\hat{\mathcal{N}}_+} + (1+z^2)P_{\hat{\mathcal{N}}_+}(\widehat{H} - z)^{-1}P_{\hat{\mathcal{N}}_+}\big|_{\hat{\mathcal{N}}_+})(\cdot - i)^{-1}\eta)_{\hat{\mathcal{N}}_+} \\
&= \int_{\mathbb{R}} d(\xi, \Omega(\lambda)\eta)_{\mathcal{N}} z(1+\lambda^2)^{-1} + \int_{\mathbb{R}} d(\xi, \Omega(\lambda)\eta)_{\mathcal{N}} (1+z^2)(1+\lambda^2)^{-1}(\lambda - z)^{-1} \\
&= \int_{\mathbb{R}} d(\xi, \Omega(\lambda)\eta)_{\mathcal{N}} ((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}) \\
&= (\xi, M(z)\eta)_{\mathcal{N}}, \quad \xi, \eta, \in \mathcal{N}, \ z \in \mathbb{C}\backslash\mathbb{R}.
\end{aligned} \tag{4.111}$$

(ii) and (iii) then follow in the same way using Theorem 4.7. ☐

For a whole scale of Nevanlinna classes in the case where $\dot{H}$ has deficiency indices $(1,1)$ we refer to [37].

Remark 4.11. In the special case where $\dim_{\mathbb{C}}(\mathcal{N}) \in \mathbb{N}$, treated in detail in [30], we also considered at length the case where H and H_F (respectively, H_K) were relatively prime operators with respect to $\dot{H}$. In this case the limiting behavior of $M(z)$ as $\lambda \downarrow -\infty$ (respectively, $\lambda \uparrow 0$) crucially entered the corresponding results in Theorems 7.5–7.7 of [30]. These limits are given in terms of $\operatorname{Re}((P_{1,2}(i)\big|_{\mathcal{N}_+})^{-1})$ (cf. (4.15)) identifying $H_1 = H$, $H_2 = H_F$ or H_K , etc. In the present infinite-dimensional case, $(P_{1,2}(i)\big|_{\mathcal{N}_+})^{-1}$ exists if H_1 and H_2 are relatively prime with respect to $\dot{H}$. However, $(P_{1,2}(i)\big|_{\mathcal{N}_+})^{-1}$ is not necessarily a bounded operator in $\mathcal{N}_+$. In fact,

$$\operatorname{Im}((P_{1,2}(i)\big|_{\mathcal{N}_+})^{-1}) = -I_{\mathcal{N}_+}, \tag{4.112}$$

$$\operatorname{Re}((P_{1,2}(i)\big|_{\mathcal{N}_+})^{-1}) \in \mathcal{B}(\mathcal{N}_+) \text{ if and only if } \operatorname{ran}(P_{1,2}(i)) = \mathcal{N}_+ \tag{4.113}$$

as shown in Lemma 2 of [28]. This complicates matters since now the limits of $M(\lambda)$ as $\lambda \downarrow -\infty$ (or $\lambda \uparrow 0$) may exist but possibly represent unbounded self-adjoint operators in $\mathcal{N}_+$ and thus convergence of $M(\lambda)$ as $\lambda \downarrow -\infty$ (or $\lambda \uparrow 0$) in these cases is understood in the strong resolvent sense. A detailed treatment of this topic goes beyond the scope of this paper and is thus postponed.

Theorem 4.12. *Suppose $M_\ell \in \mathcal{N}_0(\mathcal{N})$, $\ell = 1,2$ and $M_1 \neq M_2$. Then M_1 and M_2 can be realized as*

$$M_\ell(z) = V^*(zI_{\mathcal{N}_+} + (1+z^2)P_{\mathcal{N}_+}(H_\ell - z)^{-1}P_{\mathcal{N}_+}\big|_{\mathcal{N}_+})V, \quad \ell = 1,2, \ z \in \mathbb{C}\backslash\mathbb{R}, \tag{4.114}$$

where H_ℓ, $\ell = 1,2$ are distinct self-adjoint extensions of one and the same densely defined closed symmetric operator $\dot{H}$ with deficiency subspaces $\mathcal{N}_\pm$ in some separable complex Hilbert space $\mathcal{H}$, and V denotes a unitary operator from $\mathcal{N}$ to $\mathcal{N}_+$, if and only if,

$$M_2(z) = e^{-i\alpha}(\cos(\alpha) + \sin(\alpha)M_1(z))(\sin(\alpha) - \cos(\alpha)M_1(z))^{-1}e^{i\alpha}, \quad z \in \mathbb{C}\backslash\mathbb{R} \tag{4.115}$$

for some self-adjoint operator α in $\mathcal{N}$.

Proof. Assuming (4.114), (4.115) is clear from (4.30). Conversely, assume (4.115). By Theorem 4.13 (i), we may realize $M_1(z)$ as

$$M_1(z) = V^*(zI_{\mathcal{N}_+} + (1+z^2)P_{\mathcal{N}_+}(H_1 - z)^{-1}P_{\mathcal{N}_+}\big|_{\mathcal{N}_+})V, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{4.116}$$

If $\widetilde{H} \neq H_1$ is another self-adjoint extension of $\dot{H}$ we introduce

$$\widetilde{M}(z) = V^*(zI_{\mathcal{N}_+} + (1+z^2)P_{\mathcal{N}_+}(\widetilde{H} - z)^{-1}P_{\mathcal{N}_+}\big|_{\mathcal{N}_+})V, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{4.117}$$

and infer from Theorem 4.3,

$$\widetilde{M}(z) = e^{-i\widetilde{\alpha}}(\cos(\widetilde{\alpha}) + \sin(\widetilde{\alpha})M_1(z))(\sin(\widetilde{\alpha}) - \cos(\widetilde{\alpha})M_1(z))^{-1}e^{i\widetilde{\alpha}}, \quad z \in \mathbb{C}\backslash\mathbb{R} \tag{4.118}$$

for some $\widetilde{\alpha} = \widetilde{\alpha}^*$ in $\mathcal{N}$.

Since $(H_1 - z)(H_1 \pm i)^{-1}$ are bounded and boundedly invertible, $P_{1,2}(z)$ in (4.4) uniquely characterizes all self-adjoint extensions $H_2 \neq H_1$ of $\dot{H}$. Moreover, by (4.5)–(4.7) and von Neumann's representation of self-adjoint extensions in terms of Cayley transforms, all self-adjoint extensions $H_2 \neq H_1$ of $\dot{H}$ are in a bijective correspondence to all self-adjoint (possibly unbounded) operators $\alpha_{1,2}$ ($\alpha_{1,2} \neq \pi/2$) in $\mathcal{N}_+$. Hence we may choose $\widetilde{H}$ such that $\widetilde{\alpha}$ equals α in (4.115) implying $\widetilde{M}(z) = M_2(z)$. □

We conclude with a result on analytic continuations of general Herglotz operators from $\mathbb{C}_+$ into a subset of $\mathbb{C}_-$ through an interval of the real line, which is independent of our emphasis of perturbation problems in Section 3 and self-adjoint extensions in the present Section 4. As is well-known, the usual convention for $M\big|_{\mathbb{C}_-}$ by means of reflection as in (1.4), in general, does not represent the analytic continuation of $M\big|_{\mathbb{C}_+}$. The following result is an adaptation of a theorem of Greenstein [31] for scalar Herglotz functions to the present operator-valued context.

Lemma 4.13. *Let $\mathcal{K}$ be a separable complex Hilbert space and M be a Herglotz operator in $\mathcal{K}$ with representation* (1.1)–(1.3). *Suppose that the operator Stieltjes integral in* (1.1) *converges in the strong operator topology of $\mathcal{K}$ and let $(\lambda_1, \lambda_2) \subseteq \mathbb{R}$, $\lambda_1 < \lambda_2$. Then a necessary condition for M to have an analytic continuation from $\mathbb{C}_+$ into a subset of $\mathbb{C}_-$ through the interval (λ_1, λ_2) is that for all $\xi \in \mathcal{K}$, the associated scalar measures $\omega_\xi = (\xi, \Omega\,\xi)_{\mathcal{K}}$ are purely absolutely continuous on (λ_1, λ_2), $\omega_\xi\big|_{(\lambda_1,\lambda_2)} = \big(\omega_\xi\big|_{(\lambda_1,\lambda_2)}\big)_{ac}$, and the corresponding density $\omega'_\xi \geq 0$ of ω_ξ is real-analytic on (λ_1, λ_2). If $\mathcal{K}$ is finite-dimensional, this condition is also sufficient. If M has such an analytic continuation into some domain $\mathcal{D}_- \subseteq \mathbb{C}_-$, then it is given by*

$$M(z) = M(\overline{z})^* + 2\pi i\Omega'(z), \quad z \in \mathcal{D}_-, \tag{4.119}$$

where $\Omega'(z)$ denotes the complex-analytic extension of $\Omega'(\lambda)$ for $\lambda \in (\lambda_1, \lambda_2)$. In particular, M can be analytically continued through (λ_1, λ_2) by reflection, that is, $M(z) = M(\overline{z})^*$ for all $z \in \mathbb{C}_-$ if Ω has no support in (λ_1, λ_2).

Proof. Suppose M has an analytic continuation from $\mathbb{C}_+$ into a subset of $\mathbb{C}_-$ through the interval (λ_1, λ_2). Then for all $\xi \in \mathcal{K}$, Greenstein's result [31] applies to the scalar Herglotz function $m_\xi(z) = (\xi, M(z)\xi)_\mathcal{K}$, $\xi \in \mathcal{K}$ associated to the measure $\omega_\xi = (\xi, \Omega\,\xi)_\mathcal{K}$. Consequently, m_ξ has an analytic continuation from $\mathbb{C}_+$ into a subset of $\mathbb{C}_-$ through the interval (λ_1, λ_2) if and only if the associated scalar measure $\omega_\xi = (\xi, \Omega\,\xi)_\mathcal{K}$ is purely absolutely continuous on (λ_1, λ_2), $\omega_\xi\big|_{(\lambda_1,\lambda_2)} = \big(\omega_\xi\big|_{(\lambda_1,\lambda_2)}\big)_{ac}$, and the corresponding density $\omega_\xi' \geq 0$ of ω_ξ is real-analytic on (λ_1, λ_2). In this case the analytic continuation of m_ξ into some domain $\mathcal{D}_{-,\xi} \subseteq \mathbb{C}_-$ is given by

$$m_\xi(z) = m_\xi(\overline{z})^* + 2\pi i\omega_\xi'(z), \quad z \in \mathcal{D}_{-,\xi}, \tag{4.120}$$

where $\omega_\xi'(z)$ denotes the complex-analytic extension of $\omega_\xi'(\lambda)$ for $\lambda \in (\lambda_1, \lambda_2)$. This can be seen as follows: If m_x can be analytically continued through (λ_1, λ_2) into some region $\mathcal{D}_- \subseteq \mathbb{C}_-$, then $\widetilde{m}_\xi(z) := m_\xi(z) - \pi i\omega_\xi'(z)$ is real-analytic on (λ_1, λ_2) and hence can be continued through (λ_1, λ_2) by reflection. Similarly, $\omega_\xi'(z)$, being real-analytic, can be continued through (λ_1, λ_2) by reflection. Hence (4.120) follows from

$$m_\xi(z) - \pi i\omega_\xi'(z) = \widetilde{m}_\xi(z) = \overline{\widetilde{m}_\xi(\overline{z})} = \overline{m_\xi(\overline{z})} + \pi i\omega_\xi'(z), \quad z \in \mathcal{D}_-. \tag{4.121}$$

Applying a standard polarization argument, we obtain that the analytic continuation of $m_{\xi,\eta}(z) = (\xi, M(z)\eta)_\mathcal{K}$, $\xi, \eta \in \mathcal{K}$ into some domain $\mathcal{D}_{-,\xi,\eta} \subseteq \mathbb{C}_-$ is given by

$$m_{\xi,\eta}(z) = m_{\xi,\eta}(\overline{z})^* + 2\pi i\omega_{\xi,\eta}'(z), \quad z \in \mathcal{D}_{-,\xi,\eta}, \tag{4.122}$$

where $\omega_{\xi,\eta}'(z) = (\xi, \Omega'(z)\,\eta)_\mathcal{K}$ is related to $\omega_{\xi\pm\eta}'(z)$ and $\omega_{\xi\pm i\eta}'(z)$ by polarization. In particular, if $M(z)$ has such an analytic continuation through the interval (λ_1, λ_2) it is necessarily of the form stated in (4.119). If $\dim_\mathbb{C}(\mathcal{K}) < \infty$, then (4.120) and (4.121) yield the weak and hence $\mathcal{B}(\mathcal{K})$-analytic continuation of M through the interval (λ_1, λ_2). $\square$

Formula (4.119) shows that any possible singularity behavior of $M\big|_{\mathbb{C}_-}$ is determined by that of $\Omega'\big|_{\mathbb{C}_-}$ since M, being Herglotz, has no singularities in $\mathbb{C}_+$. Moreover, analytic continuations through different intervals on $\mathbb{R}$ in general, will lead to different $\Omega'(z)$ and hence to branch cuts of $M\big|_{\mathbb{C}_-}$.

5. One-Dimensional Applications

In our final section we consider concrete applications of the formalism of Section 4 in the special case $\dim_\mathbb{C}(\mathcal{N}_+) = 1$. We study Schrödinger operators on a half-line, compare the corresponding Donoghue and Weyl-Titchmarsh m-functions, and prove some estimates on linear functionals associated with these Schrödinger operators. We conclude with two illustrations of Livsic's result [44] on quasi-hermitian extensions in the special case of densely defined closed prime symmetric operators with deficiency indices $(1, 1)$ in connection with first-order differential expressions $-id/dx$.

First we specialize some of the abstract material in Section 4 to the case of a densely defined closed prime symmetric operator $\dot{H}$ in a separable complex Hilbert space $\mathcal{H}$ with deficiency indices $(1,1)$. This case has been studied in detail by Donoghue [25] (see also [30]) and we partly follow his analysis.

Choose $u_\pm \in \ker(\dot{H}^* \mp i)$ with $||u_\pm||_{\mathcal{H}} = 1$ and introduce the one-parameter family H_α, $\alpha \in [0,\pi)$ of self-adjoint extensions $\dot{H}$ in $\mathcal{H}$ by

$$\begin{aligned}&H_\alpha(f + c(u_+ + e^{2i\alpha}u_-)) = \dot{H}f + c(iu_+ - ie^{2i\alpha}u_-),\\ &\operatorname{dom}(H_\alpha) = \{(f + c(u_+ + e^{2i\alpha}u_-)) \in \operatorname{dom}(\dot{H}^*) \,|\, f \in \operatorname{dom}(\dot{H}),\, c \in \mathbb{C}\}, \quad \alpha \in [0,\pi).\end{aligned} \tag{5.1}$$

Let $\{E_{H_\alpha}(\lambda)\}_{\lambda\in\mathbb{R}}$ be the family of orthogonal spectral projections of H_α and suppose that H_α has simple spectrum for one (and hence for all) $\alpha \in [0,\pi)$. (This is equivalent to the assumption that $\dot{H}$ is a prime symmetric operator and also equivalent to the fact that u_+ is a cyclic vector for H_α for all $\alpha \in [0,\pi)$.) Next we introduce the model representation $(\widehat{\dot{H}}_\alpha, \widehat{H}_\alpha)$ for $(\dot{H}, H_\alpha)$ discussed in (4.32)–(4.37), Theorem 4.4, and Theorem 4.6. However, since in the present context $\mathcal{N}_+$ is a one-dimensional subspace of $\mathcal{H}$,

$$\mathcal{N}_+ = \text{lin.span}\{u_+\}, \tag{5.2}$$

the model Hilbert space $\widehat{\mathcal{H}}_\alpha = L^2(\mathbb{R}, \mathcal{N}_+; d\Omega_{H_\alpha,\mathcal{N}_+})$, $\alpha \in [0,\pi)$ with the operator (in fact, rank-one) valued measure $\Omega_{H_\alpha,\mathcal{N}_+}$,

$$\begin{aligned}&\Omega_{H_\alpha,\mathcal{N}_+}(\lambda) = \omega_\alpha(\lambda)P_{\mathcal{N}_+}|_{\mathcal{N}_+}, \quad P_{\mathcal{N}_+} = (u_+,\cdot)u_+,\\ &\omega_\alpha(\lambda) = (1+\lambda^2)\|E_{H_\alpha}(\lambda)u_+\|^2_{\mathcal{H}}, \quad \alpha \in [0,\pi),\end{aligned} \tag{5.3}$$

can be replaced by the model space $\widetilde{\mathcal{H}}_\alpha = L^2(\mathbb{R}; d\omega_\alpha)$ with scalar measure ω_α. In particular, $\omega_\alpha(\lambda)$ can be taken as the control measure in this special case and

$$\begin{aligned}&V: \widehat{\mathcal{H}}_\alpha = L^2(\mathbb{R}, \mathcal{N}_+; d\Omega_{H_\alpha,\mathcal{N}_+}) \to \widetilde{\mathcal{H}}_\alpha = L^2(\mathbb{R}; d\omega_\alpha)\\ &\hat{f} = \{\hat{f}(\lambda) = \tilde{f}(\lambda)u_+\}_{\lambda\in\mathbb{R}} \to V\hat{f} = \tilde{f} = \{\tilde{f}(\lambda)\}_{\lambda\in\mathbb{R}}\end{aligned} \tag{5.4}$$

represents the corresponding unitary operator from $\widehat{\mathcal{H}}_\alpha = L^2(\mathbb{R}, \mathcal{N}_+; d\Omega_{H_\alpha,\mathcal{N}_+})$ to $\widetilde{\mathcal{H}}_\alpha = L^2(\mathbb{R}; d\omega_\alpha)$. Hence we translate in the following some of the results of Theorems 4.4 and 4.6 from $\widehat{\mathcal{H}}_\alpha$ to $\widetilde{\mathcal{H}}_\alpha$. However, due to the trivial nature of the unitary operator V in (5.4), we will ignore this additional isomorphism and simply keep using our $\widehat{\ }$-notation of Section 4 instead of the new $\widetilde{\ }$-notation. Thus, we consider the model Hilbert space $\widehat{\mathcal{H}}_\alpha = L^2(\mathbb{R}; d\omega_\alpha)$, $\alpha \in [0,\pi)$, where

$$\omega_\alpha(\lambda) = (1+\lambda^2)||E_{H_\alpha}(\lambda)u_+||^2_{\mathcal{H}}, \quad \alpha \in [0,\pi), \tag{5.5}$$

$$\int_{\mathbb{R}} d\omega_\alpha(\lambda)(1+\lambda^2)^{-1} = 1, \quad \int_{\mathbb{R}} d\omega_\alpha(\lambda) = \infty, \quad \alpha \in [0,\pi) \tag{5.6}$$

and define in $\widehat{\mathcal{H}}_\alpha$ the self-adjoint operator $\widehat{H}_\alpha$,

$$(\widehat{H}_\alpha \hat{f})(\lambda) = \lambda\hat{f}(\lambda), \quad \hat{f} \in \operatorname{dom}(\widehat{H}_\alpha) = L^2(\mathbb{R}; (1+\lambda^2)d\omega_\alpha) \tag{5.7}$$

and its densely defined and closed restriction $\widehat{\dot{H}}_\alpha$,

$$\operatorname{dom}(\widehat{\dot{H}}_\alpha) = \{\hat{f} \in \operatorname{dom}(\widehat{H}_\alpha) \,|\, \textstyle\int_{\mathbb{R}} d\omega_\alpha(\lambda)\hat{f}(\lambda) = 0\}, \quad \widehat{\dot{H}}_\alpha = \widehat{H}_\alpha\big|_{\operatorname{dom}(\widehat{\dot{H}}_\alpha)}. \tag{5.8}$$

Then

$$\ker(\hat{\dot{H}}^* - z) = \{c(\cdot - z)^{-1} \in \widehat{\mathcal{H}}_\alpha \,|\, c \in \mathbb{C}\} \tag{5.9}$$

and the pair $(\dot{H}, H_\alpha)$ in $\mathcal{H}$ is unitarily equivalent to the pair $(\hat{\dot{H}}_\alpha, \widehat{H}_\alpha)$ in $\widehat{\mathcal{H}}_\alpha$ (cf. Theorem 4.6). This representation of $(\dot{H}, H_\alpha)$ in terms of $(\hat{\dot{H}}_\alpha, \widehat{H}_\alpha)$ has the advantage of very simple definitions of $\widehat{H}_\alpha$ and $\hat{\dot{H}}_\alpha$, however, one has to pay a price since different $H_\alpha, \hat{\dot{H}}_\alpha$ act in different Hilbert spaces $\widehat{\mathcal{H}}_\alpha$. Hence it is desirable to determine the expression for all H_α, $\alpha \in [0, \pi)$ in connection with one fixed α say, $\alpha_0 \in [0, \pi)$, in the corresponding fixed Hilbert space $\widehat{\mathcal{H}}_{\alpha_0} = L^2(\mathbb{R}; d\omega_{\alpha_0})$ and we turn our attention to this task next.

Lemma 5.1. *Fix* $\alpha_0 \in [0, \pi)$ *and define*

$$U_{\alpha_0} : \widehat{\mathcal{H}}_{\alpha_0} \longrightarrow \mathcal{H}, \quad \hat{f} \to U_{\alpha_0} \hat{f} = \operatorname*{s-lim}_{N \to \infty} \int_{-N}^{N} d(E_{H_{\alpha_0}}(\lambda) u_+)(\lambda - i) \hat{f}(\lambda). \tag{5.10}$$

Then U_{α_0} *is a unitary operator from* $\widehat{\mathcal{H}}_{\alpha_0}$ *to* $\mathcal{H}$ *and*

$$\dot{H} = U_{\alpha_0} \hat{\dot{H}}_{\alpha_0} U_{\alpha_0}^{-1}, \quad H_{\alpha_0} = U_{\alpha_0} \widehat{H}_{\alpha_0} U_{\alpha_0}^{-1}. \tag{5.11}$$

Moreover,

$$\hat{u}_+(\lambda) = (U_{\alpha_0}^{-1} u_+)(\lambda) = (\lambda - i)^{-1}, \tag{5.12}$$

$$\hat{u}_-(\lambda) = (U_{\alpha_0}^{-1} u_-)(\lambda) = -e^{-2i\alpha_0} (\lambda + i)^{-1}, \quad \lambda \in \mathbb{R}, \tag{5.13}$$

and hence

$$(U_{\alpha_0}^{-1}(u_+ + e^{2i\alpha} u_-))(\lambda) = 2ie^{i(\alpha - \alpha_0)}(1 + \lambda^2)^{-1}(-\lambda \sin(\alpha - \alpha_0) + \cos(\alpha - \alpha_0)),$$
$$\alpha \in [0, \pi), \ \lambda \in \mathbb{R}. \tag{5.14}$$

Proof. (5.10) and (5.11) have been discussed in Theorem 4.6, (5.12) is clear from (5.10). From

$$U_{\alpha_0}^{-1} H_{\alpha_0}(u_+ + e^{2i\alpha_0} u_-) = U_{\alpha_0}^{-1} \dot{H}^*(u_+ + e^{2i\alpha_0} u_-) = i\hat{u}_+ - ie^{2i\alpha_0} \hat{u}_-, \tag{5.15}$$

$$\widehat{H}_{\alpha_0}(\hat{u}_+ + e^{2i\alpha_0} \hat{u}_-) = \lambda(\hat{u}_+ + e^{2i\alpha_0} \hat{u}_-), \tag{5.16}$$

and (5.12) one infers

$$i(\lambda - i)^{-1} - ie^{2i\alpha_0} \hat{u}_-(\lambda) = \lambda(\lambda - i)^{-1} + e^{2i\alpha_0} \lambda \hat{u}_-(\lambda) \tag{5.17}$$

and hence (5.13). Equation (5.14) then immediately follows from (5.12) and (5.13). □

Equation (5.14) confirms the fact that any two different self-adjoint extensions of $\dot{H}$ are relatively prime

$$\operatorname{dom}(H_\alpha) \cap \operatorname{dom}(H_\beta) = \operatorname{dom}(\dot{H}), \quad \alpha, \beta \in [0, \pi), \quad \alpha \neq \beta \tag{5.18}$$

since $\int_{\mathbb{R}} d\omega_{\alpha_0}(\lambda) = \infty$ and hence

$$\int_{\mathbb{R}} d\omega_{\alpha_0}(\lambda) \lambda^2 |U_{\alpha_0}^{-1}(u_+ + e^{2i\alpha} u_-)(\lambda)|^2 = \infty \text{ for all } \alpha \neq \alpha_0. \tag{5.19}$$

This is of course an artifact of our special hypothesis $\mathrm{def}(\widehat{H}) = (1,1)$.

Next, consider the normalized element (cf. (5.14) for $\alpha = \alpha_0$)

$$\hat{g}_\alpha \in \big(\ker(\widehat{\dot{H}}^* - i) \dot{+} \ker(\widehat{\dot{H}}^* + i)\big) \cap \mathrm{dom}(\widehat{H}_\alpha),$$
$$\hat{g}_\alpha(\lambda) = \bigg(\int_{\mathbb{R}} d\omega_\alpha(\nu)(1+\nu^2)^{-2}\bigg)^{-1/2}(1+\lambda^2)^{-1}, \quad ||\hat{g}_\alpha||_{\hat{\mathcal{H}}_\alpha} = 1. \tag{5.20}$$

Then

$$\mathrm{dom}(\widehat{H}_\alpha) = \mathrm{lin.span}\{\hat{g}_\alpha\} \dot{+} \mathrm{dom}(\widehat{\dot{H}}_\alpha) \tag{5.21}$$

by von Neumann's theory of self-adjoint extensions of symmetric operators (cf., e.g., [3], Ch. VII, [26], Sect. II.4, [54], Sect. 14, [55], Sect. X.1, [69]) and we may consider the linear functional $\ell_{\hat{g}_\alpha}$ on $\mathrm{dom}(\widehat{H}_\alpha)$ defined by

$$\ell_{\hat{g}_\alpha} : \mathrm{dom}(\widehat{H}_\alpha) \to \mathbb{C}, \quad \ell_{\hat{g}_\alpha}(\hat{f}) = c, \tag{5.22}$$

where

$$\hat{f} \in \mathrm{dom}(\widehat{H}_\alpha), \quad \hat{f} = c\hat{g}_\alpha + \hat{h}, \quad \hat{h} \in \mathrm{dom}(\widehat{\dot{H}}_\alpha). \tag{5.23}$$

Lemma 5.2. *Let $\alpha \in [0,\pi)$. Then*

$$\sup_{\hat{f} \in \mathrm{dom}(\hat{H}_\alpha)} \bigg(\frac{|\ell_{\hat{g}_\alpha}(\hat{f})|^2}{||\hat{f}||^2_{\hat{\mathcal{H}}_\alpha} + ||\widehat{H}_\alpha \hat{f}||^2_{\hat{\mathcal{H}}_\alpha}}\bigg) = \int_{\mathbb{R}} d\omega_\alpha(\lambda)(1+\lambda^2)^{-2}. \tag{5.24}$$

Proof. By (5.6) and (5.8) one computes

$$\int_{\mathbb{R}} d\omega_\alpha(\lambda)\hat{f}(\lambda) = c\int_{\mathbb{R}} d\omega_\alpha(\lambda)\hat{g}_\alpha(\lambda) = \ell_{\hat{g}_\alpha}(\hat{f})\bigg(\int_{\mathbb{R}} d\omega_\alpha(\lambda)(1+\lambda^2)^{-2}\bigg)^{-1/2} \tag{5.25}$$

and hence the Cauchy-Schwarz inequality applied to

$$\begin{aligned}\bigg|\int_{\mathbb{R}} d\omega_\alpha(\lambda)\hat{f}(\lambda)\bigg| &\leq \bigg(\int_{\mathbb{R}} d\omega_\alpha(\lambda)(1+\lambda^2)|\hat{f}(\lambda)|^2\bigg)^{1/2}\bigg(\int_{\mathbb{R}} d\omega_\alpha(\lambda)(1+\lambda^2)^{-1}\bigg)^{1/2} \\ &= (||\hat{f}||^2_{\hat{\mathcal{H}}_\alpha} + ||\widehat{H}_\alpha \hat{f}||^2_{\hat{\mathcal{H}}_\alpha})^{1/2}\end{aligned} \tag{5.26}$$

yields

$$\frac{|\ell_{\hat{g}_\alpha}(\hat{f})|^2}{||\hat{f}||^2_{\hat{\mathcal{H}}_\alpha} + ||\widehat{H}_\alpha \hat{f}||^2_{\hat{\mathcal{H}}_\alpha}} \leq \int_{\mathbb{R}} d\omega_\alpha(\lambda)(1+\lambda^2)^{-2}. \tag{5.27}$$

Since inequality (5.27) saturates for $\hat{f}_0(\lambda) = (1+\lambda^2)^{-1}$, $\hat{f}_0 \in \mathrm{dom}(\widehat{H}_\alpha)$, (5.24) is proved. ☐

Introducing the Donoghue-type m-function

$$m^D_\alpha(z) = \int_{\mathbb{R}} d\omega_\alpha(\lambda)((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}), \quad \alpha \in [0,\pi),\ z \in \mathbb{C}_+, \tag{5.28}$$

the analog of (4.17), one can prove the following result.

Lemma 5.3. (Donoghue [25].)

$$m^D_\beta(z) = \frac{-\sin(\beta-\alpha) + \cos(\beta-\alpha)m^D_\alpha(z)}{\cos(\beta-\alpha) + \sin(\beta-\alpha)m^D_\alpha(z)}, \quad \alpha,\beta \in [0,\pi),\ z \in \mathbb{C}_+. \tag{5.29}$$

Next we turn to Schrödinger operator on the half-line $[0,\infty)$. Let $q \in L^1([0,R])$ for all $R>0$, q real-valued and introduce the fundamental system $\phi_\gamma(z,x)$, $\theta_\gamma(z,x)$, $z \in \mathbb{C}$ of solutions of

$$-\psi''(z,x) + (q(x)-z)\psi(z,x) = 0, \quad x>0 \tag{5.30}$$

($'$ denotes d/dx) satisfying

$$\phi_\gamma(z,0_+) = -\theta'_\gamma(z,0_+) = -\sin(\gamma), \quad \phi'_\gamma(z,0_+) = \theta_\gamma(z,0_+) = \cos(\gamma), \quad \gamma \in [0,\pi). \tag{5.31}$$

Assuming that $-\frac{d^2}{dx^2}+q$ is in the limit point case at ∞, let $\psi_\gamma(z,x)$ be the unique solution of (5.30) satisfying

$$\psi_\gamma(z,\cdot) \in L^2([0,\infty);dx), \quad \sin(\gamma)\psi'_\gamma(z,0_+) + \cos(\gamma)\psi_\gamma(z,0_+) = 1, \quad \gamma \in [0,\pi),\ z \in \mathbb{C}_+. \tag{5.32}$$

Then $\psi_\gamma(z,x)$ is of the form (see, e.g., the discussion of Weyl's theory in Appendix A of [29])

$$\psi_\gamma(z,x) = \theta_\gamma(z,x) + m_\gamma^W(z)\phi_\gamma(z,x), \quad \gamma \in [0,\pi),\ z \in \mathbb{C}_+, \tag{5.33}$$

where $m_\gamma^W(z)$ denotes the Weyl-Titchmarsh m-function [64], Chs. II, III, [70] (as opposed to Donoghue's m-function $m_\alpha^D(z)$ in (5.28)) corresponding to the operator $\widetilde{H}_\gamma$ in $L^2([0,\infty);dx)$ defined by

$$\begin{aligned}
&(\widetilde{H}_\gamma f)(x) = -f''(x) + q(x)f(x), \quad x>0,\\
&f \in \operatorname{dom}(\widetilde{H}_\gamma) = \{g \in L^2([0,\infty);dx) \,|\, g,g' \in AC([0,R]) \text{ for all } R>0;\\
&\qquad \sin(\gamma)g'(0_+) + \cos(\gamma)g(0_+) = 0;\ -g''+qg \in L^2([0,\infty);dx)\}, \quad \gamma \in [0,\pi).
\end{aligned} \tag{5.34}$$

The family $\widetilde{H}_\gamma$, $\gamma \in [0,\pi)$ represents all self-adjoint extensions of the densely defined closed prime symmetric operator $\dot{\widetilde{H}}$ in $L^2([0,\infty);dx)$ of deficiency indices $(1,1)$,

$$\begin{aligned}
&(\dot{\widetilde{H}} f)(x) = -f''(x) + q(x)f(x), \quad x>0,\\
&f \in \operatorname{dom}(\dot{\widetilde{H}}_\gamma) = \{g \in L^2([0,\infty);dx)) \,|\, g,g' \in AC([0,R]) \text{ for all } R>0;\\
&\qquad g'(0_+) = g(0_+) = 0;\ -g''+qg \in L^2([0,\infty);dx)\}.
\end{aligned} \tag{5.35}$$

(Here $AC([a,b])$ denotes the set of absolutely continuous functions on $[a,b]$.) Weyl's m-function is a Herglotz function with representation

$$m_\gamma^W(z) = \begin{cases} c_\gamma + \int_{\mathbb{R}} d\omega_\gamma^W(\lambda)((\lambda-z)^{-1} - \lambda(1+\lambda^2)^{-1}), & \gamma \in [0,\pi),\\ \cot(\gamma) + \int_{\mathbb{R}} d\omega_\gamma^W(\lambda)(\lambda-z)^{-1}, & \gamma \in (0,\pi), \end{cases} \tag{5.36}$$

for some $c_\gamma \in \mathbb{R}$, where

$$\int_{\mathbb{R}} d\omega_\gamma^W(\lambda)(1+|\lambda|)^{-1} \begin{cases} <\infty, & \gamma \in (0,\pi),\\ =\infty, & \gamma = 0. \end{cases} \tag{5.37}$$

Moreover, one can prove the following result.

Lemma 5.4. (See, e.g., Aronszajn [9], [27], Sect. 2.5.)

$$m_\delta^W(z) = \frac{-\sin(\delta-\gamma) + \cos(\delta-\gamma)m_\gamma^W(z)}{\cos(\delta-\gamma) + \sin(\delta-\gamma)m_\gamma^W(z)}, \quad \delta,\gamma \in [0,\pi),\ z \in \mathbb{C}_+. \tag{5.38}$$

Moreover,

$$m_\gamma^W(z) \underset{z\to i\infty}{=} \begin{cases} \cot(\gamma) + O(z^{-1/2}), & \gamma \in [0,\pi), \\ iz^{1/2} + o(1), & \gamma = 0. \end{cases} \tag{5.39}$$

In the following we denote by H_α in $L^2([0,\infty);dx)$ the Schrödinger operator on $[0,\infty)$ defined as in (5.1) but with $\dot H$ replaced by $\dot{\widetilde H}$ in (5.35). The connection between H_α and $\widetilde H_\gamma$ and $m_\alpha^D(z)$ and $m_\gamma^W(z)$ is then determined as follows.

Theorem 5.5. *Suppose $\gamma(\alpha) \in [0,\pi)$ satisfies*

$$\cot(\gamma(\alpha)) = -\mathrm{Re}(m_0^W(i)) - \mathrm{Im}(m_0^W(i))\tan(\alpha), \quad \alpha \in [0,\pi). \tag{5.40}$$

Then

$$H_\alpha = \widetilde H_{\gamma(\alpha)}, \quad \alpha \in [0,\pi). \tag{5.41}$$

and

$$m_\alpha^D(z) = (m_{\gamma(\alpha)}^W(z) - \mathrm{Re}(m_{\gamma(\alpha)}^W(i))/\mathrm{Im}(m_{\gamma(\alpha)}^W(i)), \quad \alpha \in [0,\pi),\, z \in \mathbb{C}_+. \tag{5.42}$$

Proof. Since $\psi_\gamma(z,x)$ are just constant multiples of $\psi_0(z,x)$, it suffices to focus on $\psi_0(z,x)$. In order to prove (5.41), subject to (5.40), we need

$$\eta_\alpha = ||\psi_0(i)||^{-1}_{L^2([0,\infty);dx)}\psi_0(i) + ||\psi_0(-i)||^{-1}_{L^2([0,\infty);dx)}e^{2i\alpha}\psi_0(-i) \in \mathrm{dom}(H_\alpha) \tag{5.43}$$

according to (5.1) and the fact (cf. (5.32))

$$u_\pm = ||\psi_0(\pm i)||^{-1}_{L^2([0,\infty);dx)}\psi_0(\pm i). \tag{5.44}$$

Since it is known (see, e.g., [20], Sect. 9.2, [27], Sect. 2.2) that

$$||\psi_\gamma(z)||^2_{L^2([0,\infty);dx)} = \mathrm{Im}(m_\gamma^W(z))/\mathrm{Im}(z), \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{5.45}$$

one obtains from (5.52) and (5.33)

$$-\cot(\gamma(\alpha)) = \eta_\alpha'(0_+)/\eta_\alpha(0_+) = (1+e^{2i\alpha})^{-1}(m_0^W(i) + e^{2i\alpha}m_0^W(-i)), \tag{5.46}$$

which yields (5.40) and at the same time proves (5.41). By (5.28) and (5.36),

$$m_\alpha^D(z) = A_\alpha m_{\gamma(\alpha)}^W(z) + B_\alpha, \quad \alpha \in [0,\pi),\ z \in \mathbb{C}_+ \tag{5.47}$$

for some $A_\alpha > 0$ and $B_\alpha \in \mathbb{R}$. The fact

$$m_\alpha^D(i) = i, \quad \alpha \in [0,\pi) \tag{5.48}$$

(use (4.8) or combine the normalization $\int_{\mathbb{R}} d\omega_\alpha(\lambda)(1+\lambda^2)^{-1} = 1$ with (5.28)) immediately yields (5.42). ☐

Corollary 5.6. *Assume in addition that $\dot H \geq 0$. Then the Friedrichs extension H_F of $\dot H$ corresponds to*

$$\alpha = \alpha_F = \pi/2 \quad \text{and} \quad \gamma = \gamma_F = 0 \tag{5.49}$$

and the Krein extension H_K of $\dot H$ corresponds to

$$\tan(\alpha) = \tan(\alpha_K) = m_{\pi/2}^D(0_-) \quad \text{and} \quad \cot(\gamma) = \cot(\gamma_K) = -m_0^W(0_-) \tag{5.50}$$

in (5.1) and (5.34). The right-hand sides in (5.50) are simultaneously infinite if and only if $H_F = H_K$.

Proof. Since $\lim_{\lambda\downarrow-\infty} m_0^W(\lambda) = -\infty$ by (5.39), (5.49) follows from Corollary 4.8 (i). Similarly, (5.50) follows from (5.38) (replacing $\delta \to \gamma$ and $\gamma \to 0$) and Corollary 4.8 (ii). □

Finally we return to the functional $\ell_{\hat g_\alpha}$ in (5.22) and establish its properties in connection with the Schrödinger operator $\widetilde H_\gamma$ on $[0,\infty)$.

Lemma 5.7. *Define* $\hat g_\alpha$ *by*

$$U_\alpha^{-1}\hat g_\alpha = ||\psi_0(i) + e^{2i\alpha}\psi_0(-i))||^{-1}_{L^2([0,\infty);dx)}(\psi_0(i) + e^{2i\alpha}\psi_0(-i)), \quad \alpha \in [0,\pi). \tag{5.51}$$

Then

$$\ell_{\hat g_\alpha}(\hat f) = \begin{cases} (2i\mathrm{Im}(m_0^W(i)))^{-1}||\psi_0(i) - \psi_0(-i)||_{L^2([0,\infty);dx)}(U_{\pi/2}^{-1}\hat f)'(0_+), & \alpha = \frac{\pi}{2}, \\ (1+e^{2i\alpha})^{-1}||\psi_0(i) + e^{2i\alpha}\psi_0(-i)||_{L^2([0,\infty);dx)}(U_\alpha^{-1}\hat f)(0_+), & \alpha \in [0,\pi)\backslash\{\frac{\pi}{2}\}, \end{cases}$$
$$\hat f \in \mathrm{dom}(\widehat H_\alpha). \tag{5.52}$$

Proof. By (5.43) and (5.45),

$$\psi_0(i) + e^{2i\alpha}\psi_0(-i) \in \mathrm{dom}(H_\alpha).$$

Hence

$$f = c||\psi_0(i) + e^{2i\alpha}\psi_0(-i)||^{-1}_{L^2([0,\infty);dx)}(\psi_0(i) + e^{2i\alpha}\psi_0(-i)) + h, \tag{5.53}$$
$$f \in \mathrm{dom}(H_\alpha), \ h \in \mathrm{dom}(\dot H)$$

and

$$\ell_{\hat g_\alpha}(\hat f) = c, \quad \hat f \in \mathrm{dom}(\widehat H_\alpha). \tag{5.54}$$

Since by (5.34),

$$h'(0_+) = h(0_+) = 0, \tag{5.55}$$

one computes in the case $\alpha = \pi/2$

$$\begin{aligned} f'(0_+) &= c||\psi_0(i) - \psi_0(-i)||^{-1}_{L^2([0,\infty);dx)}(\psi_0'(i,0_+) - \psi_0'(-i,0_+)) \\ &= c||\psi_0(i) - \psi_0(-i)||^{-1}_{L^2([0,\infty);dx)}2i\mathrm{Im}(m_0^W(i)), \quad f \in \mathrm{dom}(H_{\pi/2}) \end{aligned} \tag{5.56}$$

using (5.31) and (5.33). Similarly, for $\alpha \in [0,\pi)\backslash\{\pi/2\}$ one computes

$$\begin{aligned} f(0_+) &= c||\psi_0(i) + e^{2i\alpha}\psi_0(-i)||^{-1}_{L^2([0,\infty);dx)}(\psi_0(i,0_+) + e^{2i\alpha}\psi_0(-i,0_+)) \\ &= c||\psi_0(i) + e^{2i\alpha}\psi_0(-i)||^{-1}_{L^2([0,\infty);dx)}(1+e^{2i\alpha}), \end{aligned} \tag{5.57}$$
$$f \in \mathrm{dom}(H_{\pi/2}), \ \alpha \in [0,\pi)\backslash\{\pi/2\},$$

since $\psi_0(z,0_+) = 1, z \in \mathbb{C}\backslash\mathbb{R}$ by (5.31) and (5.33). Combining (5.54) and (5.56), (5.57) proves (5.52). □

Lemmas 5.2 and 5.3 then yield the principal result of this section:

Theorem 5.8. *Let* $\alpha \in [0,\pi)$. *Then*

$$\sup_{f\in\mathrm{dom}(H_{\pi/2})}\left(\frac{|f'(0_+)|^2}{||f||^2_{L^2([0,\infty);dx)} + ||H_{\pi/2}f||^2_{L^2([0,\infty);dx)}}\right) = \mathrm{Im}(m_0^W(i)), \tag{5.58}$$

$$\sup_{f\in \mathrm{dom}(H_\alpha)}\left(\frac{|f(0_+)|^2}{||f||^2_{L^2([0,\infty);dx)}+||H_\alpha f||^2_{L^2([0,\infty);dx)}}\right)=\frac{\cos^2(\alpha)}{\mathrm{Im}(m_0^W(i))}. \tag{5.59}$$

Proof. Consider $\alpha=\pi/2$ first. Then Lemma 5.2 combined with (5.11), (5.44), and (5.52) yields

$$\begin{aligned}&\sup_{f\in \mathrm{dom}(H_{\pi/2})}\left(\frac{|f'(0_+)|^2}{||f||^2_{L^2([0,\infty);dx)}+||H_{\pi/2} f||^2_{L^2([0,\infty);dx)}}\right)\\ &=\frac{4|\mathrm{Im}(m_0^W(i))|^2}{||\psi_0(i)||^2_{L^2([0,\infty);dx)}||u_+-u_-||^2_{L^2([0,\infty);dx)}}\int_{\mathbb{R}}d\omega_{\pi/2}(\lambda)(1+\lambda^2)^{-2}.\end{aligned} \tag{5.60}$$

Since

$$||u_+-u_-||^2_{L^2([0,\infty);dx)}=||\hat u_+-\hat u_-||^2_{\hat{\mathcal{H}}_{\pi/2}}=4\int_{\mathbb{R}}d\omega_{\pi/2}(1+\lambda^2)^{-2} \tag{5.61}$$

by (5.12) (taking $\alpha_0=\pi/2$) and

$$||\psi_0(i)||^2_{L^2([0,\infty);dx)}=\mathrm{Im}(m_0^W(i)) \tag{5.62}$$

by (5.45), the right-hand side of (5.60) coincides with that in (5.58). Similarly, one computes from Lemma 5.2, (5.11), (5.44), and (5.52),

$$\begin{aligned}&\sup_{f\in \mathrm{dom}(H_\alpha)}\left(\frac{|f(0_+)|^2}{||f||^2_{L^2([0,\infty);dx)}+||H_\alpha f||^2_{L^2([0,\infty);dx)}}\right)\\ &=\frac{4\cos^2(\alpha)}{||\psi_0(i)||^2_{L^2([0,\infty);dx)}||u_++e^{2i\alpha}u_-||^2_{L^2([0,\infty);dx)}}\int_{\mathbb{R}}d\omega_\alpha(\lambda)(1+\lambda^2)^{-2}.\end{aligned} \tag{5.63}$$

Because of (5.62) and

$$||u_++e^{2i\alpha}u_-||^2_{L^2([0,\infty);dx)}=||\hat u_++e^{2i\alpha}\hat u_-||^2_{\hat{\mathcal{H}}_\alpha}=4\int_{\mathbb{R}}d\omega_\alpha(\lambda)(1+\lambda^2)^{-2}, \tag{5.64}$$

(5.63) coincides with (5.59). □

Remark 5.9. (i) In the special case $q(x)=0$, $x\geq 0$ one has

$$m_0^W(z)=i(z)^{1/2} \tag{5.65}$$

(using the branch with $\mathrm{Im}((z)^{1/2})\geq 0$, $z\in\mathbb{C}$) and hence (5.58) yields

$$|f'(0_+)|\leq 2^{-1/4}\left(\int_0^\infty dx(|f(x)|^2+|f''(x)|^2\right)^{1/2},\quad f\in H_0^{2,2}((0,\infty)), \tag{5.66}$$

with $2^{-1/4}$ best possible and

$$\begin{aligned}H_0^{2,2}((0,\infty))=\{f\in L^2([0,\infty);dx)\,|\,f,f'\in AC([0,R])\text{ for all }R>0;\\ f(0_+)=0;\ f,f''\in L^2([0,\infty);dx)\}\end{aligned} \tag{5.67}$$

the familiar Sobolev space.

(ii) Multiplying the two results (5.58) and (5.59) reveals the curious fact,

$$\begin{aligned}&\sup_{f\in \mathrm{dom}(H_{\pi/2})}\left(\frac{|f'(0_+)|^2}{||f||^2_{L^2([0,\infty);dx)}+||H_{\pi/2} f||^2_{L^2([0,\infty);dx)}}\right)\times\\ &\times\sup_{f\in \mathrm{dom}(H_\alpha)}\left(\frac{|f(0_+)|^2}{||f||^2_{L^2([0,\infty);dx)}+||H_\alpha f||^2_{L^2([0,\infty);dx)}}\right)=\cos^2(\alpha),\quad \alpha\in[0,\pi).\end{aligned} \tag{5.68}$$

Finally, we conclude with two illustrations of a well-known result of Livsic [44] on quasi-hermitian extensions in the special case of densely defined closed prime symmetric operators with deficiency indices $(1,1)$.

Following Livsic [44] one defines a closed operator H to be a *quasi-hermitian* extension of a densely defined closed prime symmetric operator $\dot{H}$ with deficiency indices $(1,1)$ if

$$\dot{H} \subsetneqq H \subsetneqq \dot{H}^* \tag{5.69}$$

and H is not self-adjoint.

A typical example of a quasi-hermitian extension is obtained as follows.

Let $\dot{T}$ denote the following first-order differential operator on the interval $[0,2a]$, $a>0$,

$$\begin{aligned}
&(\dot{T}f)(x) = -if'(x), \quad \xi \in (0,2a), \\
&f \in \operatorname{dom}(\dot{T}) = \{g \in L^2([0,2a]) \,|\, g \in AC([0,2a]);\ g(0_+) = g(2a_-) = 0; \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad g' \in L^2([0,2a])\}.
\end{aligned} \tag{5.70}$$

Then for $\rho \in \mathbb{C} \cup \{\infty\}$, $|\rho| \neq 1$ the operator T_ρ

$$\begin{aligned}
&(T_\rho f)(x) = -if'(x), \quad \xi \in (0,2a), \\
&f \in \operatorname{dom}(T_\rho) = \{g \in L^2([0,2a]) \,|\, g \in AC([0,2a]);\ g(0_+) = \rho g(2a_-); \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad g' \in L^2([0,2a])\}
\end{aligned} \tag{5.71}$$

is a quasi-hermitian extension of $\dot{T}$. (Here $\rho=\infty$ in (5.71), in obvious notation, denotes the boundary condition $g(2a_-)=0$.) Among all quasi-hermitian extensions of $\dot{T}$ there are two exceptional ones that have empty spectrum. In fact, the operator T_0 corresponding to the value $\rho=0$ in (5.71) as well as its adjoint, $T_0^* = T_\infty$, have empty spectra, that is,

$$\operatorname{spec}(T_0) = \operatorname{spec}(T_\infty) = \emptyset. \tag{5.72}$$

The following theorem proven by Livsic in 1946 provides an interesting characterization of this example.

Theorem 5.10. (Livsic [44].) *For a densely defined closed prime symmetric operator with deficiency indices $(1,1)$ to be unitarily equivalent to the differentiation operator $\dot{T}$ in $L^2([0,2a])$ for some $a>0$ it is necessary and sufficient that it admits a quasi-hermitian extension with empty spectrum.*

Using Livsic's result we are able to characterize the model representation for the pair $(\dot{H}, H)$, where $\dot{H}$ is a densely defined prime closed symmetric operator with deficiency indices $(1,1)$ which admits a quasi-hermitian extension with empty spectrum, and H a self-adjoint extension of $\dot{H}$.

Theorem 5.11. *Let ω be a Borel measure on $\mathbb{R}$ such that*

$$\int_{\mathbb{R}} \frac{d\omega(\lambda)}{1+\lambda^2} = 1, \quad \int_{\mathbb{R}} d\omega(\lambda) = \infty, \tag{5.73}$$

H the self-adjoint operator of multiplication by λ in $L^2(\mathbb{R}; d\omega)$,

$$(Hf)(\lambda) = \lambda f(\lambda), \quad f \in \operatorname{dom}(H) = L^2(\mathbb{R}; (1+\lambda^2)d\omega). \tag{5.74}$$

Define $\dot H$ to be the densely defined closed prime symmetric restriction of H,

$$\dot H = H\big|_{\mathrm{dom}(\dot H)}, \quad \mathrm{dom}(\dot H) = \{f \in \mathrm{dom}(H) \,|\, \int_{\mathbb{R}} d\omega(\lambda) f(\lambda) = 0\}, \tag{5.75}$$

with deficiency indices $(1,1)$. Then $\dot H$ admits a quasi-hermitian extension with empty spectrum if and only if for some $a > 0$ and some $\alpha \in [0,\pi)$ the following representation holds

$$\int_{\mathbb{R}} d\omega(\lambda)((z-\lambda)^{-1} - \lambda(1+\lambda^2)^{-1}) = \frac{\sin(\alpha) - \cos(\alpha)(\cot(az)/\coth(a))}{\cos(\alpha) + \sin(\alpha)(\cot(az)/\coth(a))}, \tag{5.76}$$
$$z \in \mathbb{C}\backslash\mathbb{R}.$$

In this case the measure ω is a pure point measure,

$$\omega = \frac{\coth(a)(1+\cot^2(\alpha))}{a(1+\cot^2(\alpha)\coth^2(a))} \sum_{n\in\mathbb{Z}} \mu_{\{(\beta+\pi n)/a\}}, \tag{5.77}$$

where $\mu_{\{x\}}$ denotes the Dirac measure supported at $\xi \in \mathbb{R}$ with mass one and $\beta = \beta(\alpha, a) \in [0,\pi)$ is the solution of the equation

$$\cot(\beta) + \cot(\alpha)\coth(a) = 1 \text{ if } \alpha \in (0,\pi) \text{ and } \beta = 0 \text{ if } \alpha = 0. \tag{5.78}$$

Moreover, the self-adjoint operator H given by (5.74) is unitarily equivalent to the differentiation operator T_ρ in (5.71) with

$$\rho = e^{2i\beta}. \tag{5.79}$$

Proof. That $\dot H$ is a densely defined closed prime symmetric operator with deficiency indices $(1,1)$ is proven in [25]. By Livsic's theorem, Theorem 5.10, the pair $(\dot H, H)$ is unitarily equivalent to the pair $(\dot T, T_\rho)$, where $\dot T$ is the operator (5.70) in $L^2([0,2a])$ for some $a > 0$ and T_ρ is some self-adjoint extension of $\dot T$ given by (5.71) for some ρ, $|\rho| = 1$. By (4.8) and (4.17) (cf. also (5.28)) we conclude

$$m^D_{T_\rho}(z) = \int_{\mathbb{R}} d\omega(\lambda)((z-\lambda)^{-1} - \lambda(1+\lambda^2)^{-1}) \tag{5.80}$$
$$= z + (1+z^2)(u_+, (T_\rho - z)^{-1}u_+)_{L^2(\mathbb{R};d\omega)}, \tag{5.81}$$
$$u_+ \in \ker(\dot T^* - i),\ \|u_+\|_{L^2(\mathbb{R};d\omega)} = 1,$$

where $m^D_{T_\rho}(z)$ denotes the Donoghue Weyl m-function of the operator T_ρ.
Let $\widetilde T$ be the self-adjoint extension of $\dot T$ corresponding to periodic boundary conditions,

$$\mathrm{dom}(\widetilde T) = \{g \in L^2([0,2a]) \,|\, g \in AC([0,2a]);\ g(0_+) = g(2a_-);\ g' \in L^2([0,2a])\}. \tag{5.82}$$

By Lemma 5.3 there exists an $\alpha \in [0,\pi)$ such that

$$m^D_{T_\rho}(z) = \frac{\sin(\alpha) + \cos(\alpha) m^D_{\widetilde T}(z)}{\cos(\alpha) - \sin(\alpha) m^D_{\widetilde T}(z)}, \tag{5.83}$$

where $m^D_{\widetilde T}(z)$ is the Donoghue Weyl m-function of the extension $\widetilde T$

$$m^D_{\widetilde T}(z) = z + (1+z^2)(u_+, (\widetilde T - z)^{-1}u_+)_{L^2([0,2a];dx)}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{5.84}$$

The assertion (5.76) then follows from the fact

$$m^D_{\widetilde{T}}(z) = -\frac{\cot(az)}{\coth(a)}. \tag{5.85}$$

Next we prove (5.85). First, we note that the resolvent of the operator $\widetilde{T}$ can be explicitly computed as

$$((\widetilde{T}-z)^{-1}f)(x) = ie^{izx}\bigg(\int_0^x e^{-izt}f(t)dt + \frac{e^{2iza}}{1-e^{2iza}}\int_0^{2a} e^{-izt}f(t)dt\bigg), \quad z\in\mathbb{C}\backslash\mathbb{R}. \tag{5.86}$$

Next we calculate the quadratic form of the resolvent of $\widetilde{T}$ on the element $u_+(x) = 2^{1/2}(1-e^{-4a})^{-1/2}\exp(-x)$ generating $\ker(\dot{T}^*-i)$. By (5.86) we have

$$((\widetilde{T}-z)^{-1}u_+)(x) = \frac{2^{1/2}(1-e^{-4a})^{-1/2}}{i-z}\bigg(e^{-x} - e^{izx}\frac{1-e^{-2a}}{1-e^{2iza}}\bigg) \tag{5.87}$$

and therefore,

$$(u_+,(\widetilde{T}-z)^{-1}u_+)_{L^2([0,2a];dx)} = \frac{1}{i-z}\bigg(1+\frac{2(1-e^{-2a})(1-e^{2iaz-2a})}{(iz-1)(1-e^{-4a})(1-e^{2iaz})}\bigg). \tag{5.88}$$

Equations (5.84) and (5.88) then prove (5.85).
In order to prove (5.77) we note that the right-hand side of (5.76) is a periodic Herglotz function with period π/a. Such Herglotz functions have simple poles at the points $\{(\beta+\pi n)/a\}_{n\in\mathbb{Z}}$ with residues

$$\begin{aligned}&\operatorname*{Res}_{z=(\beta+\pi n)/a}\bigg(\frac{\sin(\alpha)-\cos(\alpha)(\cot(az)/\coth(a))}{\cos(\alpha)+\sin(\alpha)(\cot(az)/\coth(a))}\bigg)\\ &= -\frac{\coth(a)(1+\cot^2(\alpha))}{a(1+\cot^2(\alpha)\coth^2(a))}, \quad n\in\mathbb{Z},\end{aligned} \tag{5.89}$$

proving (5.77).
The last assertion of the theorem follows from the fact that the support of the measure ω coincides with the spectrum of H and therefore with the one of the operator T_ρ which is unitarily equivalent to H. The spectrum of the self-adjoint operator T_ρ can explicitly be computed as

$$\operatorname{spec}(T_\rho) = \{\frac{1}{2a}\arg\rho + \frac{\pi}{a}n\}_{n\in\mathbb{Z}}. \tag{5.90}$$

Since the sets (5.90) and $\operatorname{supp}(\omega)$ coincide we conclude (5.77). ☐

Remark 5.12. We note that the weak limit as $a\to\infty$ of the measures $\omega=\omega(\alpha,a)$ (with α fixed) given by (5.77) coincides with $\pi^{-1}d\lambda$, where $d\lambda$ denotes the Lebesgue measure on $\mathbb{R}$.

The next result shows that this limiting case $d\omega=\pi^{-1}d\lambda$ is also rather exotic.

Theorem 5.13. *Let ω be a Borel measure on $\mathbb{R}$ such that*

$$\int_{\mathbb{R}}\frac{d\omega(\lambda)}{1+\lambda^2} = 1, \quad \int_{\mathbb{R}} d\omega(\lambda) = \infty, \tag{5.91}$$

H the self-adjoint operator of multiplication by λ in $L^2(\mathbb{R};d\omega)$,

$$(Hf)(\lambda) = \lambda f(\lambda), \quad f\in\operatorname{dom}(H) = L^2(\mathbb{R};(1+\lambda^2)d\omega). \tag{5.92}$$

Define $\dot{H}$ to be the densely defined closed prime symmetric restriction of H,

$$\dot{H} = H\big|_{\mathrm{dom}(\dot{H})}, \quad \mathrm{dom}(\dot{H}) = \{f \in \mathrm{dom}(H) \,|\, \int_{\mathbb{R}} f(\lambda) d\omega(\lambda) = 0\}, \tag{5.93}$$

with deficiency indices $(1,1)$. Then $\dot{H}$ admits a quasi-hermitian extension with pure point spectrum the open upper (lower) half-plane and spectrum the closed upper (lower) half-plane if and only if the following representation holds,

$$\int_{\mathbb{R}} d\omega(\lambda)((z-\lambda)^{-1} - \lambda(1+\lambda^2)^{-1}) = \begin{cases} i, & \mathrm{Im}(z) > 0, \\ -i, & \mathrm{Im}(z) < 0. \end{cases} \tag{5.94}$$

In this case

$$d\omega = \pi^{-1} d\lambda. \tag{5.95}$$

Proof. The setup in (5.91)–(5.93) is identical to that in Theorem 5.11 and hence needs no further comments. The fact that $\dot{H}$ is unitarily equivalent to the differentiation operator $\dot{T}$ acting in $L^2(\mathbb{R}; dx)$,

$$\begin{aligned} &(\dot{T}f)(x) = -if'(x), \quad \xi \in \mathbb{R}, \\ &f \in \mathrm{dom}(\dot{T}) = \{g \in L^2(\mathbb{R}; dx) \,|\, g \in AC(\mathbb{R});\ g(0) = 0;\ g' \in L^2(\mathbb{R}; dx)\} \end{aligned} \tag{5.96}$$

goes back to Livsic (see, e.g., Appendix I.5 in [3]). In fact, the quasi-hermitian extension T of $\dot{T}$ defined by

$$\begin{aligned} &(Tf)(x) = -if'(x), \quad \xi \in \mathbb{R}\backslash\{0\}, \\ &f \in \mathrm{dom}(T) = \{g \in L^2(\mathbb{R}; dx) \,|\, g \in AC([-R,0]) \cup AC([0,R]) \text{ for all } R > 0; \\ &\qquad\qquad g(0_-) = 0;\ g' \in L^2(\mathbb{R}; dx)\}. \end{aligned} \tag{5.97}$$

(and its adjoint T^* with corresponding boundary condition $g(0_+) = 0$) has spectrum the closed upper (lower) half-plane with pure point spectrum the open upper (lower) half-plane, respectively. This is easily verified from an alternative expression for T given by

$$T = \dot{T}_- \oplus T_+ \text{ in } L^2(\mathbb{R}; dx) = L^2((-\infty,0]; dx) \oplus L^2([0,\infty); dx), \tag{5.98}$$

where

$$\begin{aligned} &(\dot{T}_- f)(x) = -if'(x), \quad x < 0, \\ &f \in \mathrm{dom}(\dot{T}_-) = \{g \in L^2((-\infty,0]; dx) \,|\, g \in AC([-R,0]) \text{ for all } R > 0; \\ &\qquad\qquad g(0_-) = 0;\ g' \in L^2((-\infty,0]; dx)\}, \end{aligned} \tag{5.99}$$

$$\begin{aligned} &(T_+ f)(x) = -if'(x), \quad x > 0, \\ &f \in \mathrm{dom}(T_+) = \{g \in L^2([0,\infty); dx) \,|\, g \in AC([0,R]) \text{ for all } R > 0; \\ &\qquad\qquad g' \in L^2([0,\infty); dx)\}. \end{aligned} \tag{5.100}$$

The explicit expressions for the resolvents of $\dot{T}_-$ and T_+ (see, e.g., [38], Example III.6.9) then show that both operators have spectrum the closed upper half-plane, that is,

$$\mathrm{spec}(\dot{T}_-) = \mathrm{spec}(T_+) = \overline{\mathbb{C}_+}. \tag{5.101}$$

Together with the aforementioned result of Livsic, this shows that the pair $(\dot{H}, H)$ is unitarily equivalent to the pair $(\dot{T}, T_\rho)$, where T_ρ, $|\rho| = 1$ is some self-adjoint extension of $\dot{T}$ in $L^2(\mathbb{R}; dx)$,

$$\begin{aligned} &(T_\rho f)(x) = -if'(x), \quad \xi \in \mathbb{R}\backslash\{0\}, \; |\rho| = 1, \\ &f \in \mathrm{dom}(T_\rho) = \{g \in L^2(\mathbb{R}; dx) \,|\, g \in AC([-R, 0]) \cup AC([0, R]) \text{ for all } R > 0; \\ &\qquad\qquad g(0_-) = \rho g(0_+); \; g' \in L^2(\mathbb{R}; dx)\}. \end{aligned} \tag{5.102}$$

Since the pair $(\dot{T}, T_1)$ is unitarily equivalent to the model pair $(\dot{H}, H)$ in (5.92) and (5.93) (it suffices applying the Fourier transform), where $d\omega = \pi^{-1} d\lambda$, we can immediately compute the Donoghue Weyl m-function $m^D_{T_1}(z)$ of the self-adjoint extension T_1,

$$m^D_{T_1}(z) = \frac{1}{\pi} \int_{\mathbb{R}} d\,\lambda((z-\lambda)^{-1} - \lambda(1+\lambda^2)^{-1}) = \begin{cases} i, & \mathrm{Im}(z) > 0, \\ -i, & \mathrm{Im}(z) < 0. \end{cases} \tag{5.103}$$

Since

$$\pm i = \frac{\sin(\alpha) + \cos(\alpha)(\pm i)}{\cos(\alpha) - \sin(\alpha)(\pm i)} \text{ for all } \alpha \in [0, \pi), \tag{5.104}$$

Lemma 5.3 implies that the Donoghue Weyl m-function $m^D_{T_\rho}(z)$ of the extension T_ρ is independent of ρ, $|\rho| = 1$ and hence $m^D_{T_1}(z) = m^D_\rho(z)$. Therefore, the model representation for the pair $(\dot{T}, T_\rho)$ is given by (5.91)–(5.93) with $d\omega = \pi^{-1} d\lambda$, proving (5.95). Finally, (5.94) follows from (5.103). ☐

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