ON MATRIX-VALUED HERGLOTZ FUNCTIONS

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Abstract. We provide a comprehensive analysis of matrix-valued Herglotz functions and illustrate their applications in the spectral theory of self-adjoint Hamiltonian systems including matrix-valued Schrödinger and Dirac-type operators. Special emphasis is devoted to appropriate matrix-valued extensions of the well-known Aronszajn-Donoghue theory concerning support properties of measures in their Nevanlinna-Riesz-Herglotz representation. In particular, we study a class of linear fractional transformations $M_A(z)$ of a given $n \times n$ Herglotz matrix $M(z)$ and prove that the minimal support of the absolutely continuos part of the measure associated to $M_A(z)$ is invariant under these linear fractional transformations.

Additional applications discussed in detail include self-adjoint finite-rank perturbations of self-adjoint operators, self-adjoint extensions of densely defined symmetric linear operators (especially, Friedrichs and Krein extensions), model operators for these two cases, and associated realization theorems for certain classes of Herglotz matrices.

1. Introduction

The spectral analysis of self-adjoint ordinary differential operators, or more generally, that of self-adjoint Hamiltonian systems (including matrix-valued Schrödinger and Dirac-type operators), is well-known to be intimately connected with the Nevanlinna-Riesz-Herglotz representation of matrix-valued Herglotz functions. The latter terminology is not uniformly adopted in the literature and postponing its somewhat controversial origin to the beginning of Section 2, we recall that $M(z)$ is said to be a matrix-valued Herglotz function if $M : \mathbb{C}_+ \to M_n(\mathbb{C})$ is analytic and $\mathrm{Im}(M(z)) \geq 0$ for $z \in \mathbb{C}_+$. (Here $\mathbb{C}_+$ denotes the open complex upper half-plane, $M_n(\mathbb{C})$, $n \in \mathbb{N}$ the set of $n \times n$ matrices with entries in $\mathbb{C}$, and $\mathrm{Re}(M) = (M + M^*)/2$, $\mathrm{Im}(M(z)) = (M - M^*)/(2i)$ the real and imaginary parts of the matrix M). The Nevanlinna-Riesz-Herglotz representation of $M(z)$ is of the type

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

where

$$C = \mathrm{Re}(M(i)), \quad D = \lim_{\eta\uparrow\infty} (\frac{1}{i\eta} M(i\eta)) \geq 0, \tag{1.2}$$

and $d\Omega(\lambda)$ denotes an $n \times n$ matrix-valued measure satisfying

$$\int_{\mathbb{R}} (\underline{c}, d\Omega(\lambda)\underline{c})_{\mathbb{C}^n}\, (1+\lambda^2)^{-1} < \infty \text{ for all } \underline{c} \in \mathbb{C}^n \tag{1.3}$$

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(with $(\cdot,\cdot)_{\mathbb{C}^n}$ the scalar product in $\mathbb{C}^n$). The Stieltjes inversion formula for Ω then reads

$$\frac{1}{2}\Omega(\{\lambda_1\}) + \frac{1}{2}\Omega(\{\lambda_2\}) + \Omega((\lambda_1,\lambda_2)) = \pi^{-1}\lim_{\varepsilon\downarrow 0}\int_{\lambda_1}^{\lambda_2} d\lambda\,\mathrm{Im}(M(\lambda+i\varepsilon)) \tag{1.4}$$

and its absolutely continuous part Ω_{ac} (w.r.t. Lebesgue measure) is given by

$$d\Omega_{ac}(\lambda) = \pi^{-1}\mathrm{Im}(M(\lambda+i\varepsilon))d\lambda \tag{1.5}$$

(cf. Section 5 for a detailed exposition of these facts). Spectral analysis of ordinary differential operators (with matrix-valued coefficients) then boils down to an analysis of (matrix-valued) measures $d\Omega(\lambda)$ in the representation (1.1) for $M(z)$. These Herglotz matrices are traditionally called Weyl-Titchmarsh M-functions in honor of Weyl, who introduced the concept in the special (scalar) Sturm-Liouville case, and Titchmarsh, who recognized and first employed its function-theoretic content. Since different self-adjoint boundary conditions associated to a given formally symmetric (matrix-valued) differential expression τ yield self-adjoint realizations of τ whose corresponding M-functions are related via certain linear fractional transformations (cf. [102]), we study in depth transformations of the type

$$M(z) \longrightarrow M_A(z) = (A_{2,1} + A_{2,2}M(z))(A_{1,1} + A_{1,2}M(z))^{-1}, \tag{1.6}$$

where

$$\begin{aligned} &A = \big(A_{p,q}\big)_{1\le p,q\le 2} \in \mathcal{A}_{2n}, \\ &\mathcal{A}_{2n} = \{A \in M_{2n}(\mathbb{C}) \mid A^* J_{2n} A = J_{2n}\}, \quad J_{2n} = \begin{pmatrix} 0 & -I_n \\ I_n & 0 \end{pmatrix} \end{aligned} \tag{1.7}$$

(I_n the identity matrix in $\mathbb{C}^n$). $M_A(z)$, $A \in \mathcal{A}_{2n}$ are Herglotz matrices whenever $M(z)$ is a Herglotz matrix. Moreover, denoting the measure in the Nevanlinna-Riesz-Herglotz representation (1.1) for $M_A(z)$ by $d\Omega_A(\lambda)$, we provide a matrix-valued extension of the well-known Aronszajn-Donoghue theory relating support properties of $d\Omega_A(\lambda)$ and $d\Omega(\lambda)$, originally inspired by Sturm-Liouville boundary value problems. As one of our principal new results we prove that the minimal support of the absolutely continuous part $d\Omega_{A,ac}(\lambda)$ of $d\Omega_A(\lambda)$ is independent of $A \in \mathcal{A}_{2n}$, which represents the proper generalization of Aronszajn's celebrated result [10] for Sturm-Liouville operators.

Concrete applications of our formalism include self-adjoint finite-rank perturbations of self-adjoint operators and self-adjoint extensions of densely defined symmetric closed linear operators H with finite deficiency indices especially emphasizing Friedrichs and Krein extensions in the special case where H is bounded from below. Moreover, we describe in detail associated model operators and realization theorems for certain classes of Herglotz matrices. These results appear to be of independent interest in operator theory.

Finally we briefly describe the content of each section. In Section 2 we review basic facts on scalar Herglotz functions and their representation theorems. Section 3 reviews the Aronszajn-Donoghue theory concerning support properties of $d\Omega_A(\lambda)$ in the scalar case and Section 4 describes a variety of applications of the scalar formalism. Some of these applications to self-adjoint extensions of symmetric operators with deficiency indices $(1,1)$ (such as Theorem 4.4 (iv) and Theorems 4.6 and 4.7) appear to be new. Section 5 provides the necessary background material for matrix-valued Herglotz functions and their representation theorems. Section 6, the principal section of this paper, is devoted to a detailed study of support properties of $d\Omega_A(\lambda)$ and Theorem 6.6 contains the invariance result of the minimal support of $d\Omega_{A,ac}(\lambda)$ with respect to $A \in \mathcal{A}_{2n}$. In our final Section 7 we again treat applications to self-adjoint finite-rank perturbations and self-adjoint extensions of symmetric operators with finite deficiency indices. We pay particular attention to Friedrichs and Krein extensions of symmetric operators bounded from below and prove a variety of realization theorems for certain classes of Herglotz matrices. To the best of our knowledge, most of the applications discussed in Section 7 are new. For the convenience of the reader we collect some examples of scalar Herglotz functions in Appendix A. Appendix B contains a detailed discussion of Krein's formula, relating self-adjoint extensions of a symmetric operator, and its application to linear fractional transformations of associated Weyl-Titchmarsh matrices.

It was our aim to provide a rather comprehensive account on matrix-valued Herglotz functions. We hope the enormous number of applications of this formalism to the theory of self-adjoint extensions of symmetric operators, the spectral theory of ordinary (matrix-valued) differential and difference operators, interpolation problems, and factorizations of matrix and operator functions [5], [14]–[16], [20], [24], [25], [27], [30], [35]– [38], [40], [47], [49]–[51], [65], [66], [69]–[80], [85], [89], [90], [96]–[99], [106]–[110], [116], [120], [122], [145], [146], inverse spectral theory [2], [6]–[8], [52], [55], [56], [59], [83], [107]–[110], [115], [117], [129]–[133], [138], [139], [144], [147]–[150], and completely integrable hierarchies of matrix-valued nonlinear evolution equations [13], [29], [39], [44], [45], [53], [82], [111], [114], [118], justifies this effort.

2. Basic Facts on Scalar Herglotz Functions

This section provides a quick review of scalar Herglotz functions and their representation theorems. These results are well-known, in fact, classical by now, and we include them for later reference to achieve a certain degree of completeness, and partly to fix our notation.

Definition 2.1. Let $\mathbb{C}_\pm = \{z \in \mathbb{C} \mid \mathrm{Im}(z) \gtrless 0\}$. $m : \mathbb{C}_+ \to \mathbb{C}$ is called a Herglotz function if m is analytic on $\mathbb{C}_+$ and $m(\mathbb{C}_+) \subseteq \mathbb{C}_+$.

It is customary to extend m to $\mathbb{C}_-$ by reflection, that is, one defines

$$m(z) = \overline{m(\overline{z})}, \quad z \in \mathbb{C}_- . \tag{2.1}$$

We will adopt this convention in this paper. While (2.1) defines an analytic function on $\mathbb{C}_-$, $m\big|_{\mathbb{C}_-}$ in (2.1), in general, does not represent the analytic continuation of $m\big|_{\mathbb{C}_+}$ (cf. Lemma 2.5 for more details in this connection).

There appears to be considerable disagreement concerning the proper name of functions satisfying the conditions in Definition 2.1. In addition to the presently used notion of Herglotz functions one can also find the names Pick, Nevanlinna, Nevanlinna-Pick, and R-functions (sometimes depending on the geographical origin of authors and occasionally whether the open upper half-plane $\mathbb{C}_+$ or the conformally equivalent open unit disk D is involved). Following a tradition in mathematical physics, we decided to adopt the notion of Herglotz functions in this paper.

If $m(z)$ and $n(z)$ are Herglotz functions, then $m(z) + n(z)$ and $m(n(z))$ are also Herglotz. Elementary examples of Herglotz functions are

$$c + id, \quad c + dz, \quad c \in \mathbb{R}, \quad d > 0, \tag{2.2}$$

$$z^r, \quad 0 < r < 1, \tag{2.3}$$
$$\ln(z), \tag{2.4}$$

choosing the obvious branches in (2.3) and (2.4),

$$\tan(z), \quad -\cot(z), \tag{2.5}$$
$$\frac{a_{2,1} + a_{2,2}z}{a_{1,1} + a_{1,2}z}, \tag{2.6}$$
$$a = \begin{pmatrix} a_{1,1} & a_{1,2} \\ a_{2,1} & a_{2,2} \end{pmatrix} \in M_2(\mathbb{C}), \quad a^* j_2 a = j_2, \quad j_2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \tag{2.7}$$

with $M_n(\mathbb{C})$ the set of $n \times n$ matrices with entries in $\mathbb{C}$, and hence

$$-1/z \tag{2.8}$$

as a special case of (2.6). Equations (2.6) and (2.7) define the group of automorphisms on $\mathbb{C}_+$ (or $\mathbb{C}_-$). Finally, we mention a less elementary example, the digamma function [1], Ch. 6,

$$\psi(z) = \Gamma'(z)/\Gamma(z), \tag{2.9}$$

with $\Gamma(z)$ Euler's gamma function. Further examples are described in detail in Appendix A.

As a consequence,

$$-1/m(z), \quad m(-1/z), \tag{2.10}$$
$$\ln(m(z)), \tag{2.11}$$

and

$$m_a(z) = \frac{a_{2,1} + a_{2,2}m(z)}{a_{1,1} + a_{1,2}m(z)}, \tag{2.12}$$

with $a \in M_2(\mathbb{C})$ satisfying (2.7), are all Herglotz functions whenever $m(z)$ is Herglotz. More generally, and most relevant in the context of spectral theory for linear operators, let H be a self-adjoint operator in a (complex, separable) Hilbert space $\mathcal{H}$ with $(\cdot,\cdot)_{\mathcal{H}}$ the scalar product on $\mathcal{H} \times \mathcal{H}$ linear in the second factor. Let $(H-z)^{-1}$, $z \in \mathbb{C}\backslash\mathbb{R}$ denote the resolvent of H. Then for all $f \in \mathcal{H}$,

$$(f, (H-z)^{-1} f)_{\mathcal{H}} \tag{2.13}$$

is a scalar Herglotz function (it suffices to appeal to the spectral theorem for H and apply the functional calculus to $(H-z)^{-1}$), while $(H-z)^{-1}$ represents a $\mathcal{B}(\mathcal{H})$-valued Herglotz function ($\mathcal{B}(\mathcal{H})$ the set of bounded linear operators mapping $\mathcal{H}$ to itself).

The fundamental result on Herglotz functions and their representations on Borel transforms, in part due to Fatou, Herglotz, Luzin, Nevanlinna, Plessner, Privalov, de la Vallée Poussin, Riesz, and others, then reads as follows.

Theorem 2.2. ([3], Ch. VI, [11], [43], Chs. II, IV, [87], [91], Ch. 6, [125], Chs. II, IV, [128], Ch. 5). *Let $m(z)$ be a Herglotz function. Then*
(i). $m(z)$ has finite normal limits $m(\lambda \pm i0) = \lim_{\varepsilon \downarrow 0} m(\lambda \pm i\varepsilon)$ for a.e. $\lambda \in \mathbb{R}$.
(ii). If $m(z)$ has a zero normal limit on a subset of $\mathbb{R}$ having positive Lebesgue measure, then $m \equiv 0$.

(iii). There exists a Borel measure ω on $\mathbb{R}$ satisfying

$$\int_{\mathbb{R}} d\omega(\lambda)(1+\lambda^2)^{-1} < \infty \tag{2.14}$$

such that the Nevanlinna, respectively, Riesz-Herglotz representation

$$\begin{aligned} m(z) &= c + dz + \int_{\mathbb{R}} d\omega(\lambda)((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}), \quad z \in \mathbb{C}_+, \\ c &= Re(m(i)), \quad d = \lim_{\eta\uparrow\infty} m(i\eta)/(i\eta) \geq 0 \end{aligned} \tag{2.15}$$

holds.
(iv). Let $(\lambda_1, \lambda_2) \subset \mathbb{R}$, then the Stieltjes inversion formula for ω reads

$$\frac{1}{2}\omega(\{\lambda_1\}) + \frac{1}{2}\omega(\{\lambda_2\}) + \omega((\lambda_1, \lambda_2)) = \pi^{-1} \lim_{\varepsilon\downarrow 0} \int_{\lambda_1}^{\lambda_2} d\lambda \, \mathrm{Im}(m(\lambda + i\varepsilon)). \tag{2.16}$$

(v). The absolutely continuous (ac) part ω_{ac} of ω with respect to Lebesgue measure $d\lambda$ on $\mathbb{R}$ is given by

$$d\omega_{ac}(\lambda) = \pi^{-1} \mathrm{Im}(m(\lambda + i0)) d\lambda. \tag{2.17}$$

(vi). Any poles and isolated zeros of m are simple and located on the real axis, the residues at poles being negative.

It is quite illustrative to compare the various measures ω for the examples in (2.2)–(2.6), (2.8), and (2.9) and hence we provide these details and also a few more sophisticated examples in Appendix A.

Further properties of Herglotz functions are collected in the following theorem. We denote by $\omega = \omega_{ac} + \omega_s = \omega_{ac} + \omega_{sc} + \omega_{pp}$ the decomposition of ω into its absolutely continuous (ac), singularly continuous (sc), pure point (pp), and singular (s) parts with respect to Lebesgue measure on $\mathbb{R}$.

Theorem 2.3 ([11], [87], [134], [135]). *Let $m(z)$ be a Herglotz function with representation* (2.15)*. Then*
(i).

$$\begin{aligned} &d = 0 \text{ and } \int_{\mathbb{R}} d\omega(\lambda)(1+|\lambda|^s)^{-1} < \infty \text{ for some } s \in (0,2) \\ &\text{if and only if } \int_1^\infty d\eta \, \eta^{-s} \, \mathrm{Im}(m(i\eta)) < \infty. \end{aligned} \tag{2.18}$$

(ii). Let $(\lambda_1, \lambda_2) \subset \mathbb{R}$, $\eta_1 > 0$. Then there is a constant $C(\lambda_1, \lambda_2, \eta_1) > 0$ such that

$$\eta |m(\lambda + i\eta)| \leq C(\lambda_1, \lambda_2, \eta_1), \quad (\lambda, \eta) \in [\lambda_1, \lambda_2] \times (0, \eta_1). \tag{2.19}$$

(iii).

$$\begin{aligned} \sup_{\eta>0} \eta |m(i\eta)| < \infty \text{ if and only if } m(z) &= \int_{\mathbb{R}} d\omega(\lambda)(\lambda - z)^{-1} \\ \text{and } &\int_{\mathbb{R}} d\omega(\lambda) < \infty. \end{aligned} \tag{2.20}$$

In this case,

$$\int_{\mathbb{R}} d\omega(\lambda) = \sup_{\eta>0} \eta |m(i\eta)| = -i \lim_{\eta\uparrow\infty} \eta m(i\eta). \tag{2.21}$$

(iv). For all $\lambda \in \mathbb{R}$*,*

$$\lim_{\varepsilon \downarrow 0} \varepsilon \mathrm{Re}(m(\lambda + i\varepsilon)) = 0, \tag{2.22}$$

$$\omega(\{\lambda\}) = \lim_{\varepsilon \downarrow 0} \varepsilon \mathrm{Im}(m(\lambda + i\varepsilon)) = -i \lim_{\varepsilon \downarrow 0} \varepsilon m(\lambda + i\varepsilon). \tag{2.23}$$

(v). Let $L > 0$ *and suppose* $0 \leq \mathrm{Im}(m(z)) \leq L$ *for all* $z \in \mathbb{C}_+$*. Then* $d = 0$*,* ω *is purely absolutely continuous,* $\omega = \omega_{ac}$*, and*

$$0 \leq \frac{d\omega(\lambda)}{d\lambda} = \pi^{-1} \lim_{\varepsilon \downarrow 0} \mathrm{Im}(m(\lambda + i\varepsilon)) \leq \pi^{-1} L \text{ for a.e. } \lambda \in \mathbb{R}. \tag{2.24}$$

(vi). Let $p \in (1, \infty)$*,* $[\lambda_3, \lambda_4] \subset (\lambda_1, \lambda_2)$*,* $[\lambda_1, \lambda_2] \subset (\lambda_5, \lambda_6)$*. If*

$$\sup_{0 < \varepsilon < 1} \int_{\lambda_1}^{\lambda_2} d\lambda |\mathrm{Im}(m(\lambda + i\varepsilon))|^p < \infty, \tag{2.25}$$

then $\omega = \omega_{ac}$ *is purely absolutely continuous on* (λ_1, λ_2)*,* $\frac{d\omega_{ac}}{d\lambda} \in L^p((\lambda_1, \lambda_2); d\lambda)$*, and*

$$\lim_{\varepsilon \downarrow 0} \|\pi^{-1} \mathrm{Im}(m(\cdot + i\varepsilon)) - \frac{d\omega_{ac}}{d\lambda}\|_{L^p((\lambda_3, \lambda_4); d\lambda)} = 0. \tag{2.26}$$

Conversely, if ω *is purely absolutely continuous on* (λ_5, λ_6)*, and if* $\frac{d\omega_{ac}}{d\lambda} \in L^p((\lambda_5, \lambda_6); d\lambda)$*, then* (2.25) *holds.*
(vii). Let $(\lambda_1, \lambda_2) \subset \mathbb{R}$*. Then a local version of Wiener's theorem reads for* $p \in (1, \infty)$*,*

$$\begin{aligned} &\lim_{\varepsilon \downarrow 0} \varepsilon^{p-1} \int_{\lambda_1}^{\lambda_2} d\lambda |\mathrm{Im}(m(\lambda + i\varepsilon))|^p \\ &= \frac{\Gamma(\frac{1}{2})\Gamma(p - \frac{1}{2})}{\Gamma(p)} \Big(\frac{1}{2}\omega(\{\lambda_1\})^p + \frac{1}{2}\omega(\{\lambda_2\})^p + \sum_{\lambda \in (\lambda_1, \lambda_2)} \omega(\{\lambda\})^p \Big). \end{aligned} \tag{2.27}$$

Moreover, for $0 < p < 1$*,*

$$\lim_{\varepsilon \downarrow 0} \int_{\lambda_1}^{\lambda_2} d\lambda |\pi^{-1} \mathrm{Im}(m(\lambda + i\varepsilon))|^p = \int_{\lambda_1}^{\lambda_2} d\lambda \left| \frac{d\omega_{ac}(\lambda)}{d\lambda} \right|^p. \tag{2.28}$$

It should be stressed that Theorems 2.2 and 2.3 record only the tip of an iceberg of results in this area. In addition to the references already mentioned, the reader will find a great deal of interesting results, for instance, in [12], [33], [34], [41], [43], [62], [69]–[74], [121], Ch. III, [123], [136].

Together with $m(z)$, $\ln(m(z))$ is a Herglotz function by (2.11). Moreover, since

$$0 \leq \mathrm{Im}(\ln(m(z)) = \arg(m(z)) \leq \pi, \quad z \in \mathbb{C}_+, \tag{2.29}$$

the measure $\widehat{\omega}$ in the representation (2.15) of $\ln(m(z))$, that is, in the exponential representation of $m(z)$, is purely absolutely continuous by Theorem 2.3 (v), $d\widehat{\omega}(\lambda) = \xi(\lambda) d\lambda$ for some $0 \leq \xi \leq 1$. These exponential representations have been studied in detail by Aronszajn and Donoghue [11], [12] and we record a few of their properties below.

Theorem 2.4 ([11], [12])**.** *Suppose* $m(z)$ *is a Herglotz function with representation* (2.15)*. Then*
(i). There exists a $\xi \in L^\infty(\mathbb{R})$*,* $0 \leq \xi \leq 1$ *a.e., such that*

$$\ln(m(z)) = k + \int_{\mathbb{R}} d\lambda \, \xi(\lambda)((\lambda - z)^{-1} - \lambda(1 + \lambda^2)^{-1}), \quad z \in \mathbb{C}_+, \tag{2.30}$$

$$k = \mathrm{Re}(\ln(m(i))),$$

where

$$\xi(\lambda) = \pi^{-1} \lim_{\varepsilon \downarrow 0} \mathrm{Im}(\ln(m(\lambda + i\varepsilon))) \ a.e. \tag{2.31}$$

(ii). Let $\ell_1, \ell_2 \in \mathbb{N}$ and $d = 0$ in (2.15)*. Then*

$$\int_{-\infty}^{0} d\lambda\, \xi(\lambda) |\lambda|^{\ell_1} (1+\lambda^2)^{-1} + \int_0^\infty d\lambda\, \xi(\lambda)|\lambda|^{\ell_2}(1+\lambda^2)^{-1} < \infty \text{ if and only if}$$
$$\int_{-\infty}^{0} d\omega(\lambda)|\lambda|^{\ell_1}(1+\lambda^2)^{-1} + \int_0^\infty d\omega(\lambda)|\lambda|^{\ell_2}(1+\lambda^2)^{-1} < \infty$$
$$\text{and } \lim_{z\to i\infty} m(z) = c - \int_{\mathbb{R}} d\omega(\lambda)\, \lambda(1+\lambda^2)^{-1} > 0. \tag{2.32}$$

(iii).

$$\begin{aligned}&\xi(\lambda) = 0 \text{ for } \lambda < 0 \text{ if and only if}\\ &d = 0, \quad [0,\infty) \text{ is a support for } \omega \text{ (i.e., } \omega((-\infty,0)) = 0),\\ &\int_0^\infty d\omega(1+\lambda)^{-1} < \infty, \text{ and } c \geq \int_0^\infty d\omega(\lambda)\lambda(1+\lambda^2)^{-1}.\end{aligned} \tag{2.33}$$

In this case

$$\lim_{\lambda \downarrow -\infty} m(\lambda) = c - \int_0^\infty d\omega(\lambda')\lambda'(1+{\lambda'}^2)^{-1} \tag{2.34}$$

and

$$c > \int_0^\infty d\omega(\lambda)\lambda(1+\lambda^2)^{-1} \text{ if and only if } \int_0^\infty d\lambda\, \xi(\lambda)(1+\lambda)^{-1} < \infty. \tag{2.35}$$

(iv). Let $(\lambda_1, \lambda_2) \subset \mathbb{R}$ and suppose $0 \leq A \leq \xi(\lambda) \leq B \leq 1$ for a.e. $\lambda \in (\lambda_1, \lambda_2)$ with $(B - A) < 1$. Then ω is purely absolutely continuous in (λ_1, λ_2) and $\frac{d\omega}{d\lambda} \in L^p((\lambda_3, \lambda_4); d\lambda)$ for $[\lambda_3, \lambda_4] \subset (\lambda_1, \lambda_2)$ and all $p < (B-A)^{-1}$.
(v). The measure ω is purely singular, $\omega = \omega_s$, $\omega_{ac} = 0$ if and only if ξ equals the characteristic function of a measurable subset $A \subseteq \mathbb{R}$, that is, $\xi = \chi_A$.

As mentioned after Definition 2.1, the definition of $m|_{\mathbb{C}_-}$ by means of reflection as in (2.2), in general, does not represent the analytic continuation of $m|_{\mathbb{C}_+}$. The following result of Greenstein [67] clarifies those circumstances under which m can be analytically continued from $\mathbb{C}_+$ into a subset of $\mathbb{C}_-$ through an interval $(\lambda_1, \lambda_2) \subseteq \mathbb{R}$.

Lemma 2.5 ([67])**.** *Let m be a Herglotz function with representation* (2.15) *and $(\lambda_1, \lambda_2) \subseteq \mathbb{R}$, $\lambda_1 < \lambda_2$. Then m can be analytically continued from $\mathbb{C}_+$ into a subset of $\mathbb{C}_-$ through the interval (λ_1, λ_2) if and only if the associated measure ω is purely absolutely continuous on (λ_1, λ_2), $\omega|_{(\lambda_1,\lambda_2)} = \omega|_{(\lambda_1,\lambda_2),ac}$, and the density ω' of ω is real-analytic on (λ_1, λ_2). In this case, the analytic continuation of m into some domain $\mathcal{D}_- \subseteq \mathbb{C}_-$ is given by*

$$m(z) = \overline{m(\overline{z})} + 2\pi i \omega'(z), \quad z \in \mathcal{D}_-, \tag{2.36}$$

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, $m(z) = \overline{m(\overline{z})}$ for all $z \in \mathbb{C}_-$ if and only if ω has no support in (λ_1, λ_2).

If m can be analytically continued through (λ_1, λ_2) into some region $\mathcal{D}_- \subseteq \mathbb{C}_-$, then $\widetilde{m}(z) := m(z) - \pi i\omega'(z)$ is real-analytic on (λ_1, λ_2) and hence can be continued through (λ_1, λ_2) by reflection. Similarly, $\omega'(z)$, being real-analytic, can be continued through (λ_1, λ_2) by reflection. Hence (2.36) follows from

$$m(z) - \pi i\omega'(z) = \widetilde{m}(z) = \overline{\widetilde{m}(\overline{z})} = \overline{m(\overline{z})} + \pi i\omega'(z), \quad z \in \mathcal{D}_-. \tag{2.37}$$

Formula (2.36) shows that any possible singularity behavior of $m\big|_{\mathbb{C}_-}$ is determined by that of $\omega'\big|_{\mathbb{C}_-}$. (Note that m, being Herglotz, has no singularities in $\mathbb{C}_+$.) Moreover, analytic continuations through different intervals on $\mathbb{R}$ may lead to different $\omega'(z)$ and hence to branch cuts of $m\big|_{\mathbb{C}_-}$.

The following result of Kotani [92], [94] is fundamental in connection with applications of Herglotz functions to reflectionless Schrödinger and Dirac-type operators on $\mathbb{R}$ (i.e., solitonic, periodic, and certain classes of quasi-periodic and almost-periodic operators [32], [56], [57], [61], [92], [94], [95], [104]).

Lemma 2.6 ([92], [94])**.** *Let m be a Herglotz function and $(\lambda_1, \lambda_2) \subseteq \mathbb{R}$, $\lambda_1 < \lambda_2$. Suppose $\lim_{\varepsilon\to 0} \mathrm{Re}(m(\lambda+i\varepsilon)) = 0$ for a.e. $\lambda \in (\lambda_1, \lambda_2)$. Then m can be analytically continued from $\mathbb{C}_+$ into $\mathbb{C}_-$ through the interval (λ_1, λ_2) and*

$$m(z) = -\overline{m(\overline{z})}. \tag{2.38}$$

In addition, $\mathrm{Im}(m(\lambda + i0)) > 0$, $\mathrm{Re}(m(\lambda + i0)) = 0$ *for all* $\lambda \in (\lambda_1, \lambda_2)$.

3. Support Theorems in the Scalar Case

This section further reviews the case of scalar Herglotz functions and focuses on support theorems for ω, ω_{ac}, ω_s, etc., in (2.15). In addition, we recall the main results of the Aronszajn-Donoghue theory relating $m_a(z)$, $a \in \mathcal{A}_2$ (cf. (1.7)) and $m(z)$ as in (2.12).

Let μ, ν be Borel measures on $\mathbb{R}$. We recall that S_μ is called a support of μ if $\mu(\mathbb{R}\backslash S_\mu) = 0$. The topological support S_μ^{cl} of μ is then the smallest closed support of μ. In addition, a support S_μ of μ is called minimal relative to ν if for any smaller support $T_\mu \subseteq S_\mu$ of μ, $\nu(S_\mu\backslash T_\mu) = 0$ (or equivalently, $\widetilde{T} \subset S_\mu$ with $\mu(\widetilde{T}) = 0$ implies $\nu(\widetilde{T}) = 0$). Minimal supports are unique up to sets of μ and ν measure zero and

$$S \sim T \quad \text{if and only if} \quad \mu(S \vartriangle T) = 0 = \nu(S \vartriangle T) \tag{3.1}$$

defines an equivalence class $\mathcal{E}_\nu(\mu)$ of minimal supports of μ relative to ν (with $S \vartriangle T = (S\backslash T) \cup (T\backslash S)$ the symmetric difference of S and T).

Two measures, μ and ν, are called orthogonal, $\mu\perp\nu$, if some of their supports are disjoint.

If μ_1, μ_2 are absolutely continuous with respect to ν, $\mu_j \ll \nu$, $j = 1, 2$, and μ_1 and μ_2 have a common support minimal relative to ν, then μ_1 and μ_2 are equivalent, $\mu_1 \sim \mu_2$.

¿From now on the reference measure ν will be chosen to be Lebesgue measure on $\mathbb{R}$, "minimal" without further qualifications will always refer to minimal relative to Lebesgue measure on $\mathbb{R}$, and the corresponding equivalence class $\mathcal{E}_\nu(\mu)$ will simply be denoted by $\mathcal{E}(\mu)$.

For pure point measures $\mu = \mu_{pp}$ we agree to consider only the smallest support (i.e., the countable set of points with positive μ_{pp} measure). If the support of a pure point measure $\mu = \mu_{pp}$ contains no finite accumulation points we call it a discrete point measure and denote it by μ_d.

It can be shown that there always exists a minimal support S_μ of μ such that $\overline{S_\mu} = S_\mu^{cl}$ (cf. [64], Lemma 5), but in general, a minimal support and the corresponding topological support S_μ^{cl} may differ by a set of positive Lebesgue measure. Frequently, minimal supports are called essential supports in the literature.

Theorem 3.1 ([10], [61], [63], [64]). *Let m be a Herglotz function with representations* (2.15) *and* (2.30). *Then*
(i).

$$S_{\omega_{ac}} = \{\lambda \in \mathbb{R} \,|\, \lim_{\varepsilon\downarrow 0} \mathrm{Im}(m(\lambda + i\varepsilon)) \text{ exists finitely and } 0 < \mathrm{Im}(m(\lambda + i0)) < \infty\} \tag{3.2}$$

is a minimal support of ω_{ac}.
(ii).

$$S_{\omega_s} = \{\lambda \in \mathbb{R} \,|\, \lim_{\varepsilon\downarrow 0} \mathrm{Im}(m(\lambda + i\varepsilon)) = +\infty\} \tag{3.3}$$

and

$$S_{\omega_{sc}} = \{\lambda \in S_{\omega_s} \,|\, \lim_{\varepsilon\downarrow 0} \varepsilon \mathrm{Im}(m(\lambda + i\varepsilon)) = 0\} \tag{3.4}$$

are minimal supports of ω_s and ω_{sc}, respectively.
(iii).

$$S_{\omega_{pp}} = \{\lambda \in \mathbb{R} \,|\, \lim_{\varepsilon\downarrow 0} \varepsilon \mathrm{Im}(m(\lambda + i\varepsilon)) = -i \lim_{\varepsilon\downarrow 0} \varepsilon m(\lambda + i\varepsilon) > 0\} \tag{3.5}$$

is the smallest support of ω_{pp}.
(iv). $S_{\omega_{ac}}$, $S_{\omega_{sc}}$, and $S_{\omega_{pp}}$ are mutually disjoint minimal supports and

$$\begin{aligned} S_\omega &= \{\lambda \in \mathbb{R} \,|\, \lim_{\varepsilon\downarrow 0} \mathrm{Im}(m(\lambda + i\varepsilon)) \leq +\infty \text{ exists and } 0 < \mathrm{Im}(m(\lambda + i0)) \leq +\infty\} \\ &= S_{\omega_{ac}} \cup S_{\omega_s} \end{aligned} \tag{3.6}$$

is a minimal support for ω.
(v).

$$\widetilde{S}_{\omega_{ac}} = \{\lambda \in \mathbb{R} \,|\, 0 < \xi(\lambda) < 1\} \tag{3.7}$$

is a minimal support for ω_{ac}.

Of course

$$\widehat{S}_{\omega_{ac}} = \{\lambda \in \mathbb{R} \,|\, \lim_{\varepsilon\downarrow 0} m(\lambda + i\varepsilon) \text{ exists finitely and } 0 < \mathrm{Im}(m(\lambda + i0)) < \infty\} \tag{3.8}$$

is also a minimal support of ω_{ac}. Later on we shall use the analog of (3.8) in the matrix-valued context (cf. Section 6).

The equivalence relation (3.1) motivates the introduction of equivalence classes associated with ω and its decompositions ω_{ac}, ω_s, etc. We will, in particular use the following two equivalence classes

$$\mathcal{E}(\omega_{\substack{ac\\s}}) := \text{the equivalence class of minimal supports of } \omega_{\substack{ac\\s}} \tag{3.9}$$

in Theorem 3.2 below.

Next, we turn our attention to $m_a(z)$ in (2.12), with $a \in M_2(\mathbb{C})$ satisfying (2.7). We abbreviate the identity matrix in $M_n(\mathbb{C})$ by I_n, the unit circle in $\mathbb{C}$ by $S^1 = \partial D$, and introduce the set (cf. (2.7)),

$$\mathcal{A}_2 = \{a \in M_2(\mathbb{C}) |\, a^* j_2 a = j_2\}. \tag{3.10}$$

We note that

$$|\det(a)| = 1, \quad a \in \mathcal{A}_2, \tag{3.11}$$

and

$$(a_{1,1}/a_{1,2}), (a_{1,1}/a_{2,1}), (a_{2,2}/a_{1,2}), (a_{2,2}/a_{2,1}) \in \mathbb{R}, \quad a \in \mathcal{A}_2 \tag{3.12}$$

as long as $a_{1,2} \neq 0$, respectively, $a_{2,1} \neq 0$. Moreover, we recall (cf. (2.12)),

$$m_a(z) = \frac{a_{2,1} + a_{2,2} m(z)}{a_{1,1} + a_{1,2} m(z)}, \quad z \in \mathbb{C}_+ \tag{3.13}$$

and its general version

$$m_a(z) = \frac{(ab^{-1})_{2,1} + (ab^{-1})_{2,2} m_b(z)}{(ab^{-1})_{1,1} + (ab^{-1})_{1,2} m_b(z)}, \quad a, b \in \mathcal{A}_2,\ z \in \mathbb{C}_+. \tag{3.14}$$

The corresponding equivalence classes of minimal supports of $\omega_{\underset{s}{ac}}$ and $\omega_{a,\underset{s}{ac}}$ are then denoted by $\mathcal{E}(\omega_{\underset{s}{ac}})$ and $\mathcal{E}(\omega_{a,\underset{s}{ac}})$.

The celebrated Aronszajn-Donoghue theory then revolves around the following result.

Theorem 3.2 ([10], [42], see also [64], [136]). *Let $m(z)$ and $m_a(z)$, $a \in \mathcal{A}_2$ be Herglotz functions related by* (3.13), *with corresponding measures ω and ω_a, respectively. Then*
(i). For all $a \in \mathcal{A}_2$,

$$\mathcal{E}(\omega_{a,ac}) = \mathcal{E}(\omega_{ac}), \tag{3.15}$$

that is, $\mathcal{E}(\omega_{a,ac})$ is independent of $a \in \mathcal{A}_2$ (and hence denoted by $\mathcal{E}_{ac}$ below) and $\omega_{a,ac} \sim \omega_{ac}$ for all $a \in \mathcal{A}_2$.
(ii). Suppose ω_b is a discrete point measure, $\omega_b = \omega_{b,d}$, for some $b \in \mathcal{A}_2$. Then $\omega_a = \omega_{a,d}$ is a discrete point measure for all $a \in \mathcal{A}_2$.
(iii). Define

$$S = \{\lambda \in \mathbb{R} |\, \text{there is no } a \in \mathcal{A}_2 \text{ for which } \operatorname{Im}(m_a(\lambda + i0)) \text{ exists and equals } 0\}. \tag{3.16}$$

Then $S \in \mathcal{E}_{ac}$.
(iv). Suppose $a_{1,2} \neq 0$ (i.e., $a \in \mathcal{A}_2 \backslash \{\gamma I_2\}$, $\gamma \in S^1$). If $\omega_{a,s}(\mathbb{R}) > 0$ or $\omega_s(\mathbb{R}) > 0$, then $\mathcal{E}(\omega_{a,s}) \neq \mathcal{E}(\omega_s)$ and there exist $S_{a,s} \in \mathcal{E}(\omega_{a,s})$, $S_s \in \mathcal{E}(\omega_s)$ such that $S_{a,s} \cap S_s = \emptyset$ (i.e., $\omega_{a,s} \perp \omega_s$). In particular,

$$\widetilde{S}_{\omega_{a,s}} = \{\lambda \in \mathbb{R} |\, \lim_{\varepsilon \downarrow 0} m(\lambda + i\varepsilon) = -a_{1,1}/a_{1,2}\} \tag{3.17}$$

is a minimal support for $\omega_{a,s}$ and the smallest support of $\omega_{a,pp}$ equals

$$S_{\omega_{a,pp}} = \{\lambda \in \mathbb{R} |\, \lim_{\varepsilon \downarrow 0} m(\lambda + i\varepsilon) = -a_{1,1}/a_{1,2}, \int_{\mathbb{R}} d\omega(\lambda')(\lambda' - \lambda)^{-2} < \infty\}. \tag{3.18}$$

Moreover,

$$\omega_a(\{\lambda\}) = |a_{1,2})|^{-2} \left(d + \int_{\mathbb{R}} d\omega(\lambda')(\lambda' - \lambda)^{-2} \right)^{-1}, \quad \lambda \in \mathbb{R}. \tag{3.19}$$

(v). Suppose ω_b is a discrete point measure for some (and hence for all) $b \in \mathcal{A}_2$. Assume that $\operatorname{supp}(\omega) = \{\lambda_{I_2,n}\}_{n\in\mathcal{I}}$ *and* $\operatorname{supp}(\omega_a) = \{\lambda_{a,n}\}_{n\in\mathcal{I}}$ *for some $a \in \mathcal{A}_2$ with $a_{1,2} \neq 0$ are given, where $\mathcal{I}$ is either $\mathbb{N}$, $\mathbb{Z}$, or a finite non-empty index set. Suppose in addition that one of the following conditions hold: (1) $\omega(\mathbb{R})$ is known, or (2) $m(z_0)$ is known for some $z_0 \in \mathbb{C}_+$, or (3)* $\lim_{z\to i\infty}(m(z)-m^0(z)) = 0$, *where $m^0(z)$ is a known Herglotz function. Then the system of measures $\{\omega_b\}_{b\in\mathcal{A}_2}$ and hence the system of Herglotz functions $\{m_b(z)\}_{b\in\mathcal{A}_2}$ is uniquely determined.*

Sketch of Proof. (i), (iii), and (iv) follow from (3.10) and (3.13) which imply

$$\operatorname{Im}(m_a(z)) = \frac{\operatorname{Im}(m(z))}{|a_{1,1} + a_{1,2}m(z)|^2}, \tag{3.20}$$

from Theorem 2.2 (i), (ii), and from Theorem 3.1. Note that $a_{1,1} = a_{1,2} = 0$ cannot occur in (3.20) since this would contradict (3.10). (ii) follows from (3.14) and the fact that $\omega_a = \omega_{a,d}$ if and only if $m_a(z)$ is meromorphic on $\mathbb{C}$. In order to prove (v) we define

$$F(z) = m(z) + \frac{a_{1,1}}{a_{1,2}}, \quad z \in \mathbb{C}_+. \tag{3.21}$$

Then F is a meromorphic Herglotz function with simple zeros at $\{\lambda_{a,n}\}_{n\in\mathcal{I}}$ and simple poles at $\{\lambda_{I_2,n}\}_{n\in\mathcal{I}}$. In particular, its zeros and poles necessarily interlace and the exponential Herglotz representation (2.30) for F then yields

$$F(z) = \exp\big(k + \int_{\mathbb{R}} d\lambda\, \xi(\lambda)((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1})\big), \tag{3.22}$$

with ξ a piecewise constant function. Analyzing (2.31) shows that

$$\xi(\lambda) = \chi_{\{\lambda\in\mathbb{R}\,|\,F(\lambda)<0\}}(\lambda), \tag{3.23}$$

where $\chi_{\mathcal{M}}$ denotes the characteristic function of a set $\mathcal{M} \subseteq \mathbb{R}$ and hence ξ is uniquely determined by $\operatorname{supp}(\omega)$ and $\operatorname{supp}(\omega_a)$. Thus $F(z)$ is uniquely determined except for the constant $k \in \mathbb{R}$ (which cannot be determined from $\operatorname{supp}(\omega)$ and $\operatorname{supp}(\omega_a)$). Either one of the conditions (1)–(3) then will determine k and hence $F(z)$, $z \in \mathbb{C}_+$. Thus $m(z)$, and hence by (3.13) $m_b(z)$ for all $b \in \mathcal{A}_2$, are uniquely determined, which in turn determine ω_b for all $b \in \mathcal{A}_2$. □

For connections between Theorem 3.2 (iv) and Hankel operators see [117], Sect. III.10.

The relationship between $\operatorname{Im}(\ln(m_a(z)))$ (respectively, $\xi_a(\lambda)$) and $\operatorname{Im}(\ln(m(z)))$ (respectively, $\xi(\lambda)$), analogous to (3.13), in general, is quite involved. The special case $a = j_2$, that is,

$$m_{j_2}(z) = -1/m(z), \tag{3.24}$$

however, is particularly simple and leads to

$$\xi_{j_2}(\lambda) = 1 - \xi(\lambda) \text{ for a.e. } \lambda \in \mathbb{R}. \tag{3.25}$$

We also state the following elementary result.

Lemma 3.3. *Suppose $a, b \in \mathcal{A}_2$ and that $m_a(z)$ is a nonconstant Herglotz function. Then $m_a(z) = m_b(z)$ for all $z \in \mathbb{C}_+$ if and only if $a = \gamma b$ for some $\gamma \in S^1$.*

Proof. First we note that (2.6) and (2.7) determine a subgroup of the group of Möbius transformations (characterized by leaving $\mathbb{C}_\pm$ invariant and normalized by $|\det(a)| = 1$). Hence $m_a(z) = m_b(z)$ if and only if $a = \gamma b$ for some $\gamma \in \mathbb{C}\backslash\{0\}$. The normalization $|\det(a)| = |\det(b)| = 1$ then yields $\gamma \in S^1$. □

4. Further Applications of Scalar Herglotz Functions

For additional applications of the Aronszajn-Donoghue theory described in Theorem 3.2 we now consider self-adjoint rank-one perturbations of self-adjoint operators, Friedrichs and Krein extensions of densely defined symmetric operators bounded from below with deficiency indices $(1,1)$, and Sturm-Liouville operators on a half-line.

Some of the following results are well-known (the material mainly being taken from [35], [37], [38], [42], [100], [135], [136], and [137]) and hence this section is partially expository in character. However, we do supply simplified proofs of various results below and prove several realization results for different classes of Herglotz functions which appear to be new. Additional material connecting rank-one perturbations with Hankel operators, respectively, Krein's spectral shift function can be found in [117], Sect. III.10, respectively, [124].

We start with self-adjoint rank-one perturbations of self-adjoint operators (following [42] and [136]). Let $\mathcal{H}$ be a separable complex Hilbert space with scalar product $(\cdot,\cdot)_\mathcal{H}$, H_0 a self-adjoint operator in $\mathcal{H}$ (which may or may not be bounded) with simple spectrum. Suppose $f_1 \in \mathcal{H}$, $\|f_1\|_\mathcal{H} = 1$ is a cyclic vector for H_0 (i.e., $\mathcal{H} = \overline{\text{linspan}\{(H_0 - z)^{-1} f_1 \in \mathcal{H} \,|\, z \in \mathbb{C}\backslash\mathbb{R}\}}$, or equivalently, $\mathcal{H} = \overline{\text{linspan}\{E_0(\lambda) f_1 \in \mathcal{H} \,|\, \lambda \in \mathbb{R}\}}$, $E_0(\cdot)$ the family of orthogonal spectral projections of H_0) and define

$$H_\alpha = H_0 + \alpha P_1, \quad P_1 = (f_1, \cdot)_\mathcal{H} f_1, \quad \alpha \in \mathbb{R}, \tag{4.1}$$

with $\mathcal{D}(H_\alpha) = \mathcal{D}(H_0)$, $\alpha \in \mathbb{R}$ ($\mathcal{D}(\cdot)$ abbreviating the domain of a linear operator). Denote by $E_\alpha(\cdot)$ the family of orthogonal spectral projections of H_α and define

$$d\omega_\alpha(\lambda) = d\|E_\alpha(\lambda) f_1\|^2_\mathcal{H}, \quad \int_\mathbb{R} d\omega_\alpha(\lambda) = \|f_1\|^2_\mathcal{H} = 1. \tag{4.2}$$

By the spectral theorem for self-adjoint operators (cf., e.g., [119], Ch. VI), H_α in $\mathcal{H}$ is unitarily equivalent to $\widehat{H}_\alpha$ in $\widehat{\mathcal{H}}_\alpha = L^2(\mathbb{R}; d\omega_\alpha)$, where

$$(\widehat{H}_\alpha \hat{g})(\lambda) = \lambda \hat{g}(\lambda), \quad \hat{g} \in \mathcal{D}(\widehat{H}_\alpha) = L^2(\mathbb{R}; (1+\lambda^2) d\omega_\alpha), \tag{4.3}$$

$$H_\alpha = U_\alpha \widehat{H}_\alpha U_\alpha^{-1}, \quad \mathcal{H} = U_\alpha L^2(\mathbb{R}; d\omega_\alpha), \tag{4.4}$$

with U_α unitary,

$$U_\alpha : \widehat{\mathcal{H}}_\alpha = L^2(\mathbb{R}; d\omega_\alpha) \to \mathcal{H}, \quad \hat{g} \to (U_\alpha \hat{g}) = \operatorname*{s-lim}_{N\to\infty} \int_{-N}^N d(E_\alpha(\lambda) f_1) \hat{g}(\lambda). \tag{4.5}$$

Moreover,

$$f_1 = U_\alpha \hat{f}_1, \quad \hat{f}_1(\lambda) = 1, \quad \lambda \in \mathbb{R}. \tag{4.6}$$

The family of spectral projections $\widehat{E}_\alpha(\lambda)$, $\lambda \in \mathbb{R}$ of $\widehat{H}_\alpha$ is then given by

$$(\widehat{E}_\alpha(\lambda)\hat{g})(\mu) = \theta(\lambda - \mu)\hat{g}(\mu) \text{ for } \omega_\alpha\text{–a.e. } \mu \in \mathbb{R}, \ \hat{g} \in L^2(\mathbb{R}; d\omega_\alpha), \tag{4.7}$$

$$\theta(x) = \begin{cases} 1, & x \geq 0 \\ 0, & x < 0. \end{cases}$$

Introducing the Herglotz function

$$m_\alpha(z) = (f_1, (H_\alpha - z)^{-1} f_1)_{\mathcal{H}} = \int_{\mathbb{R}} \frac{d\omega_\alpha}{\lambda - z}, \quad z \in \mathbb{C}_+, \tag{4.8}$$

one verifies

$$m_\beta(z) = \frac{m_\alpha(z)}{1 + (\beta - \alpha) m_\alpha(z)}, \quad \alpha, \beta \in \mathbb{R}. \tag{4.9}$$

A comparison of (4.9) and (3.13) suggests an introduction of

$$a(\alpha, \beta) = \begin{pmatrix} 1 & \beta - \alpha \\ 0 & 1 \end{pmatrix} \in \mathcal{A}_2, \quad \alpha, \beta \in \mathbb{R}. \tag{4.10}$$

Moreover, since $\omega_\alpha(\mathbb{R}) = 1$, Theorem 3.2 applies (with $a_{1,1}(\alpha, \beta) = a_{2,2}(\alpha, \beta) = 1$, $a_{1,2}(\alpha, \beta) = \beta - \alpha$, $a_{2,1}(\alpha, \beta) = 0$).

If f_1 is not a cyclic vector for H_0, then as discussed in [42], $\mathcal{H}$ (not necessarily assumed to be separable at this point) decomposes into two orthogonal subspaces $\mathcal{H}^1$ and $\mathcal{H}^{1,\perp}$,

$$\mathcal{H} = \mathcal{H}^1 \oplus \mathcal{H}^{1,\perp}, \tag{4.11}$$

with $\mathcal{H}^1$ separable, each of which is a reducing subspace for all H_α, $\alpha \in \mathbb{R}$. One then has $\mathcal{H}^1 = \overline{\text{linspan}\,\{(H_0 - z)^{-1} f_1 \in \mathcal{H} \,|\, z \in \mathbb{C}\backslash\mathbb{R}\}}$ and

$$H_\alpha = H_\beta \text{ on } \mathcal{D}(H_0) \cap \mathcal{H}^{1,\perp} \text{ for all } \alpha, \beta \in \mathbb{R}. \tag{4.12}$$

In particular,

$$H_0 = H_0^1 \oplus H_0^{1,\perp}, \quad H_\alpha = H_\alpha^1 \oplus H_0^{1,\perp}, \quad \alpha \in \mathbb{R}, \tag{4.13}$$

$$f_1 = f_1^1 \oplus 0, \tag{4.14}$$

where

$$H_0^1 = H\big|_{\mathcal{D}(H_0)\cap\mathcal{H}^1}, \quad H_0^{1,\perp} = H_0\big|_{\mathcal{D}(H_0)\cap\mathcal{H}^{1,\perp}}, \tag{4.15}$$

implying

$$(f_1, (H_\alpha - z)^{-1} f_1)_{\mathcal{H}} = (f_1^1, (H_\alpha^1 - z)^{-1} f_1^1)_{\mathcal{H}^1} = m_\alpha^1(z), \quad \alpha \in \mathbb{R}. \tag{4.16}$$

Thus, α-dependent spectral properties of H_α in $\mathcal{H}$ are effectively reduced to those of H_α^1 in $\mathcal{H}^1$, where H_α^1 are self-adjoint operators with simple spectra and cyclic vector $f_1^1 \in \mathcal{H}^1$.

Introducing the following set of Herglotz functions (we will choose the usual symbol $\mathcal{N}$ for these sets in honor of R. Nevanlinna)

$$\mathcal{N}_1 = \{m : \mathbb{C}_+ \to \mathbb{C}_+ \text{ analytic} \,|\, m(z) = \int_{\mathbb{R}} d\omega(\lambda)(\lambda - z)^{-1}, \ \int_{\mathbb{R}} d\omega(\lambda) < \infty\}, \tag{4.17}$$

we now turn to a realization theorem for Herglotz functions of the type (4.8).

Theorem 4.1.
(i). Any $m \in \mathcal{N}_1$ with associated measure ω can be realized in the form

$$m(z) = (f_1, (H - z)^{-1} f_1)_{\mathcal{H}}, \quad z \in \mathbb{C}_+, \tag{4.18}$$

where H denotes a self-adjoint operator in some separable complex Hilbert space $\mathcal{H}$, $f_1 \in \mathcal{H}$, and

$$\int_{\mathbb{R}} d\omega(\lambda) = \|f_1\|^2_{\mathcal{H}}. \tag{4.19}$$

(ii). Suppose $m_\ell \in \mathcal{N}_1$ with corresponding measures ω_ℓ, $\ell = 1,2$, and $m_1 \neq m_2$. Then m_1 and m_2 can be realized as

$$m_\ell(z) = (f_1, (H_\ell - z)^{-1} f_1)_{\mathcal{H}}, \quad \ell = 1,2,\ z \in \mathbb{C}_+, \tag{4.20}$$

where H_ℓ, $\ell = 1,2$ are self-adjoint rank-one perturbations of one and the same self-adjoint operator H_0 in some complex Hilbert space $\mathcal{H}$ (which may be chosen separable) with $f_1 \in \mathcal{H}$, that is,

$$H_\ell = H_0 + \alpha_\ell P_1, \quad P_1 = (f_1, \cdot)_{\mathcal{H}} f_1 \tag{4.21}$$

for some $\alpha_\ell \in \mathbb{R}$, $\ell = 1,2$, if and only if the following conditions hold:

$$\int_{\mathbb{R}} d\omega_1(\lambda) = \int_{\mathbb{R}} d\omega_2(\lambda) = \|f_1\|^2_{\mathcal{H}}, \tag{4.22}$$

and for all $z \in \mathbb{C}_+$,

$$m_2(z) = \frac{m_1(z)}{1 + \|f_1\|^{-2}_{\mathcal{H}}(\alpha_2 - \alpha_1) m_1(z)}. \tag{4.23}$$

Proof. Define the self-adjoint operator H_0 of multiplication by λ in $\mathcal{H} = L^2(\mathbb{R}; d\omega)$ by

$$(H_0 g)(\lambda) = \lambda g(\lambda), \quad g \in \mathcal{D}(H_0) = L^2(\mathbb{R}; (1+\lambda^2)d\omega), \tag{4.24}$$

where ω denotes the measure in the Herglotz representation of $m(z)$, and consider $f_1 = 1 \in \mathcal{H}$. One infers

$$(f_1, (H_0 - z)^{-1} f_1)_{\mathcal{H}} = \int_{\mathbb{R}} d\omega(\lambda)(\lambda - z)^{-1} = m(z). \tag{4.25}$$

Since $\text{w-lim}_{z\to i\infty}(-z)(H_0 - z)^{-1} = I_{\mathcal{H}}$, the identity in $\mathcal{H}$, and $|iy(\lambda - iy)^{-1}| \leq 1$, Lebesgue's dominated convergence theorem yields (4.19) and hence part (i). The necessity of condition (4.23) in part (ii) was proved by Donoghue [42] (assuming $\|f_1\|_{\mathcal{H}} = 1$). Indeed, applying the last part in the argument proving (i) to $m_1(z)$ and $m_2(z)$ immediately proves (4.22). Identifying $\alpha_1 = \alpha$, $\alpha_2 = \beta$, $H_1 = H_\alpha$, $H_2 = H_\beta$, $\|f_1\|^{-2}_{\mathcal{H}} m_1(z) = m_\alpha(z)$, and $\|f_1\|^{-2}_{\mathcal{H}} m_2(z) = m_\beta(z)$, (4.23) is easily seen to be equivalent to (4.9). Conversely, assume (4.22) and (4.23). By part (i), we may realize $m_1(z)$ as

$$\|f_1\|^{-2}_{\mathcal{H}} m_1(z) = \|f_1\|^{-2}_{\mathcal{H}} (f_1, (H_1 - z)^{-1} f_1)_{\mathcal{H}}. \tag{4.26}$$

By (4.16) we may assume that $\mathcal{H}$ is separable and H_1 has simple spectrum and hence identify it with H_α in (4.1). Define H_β as in (4.1) for $\beta \in \mathbb{R}\backslash\{\alpha\}$ and consider

$$m_\beta(z) = \|f_1\|^{-2}_{\mathcal{H}} (f_1, (H_\beta - z)^{-1} f_1)_{\mathcal{H}}. \tag{4.27}$$

By (4.9) one obtains ($m_\alpha(z) = \|f_1\|^{-2}_{\mathcal{H}} m_1(z)$)

$$m_\beta(z) = \frac{\|f_1\|^{-2}_{\mathcal{H}} m_1(z)}{1 + (\beta - \alpha)\|f_1\|^{-2}_{\mathcal{H}} m_1(z)}. \tag{4.28}$$

A comparison of (4.28) and (4.9) then yields $\|f_1\|^2_{\mathcal{H}} m_\beta(z) = m_2(z)$ for $(\alpha_2 - \alpha_1) = (\beta - \alpha)$, completing the proof. $\square$

Of course we could have normalized f_1, $\|f_1\|_{\mathcal{H}} = 1$, and then added the constraint $\int_{\mathbb{R}} d\omega(\lambda) = 1$ to (4.17). By (4.16), (4.18) can be realized in nonseparable Hilbert spaces.

Next we turn to a characterization of Friedrichs and Krein extensions of densely defined operators bounded from below with deficiency indices $(1,1)$ (following [35], [37], [38], [42], [100], [101], [137], and [142]).

We start by describing a canonical representation of densely defined closed symmetric operators with deficiency indices $(1,1)$ as discussed by [42]. Let $\mathcal{H}$ be a separable complex Hilbert space, H a closed densely defined symmetric operator with domain $\mathcal{D}(H)$ and deficiency indices $(1,1)$. Choose $u_\pm \in \ker(H^* \mp i)$ with $\|u_\pm\|_{\mathcal{H}} = 1$ and denote by H_α, $\alpha \in [0,\pi)$ all self-adjoint extensions of H, that is,

$$\begin{aligned} &H_\alpha(g + u_+ + e^{2i\alpha}u_-) = Hg + iu_+ - ie^{2i\alpha}u_-, \\ &\mathcal{D}(H_\alpha) = \{(g + u_+ + e^{2i\alpha}u_-) \in \mathcal{D}(H^*) \,|\, g \in \mathcal{D}(H),\, u_\pm \in \ker(H^* \mp i)\} \end{aligned} \tag{4.29}$$

by von Neumann's formula for self-adjoint extensions of H. Let $E_\alpha(\cdot)$ be the family of spectral projections of H_α and suppose H_α has simple spectrum for some (and hence for all) $\alpha \in [0,\pi)$ (i.e., u_+ is a cyclic vector for H_α for all $\alpha \in [0,\pi)$). Define

$$d\nu_\alpha(\lambda) = d\|E_\alpha(\lambda)u_+\|^2_{\mathcal{H}}, \quad \int_{\mathbb{R}} d\nu_\alpha(\lambda) = \|u_+\|^2_{\mathcal{H}} = 1, \quad \alpha \in [0,\pi), \tag{4.30}$$

then H_α is unitarily equivalent to multiplication by λ in $L^2(\mathbb{R}; d\nu_\alpha)$ and u_+ can be mapped into the function identically 1. However, it is more convenient to define

$$d\omega_\alpha(\lambda) = (1+\lambda^2)d\nu_\alpha(\lambda), \tag{4.31}$$

such that

$$\int_{\mathbb{R}} \frac{d\omega_\alpha(\lambda)}{1+\lambda^2} = 1, \quad \int_{\mathbb{R}} d\omega_\alpha(\lambda) = \infty, \quad \alpha \in [0,\pi) \tag{4.32}$$

(by (4.30) and the fact that $u_+ \notin \mathcal{D}(H_\alpha)$). Thus, H_α is unitarily equivalent to $\widehat{H}_\alpha$ in $\widehat{\mathcal{H}}_\alpha = L^2(\mathbb{R}; d\omega_\alpha)$, where

$$(\widehat{H}_\alpha \hat{g})(\lambda) = \lambda\hat{g}(\lambda), \quad \hat{g} \in \mathcal{D}(\widehat{H}_\alpha) = L^2(\mathbb{R}; (1+\lambda^2)d\omega_\alpha), \tag{4.33}$$

$$H_\alpha = U_\alpha \widehat{H}_\alpha U_\alpha^{-1}, \quad \mathcal{H} = U_\alpha L^2(\mathbb{R}; d\omega_\alpha), \tag{4.34}$$

with U_α unitary,

$$\begin{aligned} &U_\alpha : \widehat{\mathcal{H}}_\alpha = L^2(\mathbb{R}; d\omega_\alpha) \to \mathcal{H}, \\ &\hat{g} \to U_\alpha \hat{g} = \operatorname*{s-lim}_{N\to\infty} \int_{-N}^{N} d(E_\alpha(\lambda)u_+)(\lambda - i)\hat{g}(\lambda). \end{aligned} \tag{4.35}$$

Moreover,

$$u_+ = U_\alpha \hat{u}_+, \quad \hat{u}_+(\lambda) = (\lambda - i)^{-1}, \tag{4.36}$$

and

$$(\widehat{H}(\alpha)\hat{g})(\lambda) = \lambda\hat{g}(\lambda), \quad \hat{g} \in \mathcal{D}(\widehat{H}(\alpha)) = \{\hat{h} \in \mathcal{D}(\widehat{H}_\alpha) \,|\, \textstyle\int_{\mathbb{R}} d\omega_\alpha(\lambda)\hat{h}(\lambda) = 0\}, \tag{4.37}$$

where

$$H = U_\alpha \widehat{H}(\alpha) U_\alpha^{-1}. \tag{4.38}$$

Thus $\widehat{H}(\alpha)$ in $L^2(\mathbb{R}; d\omega_\alpha)$ is a canonical representation for a densely defined closed symmetric operator H with deficiency indices $(1,1)$ in a separable Hilbert space $\mathcal{H}$ with cyclic deficiency vector $u_+ \in \ker(H^* - i)$. We shall prove in Theorem 4.2 below that $\widehat{H}(\alpha)$ in $L^2(\mathbb{R}; d\omega_\alpha)$ is actually a model for all such operators. Moreover, since

$$((H - \overline{z})g, U_\alpha(\cdot - z)^{-1})_{\mathcal{H}} = \int_{\mathbb{R}} d\omega_\alpha(\lambda)(\lambda - z)\overline{(U_\alpha^{-1} g)(\lambda)}(\lambda - z)^{-1} = 0, \tag{4.39}$$
$$g \in \mathcal{D}(H), \ z \in \mathbb{C}\backslash\mathbb{R}$$

by (4.37), one infers that $U_\alpha(\cdot - z)^{-1} \in \mathcal{D}(H^*)$. Since $\mathcal{D}(H)$ is dense in $\mathcal{H}$, one concludes

$$\ker(\widehat{H}(\alpha)^* - z) = \{c(\cdot - z)^{-1} \,|\, c \in \mathbb{C}\}, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{4.40}$$

where

$$H^* = U_\alpha \widehat{H}(\alpha)^* U_\alpha^{-1}. \tag{4.41}$$

If u_+ is not cyclic for H_α then, as shown in [42], $\mathcal{H}$ (not necessarily assumed to be separable at this point) decomposes into two orthogonal subspaces $\mathcal{H}^0$ and $\mathcal{H}^{0,\perp}$,

$$\mathcal{H} = \mathcal{H}^0 \oplus \mathcal{H}^{0,\perp}, \tag{4.42}$$

with $\mathcal{H}^0$ separable, each of which is a reducing subspace for all H_α, $\alpha \in [0,\pi)$ and

$$\mathcal{H}^0 = \overline{\operatorname{linspan}\{(H_\alpha - z)^{-1}u_+ \in \mathcal{H} \,|\, z \in \mathbb{C}\backslash\mathbb{R}\}} \text{ is independent of } \alpha \in [0,\pi), \tag{4.43}$$

$$(H_\alpha - z)^{-1} = (H_\beta - z)^{-1} \text{ on } \mathcal{H}^{0,\perp} \text{ for all } \alpha,\beta \in [0,\pi), \ z \in \mathbb{C}_+. \tag{4.44}$$

In particular, the part $H^{0,\perp}$ of H in $\mathcal{H}^{0,\perp}$ is then self-adjoint,

$$H = H^0 \oplus H^{0,\perp}, \quad H_\alpha = H_\alpha^0 \oplus H^{0,\perp}, \quad \alpha \in [0,\pi), \tag{4.45}$$

$$\operatorname{ran}(H^{0,\perp} - z) = \mathcal{H}^{0,\perp}, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{4.46}$$

$$u_+ = u_+^0 \oplus 0, \tag{4.47}$$

with H^0 a densely defined closed symmetric operator in $\mathcal{H}^0$ and deficiency indices $(1,1)$. One then computes

$$\begin{aligned} &z\|u_+\|_{\mathcal{H}}^2 + (1+z^2)(u_+, (H_\alpha - z)^{-1}u_+)_{\mathcal{H}} \\ &= z\|u_+^0\|_{\mathcal{H}^0}^2 + (1+z^2)(u_+^0, (H_\alpha^0 - z)^{-1}u_+^0)_{\mathcal{H}^0}, \quad \alpha \in [0,\pi) \end{aligned} \tag{4.48}$$

and hence α-dependent spectral properties of H_α in $\mathcal{H}$ are effectively reduced to those of H_α^0 in $\mathcal{H}^0$, where H_α^0 are self-adjoint operators with simple spectra and cyclic vector $u_+^0 \in \ker((H^0)^* - i)$.

Next we show the model character of $(\widehat{\mathcal{H}}_\alpha, \widehat{H}(\alpha), \widehat{H}_\alpha)$ following the approach outlined by Donoghue [42].

Theorem 4.2 ([42]). *Let H be a densely defined closed symmetric operator with deficiency indices $(1,1)$ and normalized deficiency vectors $u_\pm \in \ker(H^* \mp i)$, $\|u_\pm\|_{\mathcal{H}} = 1$ in some separable complex Hilbert space $\mathcal{H}$. Let H_α be a self-adjoint extension of H with simple spectrum (i.e., u_+ is a cyclic vector for H_α). Then the pair (H, H_α) in $\mathcal{H}$ is unitarily equivalent to the pair $(\widehat{H}(\alpha), \widehat{H}_\alpha)$ in $\widehat{\mathcal{H}}$ defined in* (4.37) *and* (4.33) *with unitary operator* U_α *defined in* (4.35) *(cf.* (4.38) *and* (4.34)*). Conversely, given a measure* $d\widetilde{\omega}$ *satisfying*

$$\int_{\mathbb{R}} \frac{d\widetilde{\omega}(\lambda)}{1+\lambda^2} = 1, \quad \int_{\mathbb{R}} d\widetilde{\omega}(\lambda) = \infty, \tag{4.49}$$

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

$$(\widetilde{H}g)(\lambda) = \lambda g(\lambda), \quad g \in \mathcal{D}(\widetilde{H}) = L^2(\mathbb{R}; (1+\lambda^2)d\widetilde{\omega}), \tag{4.50}$$

and the linear operator H *in* $\widetilde{\mathcal{H}}$*,*

$$\mathcal{D}(H) = \{g \in \mathcal{D}(\widetilde{H}) \mid \int_{\mathbb{R}} d\widetilde{\omega}(\lambda) g(\lambda) = 0\}, \quad H = \widetilde{H}\big|_{\mathcal{D}(H)}. \tag{4.51}$$

Then H *is a densely defined closed symmetric operator in* $\widetilde{\mathcal{H}}$ *with deficiency indices* $(1,1)$ *and deficiency spaces*

$$\ker(H^* \mp i) = \{c(\lambda \mp i)^{-1} \mid c \in \mathbb{C}\}. \tag{4.52}$$

Proof. The first part of the theorem (with the exception of the explicit expression for the unitary operator U_α in (4.35)) is due to Donoghue [42] and we essentially sketched the major steps in (4.30)–(4.48) above. For the sake of completeness we add two more details. First, in connection with proving the unitary equivalence stated in (4.34), one observes that $U_\alpha(\widehat{H}_\alpha - z)^{-1}\hat{u}_+ = (H_\alpha - z)^{-1}u_+$. Using the first resolvent identity for $\widehat{H}_\alpha$ and H_α then yields $U_\alpha(\widehat{H}_\alpha - z)^{-1}((\widehat{H}_\alpha - z')^{-1}\hat{u}_+) = (H_\alpha - z)^{-1}((H_\alpha - z')^{-1}u_+)$. Since $z' \in \mathbb{C}\backslash\mathbb{R}$ is arbitrary, one obtains (4.34) from the fact that u_+ is cyclic for H_α . Secondly, in connection with the domain of $\widehat{H}(\alpha)$ in (4.37) one makes use of the well-known fact that $\hat{h} \in \widehat{\mathcal{H}}_\alpha$ belongs to $\mathcal{D}(\widehat{H}(\alpha))$ if and only if $\hat{h} \in \mathcal{D}(\widehat{H}_\alpha)$ and $\hat{h}$ is orthogonal to $\ker(\widehat{H}^* - i)$ in the topology of the graph of $\widehat{H}^*$, that is,

$$(\widehat{H}^*\hat{h}, \widehat{H}^*u_+)_{\hat{\mathcal{H}}_\alpha} + (\hat{h}, u_+)_{\hat{\mathcal{H}}_\alpha} = 0 \text{ or } i(\widehat{H}_\alpha\hat{h}, u_+)_{\hat{\mathcal{H}}_\alpha} + (\hat{h}, u_+)_{\hat{\mathcal{H}}_\alpha} = 0. \tag{4.53}$$

This is easily seen to be equivalent to $\int_{\mathbb{R}} d\omega_\alpha(\lambda)\hat{h}(\lambda) = 0$ in (4.37).

Since the second part of Theorem 4.2 is stated but not explicitly proved in [42], we now sketch such a proof.

Define $\widetilde{\mathcal{H}}_{2r} = L^2(\mathbb{R}; (1+\lambda^2)^r d\widetilde{\omega})$, $r \in \mathbb{R}$, $\widetilde{\mathcal{H}}_0 = \widetilde{\mathcal{H}}$ and consider the isometric isomorphism (unitary operator) R from $\widetilde{\mathcal{H}}_2$ onto $\widetilde{\mathcal{H}}_{-2}$,

$$R : \widetilde{\mathcal{H}}_2 \to \widetilde{\mathcal{H}}_{-2}, \quad \widetilde{f} \to (1+\lambda^2)\widetilde{f}, \tag{4.54}$$

$$(\widetilde{f}, \widetilde{g})_{\widetilde{\mathcal{H}}_2} = (\widetilde{f}, R\widetilde{g})_{\widetilde{\mathcal{H}}} = (R\widetilde{f}, \widetilde{g})_{\widetilde{\mathcal{H}}} = (R\widetilde{f}, R\widetilde{g})_{\widetilde{\mathcal{H}}_{-2}}, \quad \widetilde{f}, \widetilde{g} \in \widetilde{\mathcal{H}}_2, \tag{4.55}$$

$$(\widetilde{u}, \widetilde{v})_{\widetilde{\mathcal{H}}_{-2}} = (\widetilde{u}, R^{-1}\widetilde{v})_{\widetilde{\mathcal{H}}} = (R^{-1}\widetilde{u}, \widetilde{v})_{\widetilde{\mathcal{H}}} = (R^{-1}\widetilde{u}, R^{-1}\widetilde{v})_{\widetilde{\mathcal{H}}_2}, \quad \widetilde{u}, \widetilde{v} \in \widetilde{\mathcal{H}}_{-2}. \tag{4.56}$$

We note that $\mathbb{C} \subset \widetilde{\mathcal{H}}_{-2}$. Since $\widetilde{g} \in \widetilde{\mathcal{H}}_2$ implies $\widetilde{g} \in L^1(\mathbb{R}; d\widetilde{\omega})$ using $|\widetilde{g}(\lambda)| = (1+\lambda^2)^{-1/2}(1+\lambda^2)^{1/2}|\widetilde{g}(\lambda)|$ and Cauchy's inequality, $\mathcal{D}(H)$ is well-defined. Moreover, as a restriction of the self-adjoint operator $\widetilde{H}$, H is clearly symmetric. One infers from (4.54) and (4.51) that

$$\mathcal{D}(\widetilde{H}) = \widetilde{\mathcal{H}}_2 = \mathcal{D}(H) \oplus_{\widetilde{\mathcal{H}}_2} R^{-1}\mathbb{C}, \tag{4.57}$$

where, in obvious notation, $\oplus_{\widetilde{\mathcal{H}}_2}$ denotes the direct orthogonal sum in $\widetilde{\mathcal{H}}_2$. Next, to prove that $\mathcal{D}(H)$ is dense in $\widetilde{\mathcal{H}}$, suppose there exists a $\widetilde{g} \in \widetilde{\mathcal{H}}$ such that $\widetilde{g} \perp \mathcal{D}(H)$.

Then

$$0 = (\widetilde{f}, \widetilde{g})_{\widetilde{\mathcal{H}}} = (\widetilde{f}, R^{-1}\widetilde{g})_{\widetilde{\mathcal{H}}_2} \text{ for all } \widetilde{f} \in \mathcal{D}(H) \tag{4.58}$$

and hence $R^{-1}\widetilde{g} \in R^{-1}\mathbb{C}$, that is, $\widetilde{g} = c \in \mathbb{C}$ a.e. by (4.57), and consequently, $\widetilde{g} \in \widetilde{\mathcal{H}}$ if and only if $c = \widetilde{g} = 0$. Next, H is a closed operator, either by (4.57) or directly by its definition (4.51) ($\lim_{n\to\infty} \|\widetilde{f}_n - \widetilde{g}\|_{\widetilde{\mathcal{H}}} = 0$, $\lim_{n\to\infty} \|H\widetilde{f}_n - \widetilde{g}\|_{\widetilde{\mathcal{H}}} = 0$ for $\{\widetilde{f}_n\}_{n\in\mathbb{N}} \subset \mathcal{D}(H)$, $\widetilde{f}, \widetilde{g} \in \widetilde{\mathcal{H}}$ imply $\widetilde{f} \in \widetilde{\mathcal{H}}_2$ and $\widetilde{g} = \widetilde{H}\widetilde{f}$ by passing to appropriate subsequences of $\{\widetilde{f}_n\}_{n\in\mathbb{N}}$ and $\{H\widetilde{f}_n\}_{n\in\mathbb{N}}$, and $\int_{\mathbb{R}} d\widetilde{\omega}(\lambda)\widetilde{f}(\lambda) = (R^{-1}1, \widetilde{f})_{\widetilde{\mathcal{H}}_2} = \lim_{n\to\infty}(R^{-1}1, \widetilde{f}_n)_{\widetilde{\mathcal{H}}_2} = 0$ then yields $\widetilde{f} \in \mathcal{D}(H)$). Since $\widetilde{H}$ is self-adjoint, $\operatorname{ran}(\widetilde{H} - z) = \widetilde{\mathcal{H}}$ for all $z \in \mathbb{C}\backslash\mathbb{R}$, and $(\widetilde{H} \pm i) : \widetilde{\mathcal{H}}_2 \to \widetilde{\mathcal{H}}$ is unitary,

$$((\widetilde{H} \pm i)\widetilde{f}, (\widetilde{H} \pm i)\widetilde{g}))_{\widetilde{\mathcal{H}}} = \int_{\mathbb{R}} (1 + \lambda^2) d\omega(\lambda)\overline{\widetilde{f}(\lambda)}\widetilde{g}(\lambda) = (\widetilde{f}, \widetilde{g})_{\widetilde{\mathcal{H}}_2}, \quad \widetilde{f}, \widetilde{g} \in \widetilde{\mathcal{H}}_2. \tag{4.59}$$

Thus, (4.57) and (4.59) yield

$$\begin{aligned} \widetilde{\mathcal{H}} &= (\widetilde{H} \pm i)\widetilde{\mathcal{H}}_2 = (\widetilde{H} \pm i)(\mathcal{D}(H) \oplus_{\widetilde{\mathcal{H}}_2} R^{-1}\mathbb{C}) = (H \pm i)\mathcal{D}(H) \oplus_{\widetilde{\mathcal{H}}} \{\tfrac{\lambda \pm i}{1+\lambda^2} c \,|\, c \in \mathbb{C}\} \\ &= \operatorname{ran}(H \pm i) \oplus_{\widetilde{\mathcal{H}}} \{c(\lambda \mp i)^{-1} \,|\, c \in \mathbb{C}\} \end{aligned} \tag{4.60}$$

and hence (4.52). □

If H_α and H_β are two distinct self-adjoint extensions of the symmetric operator H with deficiency indices $(1,1)$ considered in Theorem 4.2, then, in contrast to the case of deficiency indices (n,n) to be studied in detail in Section 7, $\mathcal{D}(H_\alpha)$ and $\mathcal{D}(H_\beta)$ have a trivial intersection, that is,

$$\mathcal{D}(H_\alpha) \cap \mathcal{D}(H_\beta) = \mathcal{D}(H) \text{ for all } \alpha, \beta \in [0, \pi), \alpha \neq \beta. \tag{4.61}$$

Introducing the Herglotz function

$$\begin{aligned} m_\alpha(z) &= \int_{\mathbb{R}} d\omega_\alpha(\lambda)((\lambda - z)^{-1} - \lambda(1 + \lambda^2)^{-1}) &(4.62)\\ &= z + (1 + z^2)(u_+, (H_\alpha - z)^{-1}u_+)_{\mathcal{H}} &(4.63)\end{aligned}$$

(the last equality being a simple consequence of $\int_{\mathbb{R}} d\omega_\alpha(\lambda)(1 + \lambda^2)^{-1} = 1$) one verifies

$$m_\beta(z) = \frac{-\sin(\beta - \alpha) + \cos(\beta - \alpha)m_\alpha(z)}{\cos(\beta - \alpha) + \sin(\beta - \alpha)m_\alpha(z)}, \quad \alpha, \beta \in [0, \pi). \tag{4.64}$$

A comparison of (4.64) and (3.13) suggests invoking

$$a(\alpha, \beta) = \begin{pmatrix} \cos(\beta - \alpha) & \sin(\beta - \alpha) \\ -\sin(\beta - \alpha) & \cos(\beta - \alpha) \end{pmatrix} \in \mathcal{A}_2, \quad \alpha, \beta \in [0, \pi). \tag{4.65}$$

Moreover, since $m_\gamma(i) = i$ for all $\gamma \in [0, \pi)$, Theorem 3.2 applies (with $a_{1,1}(\alpha, \beta) = a_{2,2}(\alpha, \beta) = \cos(\beta - \alpha)$, $a_{1,2}(\alpha, \beta) = -a_{2,1}(\alpha, \beta) = \sin(\beta - \alpha)$).

Next, assuming that H is nonnegative, $H \geq 0$, we intend to characterize the Friedrichs and Krein extensions, H_F and H_K, of H. In order to apply Krein's results [100] (see also [9], [140], [141]) in a slightly different form (see, e.g., [137], Sect. 4 for an efficient summary of Krein's results most relevant in our context) we state

Theorem 4.3.
(i). $H_\alpha = H_F$ for some $\alpha \in [0,\pi)$ if and only if $\int_R^\infty d\|E_\alpha(\lambda)u_+\|_{\mathcal{H}}^2\lambda = \infty$, or equivalently, if and only if $\int_R^\infty d\omega_\alpha(\lambda)\lambda^{-1} = \infty$ for all $R > 0$.
(ii). $H_\beta = H_K$ for some $\beta \in [0,\pi)$ if and only if $\int_0^R d\|E_\beta(\lambda)u_+\|_{\mathcal{H}}^2\lambda^{-1} = \infty$, or equivalently, if and only if $\int_0^R d\omega_\beta(\lambda)\lambda^{-1} = \infty$ for all $R > 0$.
(iii). $H_\gamma = H_F = H_K$ for some $\gamma \in [0,\pi)$ if and only if $\int_R^\infty d\|E_\gamma(\lambda)u_+\|_{\mathcal{H}}^2\lambda = \int_0^R d\|E_\gamma(\lambda)u_+\|_{\mathcal{H}}^2\lambda^{-1} = \infty$, or equivalently, if and only if $\int_R^\infty d\omega_\gamma(\lambda)\lambda^{-1} = \infty = \int_0^R d\omega_\gamma(\lambda)\lambda^{-1}$ for all $R > 0$.

Proof. In order to reduce the above statements (i)–(iii) to those in Krein [100] (as summarized in Skau [137]), it suffices to argue as follows. From $(\mu+1)^{-1} = (\mu-i)^{-1} - (1+i)(\mu+1)^{-1}(\mu-i)^{-1}$ one infers

$$\begin{aligned}\|E_\alpha(\lambda)U_\alpha(\cdot+1)^{-1}\|_{\mathcal{H}}^2 =& \|E_\alpha(\lambda)u_+\|_{\mathcal{H}}^2 + 2\|E_\alpha(\lambda)(H_\alpha+1)^{-1}u_+\|_{\mathcal{H}}^2 \\ & - 2\|E_\alpha(\lambda)(H_\alpha+1)^{-1/2}u_+\|_{\mathcal{H}}^2 \end{aligned} \tag{4.66}$$

and since

$$\int_{\mathcal{B}} d\|E_\alpha(\lambda)(H_\alpha+1)^{-r}u_+\|_{\mathcal{H}}^2 = \int_{\mathcal{B}} \frac{d\|E_\alpha(\lambda)u_+\|_{\mathcal{H}}^2}{(\lambda+1)^{2r}}, \quad r \geq 0, \tag{4.67}$$

one concludes that

$$\begin{aligned}&\int_{\mathcal{B}} d\|E_\alpha(\lambda)U_\alpha(\cdot+1)^{-1}\|_{\mathcal{H}}^2 \text{ is finite (infinite)} \\ &\text{if and only if } \int_{\mathcal{B}} d\|E_\alpha(\lambda)u_+\|_{\mathcal{H}}^2 \text{ is finite (infinite).}\end{aligned} \tag{4.68}$$

Here $\mathcal{B}$ denotes any Borel subset of $[0,\infty)$. ∎

We also recall that

$$\inf\sigma(H_F) = \inf\{(g,Hg)_{\mathcal{H}} \in \mathbb{R} \,|\, g \in \mathcal{D}(H), \|g\|_{\mathcal{H}} = 1\} \geq 0, \tag{4.69}$$

whereas

$$\inf\sigma(H_K) = 0 \tag{4.70}$$

(here $\sigma(\cdot)$ abbreviates the spectrum of a linear operator). Moreover, all nonnegative self-adjoint extensions $\widetilde{H}$ of H satisfy

$$0 \leq (H_F-\mu)^{-1} \leq (\widetilde{H}-\mu)^{-1} \leq (H_K-\mu)^{-1}, \quad \mu \in (-\infty,0). \tag{4.71}$$

and hence H has a unique nonnegative self-adjoint extension if and only if $H_K = H_F$.

Theorem 4.3 then yields the following result.

Theorem 4.4. ([35], [37], [38], [42], [101]).
(i). $H_\alpha = H_F$ for some $\alpha \in [0,\pi)$ if and only if $\lim_{\lambda\downarrow-\infty} m_\alpha(\lambda) = -\infty$.
(ii). $H_\beta = H_K$ for some $\beta \in [0,\pi)$ if and only if $\lim_{\lambda\uparrow 0} m_\beta(\lambda) = \infty$.
(iii). $H_\gamma = H_F = H_K$ for some $\gamma \in [0,\pi)$ if and only if $\lim_{\lambda\downarrow-\infty} m_\gamma(\lambda) = -\infty$ and $\lim_{\lambda\uparrow 0} m_\gamma(\lambda) = \infty$.
(iv). Suppose $\alpha_F \in [0,\pi)$ corresponds to $H_{\alpha_F} = H_F$, $\beta_K \in [0,\pi)$ to $H_{\beta_K} = H_K$, and $\gamma \in [0,\pi)$. Then

$$\lim_{\lambda\downarrow-\infty} m_\gamma(\lambda) = -\cot(\gamma-\alpha_F) = -\int_{\mathbb{R}} d\omega_\gamma(\lambda)\lambda(1+\lambda^2)^{-1}, \quad \gamma \neq \alpha_F, \tag{4.72}$$

$$\lim_{\lambda\uparrow 0} m_\gamma(\lambda) = -\cot(\gamma-\alpha_K) = \int_{\mathbb{R}} d\omega_\gamma(\lambda)(\lambda^{-1} - \lambda(1+\lambda^2)^{-1}), \quad \gamma \neq \alpha_K, \tag{4.73}$$

$$\int_{\mathbb{R}} d\omega_\gamma(\lambda)\lambda^{-1} = \cot(\gamma-\alpha_F) - \cot(\gamma-\alpha_K), \quad \gamma\neq\alpha_F,\ \gamma\neq\alpha_K. \tag{4.74}$$

Proof. If $H_\delta \geq 0$ for some $\delta \in [0,\pi)$ one infers

$$m_\delta(\lambda) = \int_0^\infty d\omega_\delta(\lambda')((\lambda'+|\lambda|)^{-1} - \lambda'(1+\lambda'^2)^{-1}), \quad \lambda < 0. \tag{4.75}$$

Next, suppose $H_\alpha = H_F$. Then, since $[\lambda'(1+\lambda'^2)^{-1} - (\lambda'+|\lambda|)^{-1}]$ is monotone increasing as $\lambda \downarrow -\infty$, $\lim_{\lambda\downarrow-\infty} m_\alpha(\lambda) = -\int_0^\infty d\omega_\alpha(\lambda')\lambda'(1+\lambda'^2)^{-1} = -\infty$ by the monotone convergence theorem and Theorem 4.2 (i). Conversely, suppose $\lim_{\lambda\downarrow-\infty} m_\alpha(\lambda) = -\infty$, then necessarily $\int_0^\infty d\omega_\alpha(\lambda)(1+\lambda)^{-1} = \infty$ and hence $H_\alpha = H_F$ again by Theorem 4.2 (i). This proves (i). Items (ii) and (iii) then follow analogously from Theorem 4.2 (ii) and (iii) above. Equation (4.72) is a direct consequence of (4.62), (4.64), (i)–(iii), and the fact that all operators H_α, $\alpha \in [0,\pi)$ are bounded from below (and hence $m_\alpha(z)$ are real-valued for $z \in (-\infty, -c(\alpha)]$ and analytic in $\mathbb{C}\backslash(-\infty,-c(\alpha)]$ for $c(\alpha) > 0$ sufficiently large). Equation (4.73) is proved in the same manner observing that $\sigma(H_\alpha)\cap(-\infty,0)$, $\alpha\in[0,\pi)$ consists of at most one eigenvalue. Finally, (4.74) is just the difference of (4.73) and (4.72). $\square$

The following represents an elementary example illustrating these concepts.

Example 4.5. Let $r \in (-1,1)$ and consider the measure

$$d\mu_r(\lambda) = \begin{cases} (2/\pi)\sin((r+1)\pi/2)\lambda^r d\lambda, & \lambda \geq 0 \\ 0, & \lambda < 0. \end{cases} \tag{4.76}$$

Then (4.32) is easily verified and

$$\int_R^\infty \frac{d\mu_r(\lambda)}{\lambda} = \begin{cases} \infty & \text{if } 0 \leq r < 1 \\ < \infty & \text{if } -1 < r < 0, \end{cases} \qquad \int_0^R \frac{d\mu_r(\lambda)}{\lambda} = \begin{cases} \infty & \text{if } -1 < r \leq 0 \\ < \infty & \text{if } 0 < r < 1 \end{cases} \tag{4.77}$$

for all $R > 0$. Define the closed symmetric operator $\widehat{H}(r) \geq 0$ in $L^2((0,\infty); d\mu_r)$ with deficiency indices $(1,1)$ by

$$(\widehat{H}(r)\hat{g})(\lambda) = \lambda\hat{g}(\lambda), \tag{4.78}$$
$$\hat{g} \in \mathcal{D}(\widehat{H}(r)) = \{\hat{h} \in L^2((0,\infty);(1+\lambda^2)d\mu_r) \,|\, \int_0^\infty d\mu_r(\lambda)\hat{h}(\lambda) = 0\}$$

and the self-adjoint (maximally defined multiplication) operator

$$(\widehat{H}_r\hat{g})(\lambda) = \lambda\hat{g}(\lambda), \quad \hat{g} \in \mathcal{D}(\widehat{H}_r) = L^2((0,\infty);(1+\lambda^2)d\mu_r). \tag{4.79}$$

Then $\widehat{H}_r$ represents the Friedrichs extension $\widehat{H}(r)_F$ of $\widehat{H}(r)$ for $0 \leq r < 1$ and the Krein extension $\widehat{H}(r)_K$ of $\widehat{H}(r)$ for $-1 < r \leq 0$. In particular, $\widehat{H}(r)_F = \widehat{H}(r)_K$ if and only if $r = 0$.

Next, we turn to a realization theorem for Herglotz functions of the type (4.63). It will be convenient to introduce the following sets of Herglotz functions,

$$\mathcal{N}_0 = \{m : \mathbb{C}_+ \to \mathbb{C}_+ \text{ analytic} \,|\, m(z) = \int_{\mathbb{R}} d\omega(\lambda)((\lambda-z)^{-1} - \lambda(1+\lambda^2)^{-1}),$$

$$\textstyle\int_{\mathbb{R}} d\omega(\lambda) = \infty, \ \int_{\mathbb{R}} d\omega(\lambda)(1+\lambda^2)^{-1} < \infty\}, \tag{4.80}$$

$$\mathcal{N}_{0,F} = \{m \in \mathcal{N}_0 \,|\, \operatorname{supp}(\omega) \subseteq [0,\infty), \ \textstyle\int_R^\infty d\omega(\lambda)\lambda^{-1} = \infty \text{ for some } R > 0\}, \tag{4.81}$$

$$\mathcal{N}_{0,K} = \{m \in \mathcal{N}_0 \,|\, \operatorname{supp}(\omega) \subseteq [0,\infty), \ \textstyle\int_0^R d\omega(\lambda)\lambda^{-1} = \infty \text{ for some } R > 0\}, \tag{4.82}$$

$$\begin{aligned}\mathcal{N}_{0,F,K} = \{m \in \mathcal{N}_0 \,|\, \operatorname{supp}(\omega) \subseteq [0,\infty), \ &\textstyle\int_R^\infty d\omega(\lambda)\lambda^{-1} = \int_0^R d\omega(\lambda)\lambda^{-1} = \infty \\ &\text{for some } R > 0\} = \mathcal{N}_{0,F} \cap \mathcal{N}_{0,K}.\end{aligned} \tag{4.83}$$

The sets $\mathcal{N}_{0,F}$, $\mathcal{N}_{0,K}$, and $\mathcal{N}_{0,F,K}$ are of course independent of $R > 0$.

Theorem 4.6.
(i). Any $\widetilde{m} \in \mathcal{N}_0$ can be realized in the form

$$\widetilde{m}(z) = z\|u_+\|^2_{\widetilde{\mathcal{H}}} + (1+z^2)(u_+, (\widetilde{H} - z)^{-1}u_+)_{\widetilde{\mathcal{H}}}, \quad z \in \mathbb{C}_+, \tag{4.84}$$

where $\widetilde{H}$ denotes the self-adjoint extension of some densely defined closed symmetric operator H with deficiency indices $(1,1)$ and deficiency vector $u_+ \in \ker(H^* - i)$ in some separable complex Hilbert space $\widetilde{\mathcal{H}}$.
(ii). Any $\widetilde{m}_{F(resp.\ K)} \in \mathcal{N}_{0,F(resp.\ K)}$ can be realized in the form

$$\widetilde{m}_{F(resp.\ K)}(z) = z\|u_+\|^2_{\widetilde{\mathcal{H}}} + (1+z^2)(u_+, (\widetilde{H}_{F(resp.\ K)} - z)^{-1}u_+)_{\widetilde{\mathcal{H}}}, \quad z \in \mathbb{C}_+, \tag{4.85}$$

where $\widetilde{H}_{F(resp.\ K)} \geq 0$ denotes the Friedrichs (respectively, Krein) extension of some densely defined closed operator $H \geq 0$ with deficiency indices $(1,1)$ and deficiency vector $u_+ \in \ker(H^* - i)$ in some separable complex Hilbert space $\widetilde{\mathcal{H}}$.
(iii). Any $\widetilde{m}_{F,K} \in \mathcal{N}_{0,F,K}$ can be realized in the form

$$\widetilde{m}_{F,K}(z) = z\|u_+\|^2_{\widetilde{\mathcal{H}}} + (1+z^2)(u_+, (\widetilde{H}_{F,K} - z)^{-1}u_+)_{\widetilde{\mathcal{H}}}, \quad z \in \mathbb{C}_+, \tag{4.86}$$

where $\widetilde{H}_{F,K} \geq 0$ denotes the unique nonnegative self-adjoint extension of some densely defined closed operator $H \geq 0$ with deficiency indices $(1,1)$ and deficiency vector $u_+ \in \ker(H^* - i)$ in some separable complex Hilbert space $\widetilde{\mathcal{H}}$.
In each case (i)–(iii) one has

$$\int_{\mathbb{R}} d\widetilde{\omega}(\lambda)(1+\lambda^2)^{-1} = \|u_+\|^2_{\widetilde{\mathcal{H}}}, \tag{4.87}$$

where $\widetilde{\omega}$ denotes the measure in the Herglotz representation of $\widetilde{m}(z)$.

Proof. We use the notation established in Theorem 4.2. Define

$$u_+(\lambda) = (\lambda - i)^{-1}, \tag{4.88}$$

then $\|u_+\|^2_{\widetilde{\mathcal{H}}} = \int_{\mathbb{R}} d\widetilde{\omega}(\lambda)(1+\lambda^2)^{-1}$ and

$$\begin{aligned}&z\|u_+\|^2_{\widetilde{\mathcal{H}}} + (1+z^2)(u_+, (\widetilde{H} - z)^{-1}u_+)_{\widetilde{\mathcal{H}}} \\ &= \int_{\mathbb{R}} d\widetilde{\omega}(\lambda)(z(1+\lambda^2)^{-1} + (1+z^2)(\lambda - z)^{-1}(1+\lambda^2)^{-1}) \\ &= \int_{\mathbb{R}} d\widetilde{\omega}(\lambda)((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}) = \widetilde{m}(z)\end{aligned} \tag{4.89}$$

proves (4.84) and hence part (i). Parts (ii) and (iii) then follow in the same manner from Theorems 4.2 and 4.3. ☐

Of course we could have normalized u_+, $\|u_+\|_{\tilde{\mathcal{H}}} = 1$, and then added the constraint $\int_{\mathbb{R}} d\omega(\lambda)(1+\lambda^2)^{-1} = 1$ to (4.80)–(4.83). By (4.48), (4.84)–(4.86) can be realized in nonseparable Hilbert spaces.

Theorem 4.7. *Suppose $m_\ell \in \mathcal{N}_0$ with corresponding measures ω_ℓ in the Herglotz representation of m_ℓ, $\ell = 1, 2$, and $m_1 \neq m_2$. Then m_1 and m_2 can be realized as*

$$m_\ell(z) = z\|u_+\|^2_{\mathcal{H}} + (1+z^2)(u_+, (H_\ell - z)^{-1}u_+)_{\mathcal{H}}, \quad \ell = 1, 2, \ z \in \mathbb{C}_+, \tag{4.90}$$

where H_ℓ, $\ell = 1, 2$ are distinct self-adjoint extensions of one and the same densely defined closed symmetric operator H with deficiency indices $(1,1)$ and deficiency vector $u_+ \in \ker(H^* - i)$ in some complex Hilbert space $\mathcal{H}$ (which may be chosen to be separable) if and only if the following conditions hold:

$$\int_{\mathbb{R}} d\omega_1(\lambda)(1+\lambda^2)^{-1} = \int_{\mathbb{R}} d\omega_2(\lambda)(1+\lambda^2)^{-1} = \|u_+\|^2_{\mathcal{H}}, \tag{4.91}$$

and for all $z \in \mathbb{C}_+$,

$$m_2(z) = \frac{-\|u_+\|^2_{\mathcal{H}} + h\, m_1(z)}{h + \|u_+\|^{-2}_{\mathcal{H}} m_1(z)} \ \textit{for some } h \in \mathbb{R}. \tag{4.92}$$

Proof. The necessity of condition (4.92) has been proved by Donoghue [42] (he assumed $\|u_+\|_{\mathcal{H}} = 1$). Indeed, assuming (4.90), the fact

$$m_\ell(i) = i\|u_+\|^2_{\mathcal{H}} = i\int_{\mathbb{R}} d\omega_\ell(\lambda)(1+\lambda^2)^{-1}, \quad \ell = 1, 2 \tag{4.93}$$

yields (4.91). Identifying $h = \cot(\beta - \alpha)$, $H_1 = H_\alpha$, $H_2 = H_\beta$, $\|u_+\|^{-2}_{\mathcal{H}} m_1(z) = m_\alpha(z)$, and $\|u_+\|^{-2}_{\mathcal{H}} m_2(z) = m_\beta(z)$, (4.92) is seen to be equivalent to (4.64). (Here we may, without loss of generality, assume that H_ℓ, $\ell = 1, 2$ have simple spectra since otherwise one can apply the reduction (4.48).) Conversely, assume (4.91) and (4.92). By Theorem 4.6 (i), we may realize $m_1(z)$ as

$$\|u_+\|^{-2}_{\mathcal{H}} m_1(z) = z + (1+z^2)\|u_+\|^{-2}_{\mathcal{H}}(u_+, (H_1 - z)^{-1}u_+)_{\mathcal{H}}. \tag{4.94}$$

Again by (4.48) we may assume that H_1 has simple spectrum and identify it with H_α, $\alpha \in [0, \pi)$ in (4.29). If H_β, $\beta \in [0, \pi)\backslash\{\alpha\}$ is any other self-adjoint extension of H defined as in (4.29) (the actual normalization of $u_\pm$ being immaterial in this context), introduce

$$m_\beta(z) = z + (1+z^2)\|u_+\|^{-2}_{\mathcal{H}}(u_+, (H_\beta - z)^{-1}u_+)_{\mathcal{H}}. \tag{4.95}$$

By (4.64) one obtains $(m_\alpha(z) = \|u_+\|^{-2}_{\mathcal{H}} m_1(z))$

$$m_\beta(z) = \frac{-1 + \cot(\beta - \alpha)\|u_+\|^{-2}_{\mathcal{H}} m_1(z)}{\cot(\beta - \alpha) + \|u_+\|^{-2}_{\mathcal{H}} m_1(z)}. \tag{4.96}$$

A comparison of (4.92) and (4.96) then yields $\|u_+\|^2_{\mathcal{H}} m_\beta(z) = m_2(z)$ for $h = \cot(\beta - \alpha)$, completing the proof. ☐

Remark 4.8. For simplicity we studied Friedrichs H_F and Krein H_K extensions of a densely defined closed operator $H \geq 0$ with deficiency indices $(1,1)$ in Theorems 4.4 and 4.6 (ii),(iii). In other words, we studied the special case where H admitted at least one self-adjoint extension with the spectral gap $(-\infty, 0)$ (in general, there is a one-parameter family of such self-adjoint extensions with H_F and H_K as extreme points, cf., (4.71)). There is no difficulty in extending all our results to the case of symmetric operators and their self-adjoint extensions with arbitrary gaps (λ_1, λ_2), $-\infty < \lambda_1 < \lambda_2 < \infty$ in their spectrum. In fact, assuming H to be densely defined and closed in some complex Hilbert space $\mathcal{H}$, the condition $H \geq 0$ is now replaced by

$$\|(H - \tfrac{\lambda_1+\lambda_2}{2})f\|_{\mathcal{H}} \geq \tfrac{\lambda_2-\lambda_1}{2}\|f\|_{\mathcal{H}}, \quad f \in \mathcal{D}(H). \tag{4.97}$$

In this situation it was proved by Krein [100] that H always admits self-adjoint extensions $\widetilde{H}$ with the same spectral gap (λ_1, λ_2). In particular, there always exist two extremal self-adjoint extensions $H_{F_{\lambda_1}}$ and $H_{K_{\lambda_2}}$ of H with the same gap (λ_1, λ_2) such that

$$(H_{F_{\lambda_1}} - \mu)^{-1} \leq (\widetilde{H} - \mu)^{-1} \leq (H_{K_{\lambda_2}} - \mu)^{-1}, \quad \mu \in (\lambda_1, \lambda_2) \tag{4.98}$$

for any self-adjoint extension $\widetilde{H}$ of H with spectral gap (λ_1, λ_2). Given the results in [9], [35], [37], [38], and [100], Theorem 4.4 immediately extends to general gaps (λ_1, λ_2) upon replacing H_F by $H_{F_{\lambda_1}}$, $\lim_{\lambda\downarrow-\infty} m_\alpha(\lambda) = -\infty$ by $\lim_{\lambda\downarrow\lambda_1,\, \lambda\in(\lambda_1,\lambda_2)} m_\alpha(\lambda) = -\infty$, H_K by $H_{K_{\lambda_2}}$, and $\lim_{\lambda\uparrow 0} m_\beta(\lambda) = \infty$ by $\lim_{\lambda\uparrow\lambda_2,\, \lambda\in(\lambda_1,\lambda_2)} m_\beta(\lambda) = \infty$, etc. Analogous remarks apply to Theorem 4.6 (ii),(iii), replacing the condition $\operatorname{supp}(\omega) \subseteq [0,\infty)$ by $\operatorname{supp}(\omega) \subseteq \mathbb{R}\backslash(\lambda_1, \lambda_2)$ in (4.81)–(4.83).

Next we briefly turn to Schrödinger operators on a half-line. Let $q \in L^1([0,R])$ for all $R > 0$, q real-valued, and introduce the fundamental system $\phi_\alpha(z,x)$, $\theta_\alpha(z,x)$, $z \in \mathbb{C}$ of solutions of ($\prime$ denotes d/dx)

$$-\psi''(z,x) + (q(x) - z)\psi(z,x) = 0, \quad x > 0, \tag{4.99}$$

satisfying

$$\phi_\alpha(z,0_+) = -\theta'_\alpha(z,0_+) = -\sin(\alpha),\ \ \phi'_\alpha(z,0_+) = \theta_\alpha(z,0_+) = \cos(\alpha),\ \ \alpha \in [0,\pi). \tag{4.100}$$

Next, pick a fixed $z_0 \in \mathbb{C}_+$ and a solution $f_0(z_0,\cdot) \in L^2([0,\infty);dx)$ of (4.99) and let $\psi_\alpha(z,x)$ be the unique solution of (4.99) satisfying

$$\begin{aligned}&\psi_\alpha(z,\cdot) \in L^2([0,\infty);dx), \quad \sin(\alpha)\psi'_\alpha(z,0_+) + \cos(\alpha)\psi_\alpha(z,0_+) = 1,\\ &\lim_{x\to\infty} W(f_0(z_0,x),\psi_\alpha(z,x)) = 0, \quad z \in \mathbb{C}_+,\end{aligned} \tag{4.101}$$

the latter condition being superfluous, i.e., automatically fulfilled, if $-\frac{d^2}{dx^2} + q$ is in the limit point case at ∞. (Here $W(f(x),g(x)) = f(x)g'(x) - f'(x)g(x)$ denotes the Wronskian of f and g.) Existence and uniqueness of $\psi_\alpha(z,x)$ is a consequence of Weyl's theory (see, e.g., the discussion in Appendix A of [60]). Then $\psi_\alpha(z,x)$ is of the form

$$\psi_\alpha(z,x) = \theta_\alpha(z,x) + m_\alpha(z)\phi_\alpha(z,x), \tag{4.102}$$

with $m_\alpha(z)$ the Weyl-Titchmarsh m-function corresponding to the operator H_α in $L^2([0,\infty);dx)$ defined by

$$\begin{aligned}&(H_\alpha g)(x) = -g''(x) + q(x)g(x), \quad x > 0, \\ &\mathcal{D}(H_\alpha) = \{g \in L^2([0,\infty);dx) \,|\, g, g' \in AC([0,R]) \text{ for all } R > 0\ ;\\ &\qquad -g'' + qg \in L^2([0,\infty);dx);\ \lim_{x\to\infty} W(f_0(z_0,x),g(x)) = 0;\\ &\qquad \sin(\alpha)g'(0_+) + \cos(\alpha)g(0_+) = 0\}, \quad \alpha \in [0,\pi).\end{aligned} \tag{4.103}$$

(Here $AC([a,b])$ denotes the set of absolutely continuous functions on $[a,b]$.) Then $m_\alpha(z)$ is a Herglotz function with representation

$$m_\alpha(z) = c_\alpha + \int_{\mathbb{R}} d\omega_\alpha(\lambda)((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}), \qquad \alpha \in [0,\pi), \tag{4.104}$$

$$= \cot(\alpha) + \int_{\mathbb{R}} d\omega_\alpha(\lambda)(\lambda - z)^{-1}, \qquad \alpha \in (0,\pi), \tag{4.105}$$

where

$$\int_{\mathbb{R}} d\omega_\alpha(\lambda)(1+|\lambda|)^{-1} \begin{cases} < \infty, & \alpha \in (0,\pi), \\ = \infty, & \alpha = 0. \end{cases} \tag{4.106}$$

Moreover, one verifies

$$m_\beta(z) = \frac{-\sin(\beta-\alpha) + \cos(\beta-\alpha)m_\alpha(z)}{\cos(\beta-\alpha) + \sin(\beta-\alpha)m_\alpha(z)}, \quad \alpha,\beta \in [0,\pi) \tag{4.107}$$

and hence the corresponding matrix $a(\alpha,\beta)$ is of the type

$$a(\alpha,\beta) = \begin{pmatrix} \cos(\beta-\alpha) & \sin(\beta-\alpha) \\ -\sin(\beta-\alpha) & \cos(\beta-\alpha) \end{pmatrix} \in \mathcal{A}_2, \quad \alpha,\beta \in [0,\pi). \tag{4.108}$$

The asymptotic behavior of $m_\alpha(z)$ is given by

$$m_\alpha(z) \underset{z\to i\infty}{=} \begin{cases} \cot(\alpha) + \frac{i}{\sin^2(\alpha)} z^{-1/2} - \frac{\cos(\alpha)}{\sin^3(\alpha)} z^{-1} + o(z^{-1}), & \alpha \in (0,\pi), \\ iz^{1/2} + o(1), & \alpha = 0. \end{cases} \tag{4.109}$$

Thus, Theorem 3.2 applies (with $a_{1,1}(\alpha,\beta) = a_{2,2}(\alpha,\beta) = \cos(\beta-\alpha)$, $a_{1,2}(\alpha,\beta) = -a_{2,1}(\alpha,\beta) = \sin(\beta-\alpha)$).

Theorem 3.2 (v), in particular, represents an alternative (abstract) approach to Borg-type uniqueness theorems [22], [23] (see also [60], [103], [104], [112] and the references therein) to the effect that two sets of spectra (varying the boundary condition at one end point but keeping it fixed at the other) uniquely determine $q(x)$. Its elegant proof using the exponential Herglotz representation for $F(z)$ is due to Donoghue [42].

For simplicity we only discussed the case of a half-line $[0,\infty)$. However, the case of a finite interval $[0,R_0]$ for some $R_0 > 0$ is completely analogous, replacing the first and third condition on $\psi_\alpha(z,x)$ in (4.101) by the boundary condition $\sin(\gamma)\psi'_\alpha(z,R_0) + \cos(\gamma)\psi_\alpha(z,R_0) = 0$ for some fixed $\gamma \in [0,\pi)$.

It is possible to characterize the set of Herglotz functions leading to Weyl-Titchmarsh m-functions for $-\frac{d^2}{dx^2} + q$ in $L^2([0,R_0];dx)$ or $L^2([0,\infty);dx)$ with real-valued q satisfying $q \in L^1([0,R_0];dx)$ or $q \in L^1([0,R);dx)$ for all $R > 0$, respectively. These realization theorems, however, are far less elementary, being based on the Gelfand-Levitan formalism of inverse spectral theory (see, e.g., [54], [104], [105], [113]). We omit further details at this point.

These considerations extend to singular coefficients q at $x = 0$ replacing $q \in L^1([0,R])$ for all $R > 0$ by $q \in L^1_{\text{loc}}((0,\infty))$. A careful investigation of the Weyl limit point/limit circle theory (see, e.g., [31], Ch. 9) then shows that the fundamental system $\phi_\alpha(z,x)$, $\theta_\alpha(z,x)$ of (4.99) can be replaced by $\phi(z,x)$, $\theta(z,x)$ satisfying (4.99) with the following properties:

(i). For all $x > 0$, $\phi(z,x)$, $\theta(z,x)$ are entire with respect to $z \in \mathbb{C}$ and real-valued for all $z \in \mathbb{R}$.

(ii). $W(\theta(z,x),\phi(z,x)) = 1$, $z \in \mathbb{C}$, $x > 0$.

(iii). $\lim_{x\downarrow 0} W(\phi(z,x),\overline{\phi(z,x)}) = \lim_{x\downarrow 0} W(\theta(z,x),\overline{\theta(z,x)}) = 0$,
$\lim_{x\downarrow 0} W(\theta(z,x),\overline{\phi(z,x)}) = 1$, $z \in \mathbb{C}$.

Introducing

$$\psi(z,x) = \theta(z,x) + m(z)\phi(z,x), \quad z \in \mathbb{C}\backslash\mathbb{R} \tag{4.110}$$

satisfying

$$\psi(z,\cdot) \in L^2([0,\infty);dx), \quad z \in \mathbb{C}\backslash\mathbb{R} \tag{4.111}$$

then yields

$$\operatorname{Im}(m(z)) = \operatorname{Im}(z)\int_0^\infty dx|\psi(z,x)|^2, \quad z \in \mathbb{C}\backslash\mathbb{R} \tag{4.112}$$

$$\text{if and only if } \lim_{x\uparrow\infty} W(\psi(z,x),\overline{\psi(z,x)}) = 0, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{4.113}$$

In particular, $m(z)$ is a Herglotz function if (4.113) is satisfied. For associated self-adjoint boundary conditions in the singular case see, for instance, [26], [84], Ch. III, and [127].

5. Basic Facts on Matrix-Valued Herglotz Functions

The main purpose of this section is to carry over some of the scalar results of Section 2 to matrix-valued Herglotz functions.

In the following we denote by $M_n(\mathbb{C})$, $n \in \mathbb{N}$ the set of $n \times n$ matrices with complex-valued entries, denote by $I_n \in M_n(\mathbb{C})$ the identity matrix, by A^* the adjoint (complex conjugate transpose) of $A \in M_n(\mathbb{C})$, and by $(\cdot,\cdot)_{\mathbb{C}^n}$ the scalar product in $\mathbb{C}^n$ associated with the standard Euclidean metric on $\mathbb{C}^n$ (antilinear in the first and linear in the second factor). We recall that a matrix $A \in M_n(\mathbb{C})$ is called nonnegative (respectively, nonpositive), $A \geq 0$ (respectively, $A \leq 0$) if $(\underline{x}, A\underline{x})_{\mathbb{C}^n} \geq 0$ (respectively, $(\underline{x}, A\underline{x})_{\mathbb{C}^n} \leq 0$) for all $\underline{x} \in \mathbb{C}^n$. Similarly, A is called positive (positive definite, or strictly positive), $A > 0$, if $(\underline{x}, A\underline{x})_{\mathbb{C}^n} > 0$ for all $\underline{x} \in \mathbb{C}^n\backslash\{0\}$. A principal submatrix of A is obtained by deleting k rows and columns, $0 \leq k \leq n-1$, which pairwise intersect at diagonal elements. Principal minors are determinants of principal submatrices. The rank, range, and kernel of A are denoted by $\operatorname{rank}(A)$, $\operatorname{ran}(A)$, and $\ker(A)$, respectively.

We start with an elementary result on nonnegative matrices which will be useful at various places later on.

Lemma 5.1 ([81], Ch. 7)**.** *Let $A = (A_{j,k})_{1\leq j,k\leq n} \in M_n(\mathbb{C})$ and assume $A \geq 0$. Then*
(i). $A \geq 0$ if and only if all principal minors of A are nonnegative. In particular, all diagonal elements of A are nonnegative,

$$A_{j,j} \geq 0, \quad 1 \leq j \leq n. \tag{5.1}$$

(ii). For all $1 \leq j,k \leq n$,

$$|A_{j,k}| \leq A_{j,j}^{1/2} A_{k,k}^{1/2} \leq \frac{1}{2}(A_{j,j} + A_{k,k}), \tag{5.2}$$

in particular, if $A_{\ell,\ell} = 0$ then the ℓth row and column of A are zero.
(iii). Let $\underline{x} \in \mathbb{C}^n$ and $(\underline{x}, A\underline{x})_{\mathbb{C}^n} = 0$. Then $A\underline{x} = 0$.
(iv). Suppose $\operatorname{rank}(A) = r < n$. Then A has an $r \times r$ positive definite principal submatrix.

Next we briefly turn to (self-adjoint) matrix-valued measures. The ones to be used below will be of the type

$$\Sigma(\mathcal{M}) = \int_{\mathcal{M}} d\Omega(\lambda)(1+\lambda^2)^{-1}, \quad \Sigma = (\Sigma_{j,k})_{1\le j,k\le n}, \quad \Omega = (\Omega_{j,k})_{1\le j,k\le n}, \quad (5.3)$$

where $\Sigma_{j,k}$, $1 \le j,k \le n$ are complex (and hence finite) Borel measures on $\mathbb{R}$ and $\Omega_{j,k}$, $1 \le j,k \le n$ are complex-valued set functions defined on the bounded Borel subsets of $\mathbb{R}$ with the properties,

(i). $\Omega(X) = (\Omega_{j,k}(X))_{1\le j,k\le n} \subset M_n(\mathbb{C})$ is nonnegative, $\Omega(X) \ge 0$, for all bounded Borel sets $X \subset \mathbb{R}$, and $\Omega(\phi) = 0$.

(ii). $\Omega_{j,k}(\cup_{\ell\in\mathbb{N}} X_\ell) = \Sigma_{\ell\in\mathbb{N}}\Omega_{j,k}(X_\ell)$, $1 \le j,k \le n$ for each sequence of disjoint Borel sets $\{X_\ell\}_{\ell\in\mathbb{N}} \subset \mathbb{R}$ with $\cup_{\ell\in\mathbb{N}} X_\ell$ bounded.

Clearly, each diagonal element $\Sigma_{j,j}$, $1 \le j \le n$ defines a positive (finite) Borel measure on $\mathbb{R}$. In addition, we denote by

$$\sigma^{tr} = \mathrm{tr}_{\mathbb{C}^n}(\Sigma) = \Sigma_{1,1} + \cdots + \Sigma_{n,n} \quad (5.4)$$

the (scalar) trace measure of Σ and note that

$$\sigma^{tr}(X) = 0 \quad \text{if and only if} \quad \Sigma(X) = 0 \quad (5.5)$$

for all Borel sets $X \subseteq \mathbb{R}$ since by (5.2) each $\Sigma_{j,k}$ is absolutely continuous with respect to $\Sigma_{j,j} + \Sigma_{k,k}$ and hence with respect to σ^{tr},

$$\Sigma_{j,k} \ll \Sigma_{j,j} + \Sigma_{k,k} \ll \sigma^{tr}, \quad 1 \le j,k \le n. \quad (5.6)$$

Below we will use the standard Lebesgue decomposition of matrix-valued measures with respect to Lebesgue measure on $\mathbb{R}$, in particular, we will use the fact that $\Omega = \Omega_{ac}$ is purely absolutely continuous with respect to Lebesgue measure $d\lambda$ if and only if $d\Omega(\lambda) = P(\lambda)d\lambda$ for some nonnegative locally integrable matrix P on $\mathbb{R}$.

Matrix-valued Herglotz functions are now defined in analogy to Definition 2.1 as follows.

Definition 5.2. $M : \mathbb{C}_+ \to M_n(\mathbb{C})$ is called a matrix-valued Herglotz function (in short, a Herglotz matrix) if M is analytic on $\mathbb{C}_+$ and $\mathrm{Im}(M(z)) \ge 0$ for all $z \in \mathbb{C}_+$.

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

$$M(z) = M(\overline{z})^*, \quad z \in \mathbb{C}_-. \quad (5.7)$$

Hence M is analytic on $\mathbb{C}\backslash\mathbb{R}$ but $M\big|_{\mathbb{C}_-}$ and $M\big|_{\mathbb{C}_+}$, in general, are not analytic continuations of each other (cf. Lemma 5.6). Here we follow the standard notation

$$\mathrm{Im}(M) = \frac{1}{2i}(M - M^*), \quad \mathrm{Re}(M) = \frac{1}{2}(M + M^*). \quad (5.8)$$

In contrast to the scalar case, we cannot in general expect strict inequality in $\mathrm{Im}(M(z)) \ge 0$. However the kernel of $\mathrm{Im}(M(z))$ has extremely simple properties. The following result and its elementary proof were communicated to us by Dirk Buschmann:

Lemma 5.3. *Let $M(z) \in M_n(\mathbb{C})$ be a matrix-valued Herglotz function. Then the kernel $\ker(\mathrm{Im}(M(z)))$ is independent of $z \in \mathbb{C}_+$, in particular, the rank r of $M(z)$*

is constant on $\mathbb{C}_+$. *Consequently, upon choosing an orthogonal basis in* $\ker(M(z))$ *and* $\ker(M(z))^\perp$, $M(z)$ *takes on the form*

$$M(z) = \begin{pmatrix} 0 & 0 \\ 0 & M_r(z) \end{pmatrix}, \tag{5.9}$$

where $M_r(z)$ *is an* $r \times r$ *matrix-valued Herglotz matrix satisfying*

$$\operatorname{Im}(M_r(z)) > 0, \quad r = n - \dim_{\mathbb{C}}(\ker(\operatorname{Im}(M(z))), \quad z \in \mathbb{C}_+. \tag{5.10}$$

Proof. Denote $N_z = \ker(\operatorname{Im}(M(z)))$, $z \in \mathbb{C}_+$. Pick a $z_0 \in \mathbb{C}_+$ and suppose $0 \neq \underline{x}_0 \in N_{z_0}$. Consider the scalar Herglotz function $m(z) = (\underline{x}_0, M(z)\underline{x}_0)_{\mathbb{C}^n}$. Then $m(z_0) \in \mathbb{R}$ shows that the Herglotz function $m(z) - m(z_0)$ has a zero at $z = z_0 \in \mathbb{C}_+$ and hence vanishes identically. Thus $m(z)$ equals a real constant for all $z \in \mathbb{C}_+$ and hence

$$0 = (\underline{x}_0, \operatorname{Im}(M(z))\underline{x}_0)_{\mathbb{C}^n} = \|(\operatorname{Im}(M(z)))^{1/2}\underline{x}_0\|^2_{\mathbb{C}^n}, \quad z \in \mathbb{C}_+ \tag{5.11}$$

yields

$$\underline{x}_0 \in \ker((\operatorname{Im}(M(z)))^{1/2}) = \ker(\operatorname{Im}(M(z))), \quad z \in \mathbb{C}_+ \tag{5.12}$$

since $\operatorname{Im}(M(z)) \geq 0$. In particular, N_z, and hence $r = \operatorname{rank}(\operatorname{Im}(M(z)))= n - \dim_{\mathbb{C}}(N_z)$ are independent of $z \in \mathbb{C}_+$. Finally, suppose $\ker(\operatorname{Im}(M(z_0))) = \{0\}$. Then $\ker(\operatorname{Im}(M(z_1))) \neq \{0\}$ for some $z_1 \in \mathbb{C}\backslash\{z_0\}$ would contradict the fact that $\dim_{\mathbb{C}}(\ker(\operatorname{Im}(M(z))))$ is constant for $z \in \mathbb{C}_+$. Thus $\ker(\operatorname{Im}(M(z))) = \{0\}$ for all $z \in \mathbb{C}_+$ thereby completing the proof. ☐

The following result, the analog of Theorem 2.2, is well-known to experts in the theory of self-adjoint extensions of symmetric operators and especially, in the spectral theory of matrix-valued Schrödinger operators, even-order Hamiltonian systems, and higher-order ordinary differential and difference operators. For relevant material we refer the reader, for instance, to [6]–[8], [14], Ch. 9, [17], [20], Sect. VI.5, [24], Sect. I.4, [25], [27], [28], [30], [35]–[37], [46], Sects. XIII.5–XIII.7, [49], [51], [65], [66], [75], [79], [80], [85], [89], [96]–[98], [99], Chs. 7, 8, [101], [116], [119], Ch. VI, [120], [129]–[133], [142], [146], Sects. 8–10.

However, since proofs are not always readily available in the literature, we briefly sketch some pertinent arguments which essentially reduce the matrix case to the scalar situation described in Theorem 2.2.

Theorem 5.4. *Let* $M(z) \in M_n(\mathbb{C})$ *be a matrix-valued Herglotz function. Then*
(i). Each diagonal element $M_{j,j}(z)$, $1 \leq j \leq n$ *of* $M(z)$ *is a (scalar) Herglotz function.*
(ii). $M(z)$ *has finite normal limits* $M(\lambda \pm i0) = \lim_{\varepsilon \downarrow 0} M(\lambda \pm i\varepsilon)$ *for a.e.* $\lambda \in \mathbb{R}$.
(iii). If each diagonal element $M_{j,j}(z)$, $1 \leq j \leq n$ *of* $M(z)$ *has a zero normal limit on a fixed subset of* $\mathbb{R}$ *having positive Lebesgue measure, then* $M(z) = C_0$, *where* $C_0 = C_0^*$ *is a constant self-adjoint* $n \times n$ *matrix with vanishing diagonal elements.*
(iv). There exists a matrix-valued measure Ω *on the bounded Borel subsets of* $\mathbb{R}$ *satisfying*

$$\int_{\mathbb{R}} (\underline{c}, d\Omega(\lambda)\underline{c})_{\mathbb{C}^n} (1+\lambda^2)^{-1} < \infty \text{ for all } \underline{c} \in \mathbb{C}^n \tag{5.13}$$

such that the Nevanlinna, respectively, Riesz-Herglotz representation

$$M(z) = C + Dz + \int_{\mathbb{R}} d\Omega(\lambda)((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}), \quad z \in \mathbb{C}_+, \tag{5.14}$$

$$C = \mathrm{Re}(M(i)), \quad D = \lim_{\eta\uparrow\infty} \big(\frac{1}{i\eta} M(i\eta)\big) \geq 0$$

holds.
(v). The Stieltjes inversion formula for Ω *reads*

$$\frac{1}{2}\Omega(\{\lambda_1\}) + \frac{1}{2}\Omega(\{\lambda_2\}) + \Omega((\lambda_1,\lambda_2)) = \pi^{-1} \lim_{\varepsilon\downarrow 0} \int_{\lambda_1}^{\lambda_2} d\lambda \, \mathrm{Im}(M(\lambda + i\varepsilon)). \tag{5.15}$$

(vi). The absolutely continuous part Ω_{ac} *of* Ω *is given by*

$$d\Omega_{ac}(\lambda) = \pi^{-1} \mathrm{Im}(M(\lambda + i0))d\lambda. \tag{5.16}$$

(vii). Any poles of M *are simple and located on the real axis, the residues at poles being nonpositive matrices (of rank* $r \in \{1, \dots, n\}$*).*

Proof. (i). Since for all $\underline{x} \in \mathbb{C}^n$,

$$(\underline{x}, M(z)\underline{x})_{\mathbb{C}^n} \quad \text{is a (scalar) Herglotz function,} \tag{5.17}$$

the choice $\underline{x} = \underline{x}_j = (x_{j,1}, \dots, x_{j,n})^t \in \mathbb{C}^n$, $x_{j,\ell} = \delta_{j,\ell}$ in (5.17) proves (i). (Here "t" denotes the transpose operation.)

(ii). Consider $\underline{x}_j = (x_{j,1}, \dots, x_{j,n})^t \in \mathbb{C}^n$, $x_{j,\ell} = \delta_{j,\ell}$ and apply the polarization identity to $(\underline{x}_j, M(z)\underline{x}_k)$, $j \neq k$ to obtain

$$\begin{aligned} M_{j,k}(z) = \frac{1}{4}\big(&((\underline{x}_j + \underline{x}_k), M(z)(\underline{x}_j + \underline{x}_k))_{\mathbb{C}^n} - ((\underline{x}_j - \underline{x}_k), M(z)(\underline{x}_j - \underline{x}_k))_{\mathbb{C}^n} \\ &+ i((\underline{x}_j - i\underline{x}_k), M(z)(\underline{x}_j - i\underline{x}_k))_{\mathbb{C}^n} - i((\underline{x}_j + i\underline{x}_k), M(z)(\underline{x}_j + i\underline{x}_k))_{\mathbb{C}^n}\big). \end{aligned} \tag{5.18}$$

Combining (5.17), (5.18), and Theorem 2.2(i) then proves (ii).

(iv),(v). By (5.17) and Theorem 2.2(iii),(iv) one infers for all $\underline{x} \in \mathbb{C}^n$ the representation

$$(\underline{x}, M(z)\underline{x})_{\mathbb{C}^n} = c_{\underline{x}} + d_{\underline{x}} z + \int_{\mathbb{R}} d\omega_{\underline{x}}(\lambda)((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}), \tag{5.19}$$

with

$$\begin{aligned} &\int_{\mathbb{R}} d\omega_{\underline{x}}(\lambda)(1+\lambda^2)^{-1} < \infty, \\ &c_{\underline{x}} = \mathrm{Re}((\underline{x}, M(i)\underline{x})_{\mathbb{C}^n}), \quad d_{\underline{x}} = \lim_{\eta\uparrow\infty} (\underline{x}, M(i\eta)\underline{x})_{\mathbb{C}^n}/(i\eta) \geq 0. \end{aligned} \tag{5.20}$$

In addition, for $(\lambda_1, \lambda_2) \subset \mathbb{R}$,

$$\frac{1}{2}\omega_{\underline{x}}(\{\lambda_1\}) + \frac{1}{2}\omega_{\underline{x}}(\{\lambda_2\}) + \omega_{\underline{x}}((\lambda_1,\lambda_2)) = \pi^{-1} \lim_{\varepsilon\downarrow 0} \int_{\lambda_1}^{\lambda_2} d\lambda \, \mathrm{Im}((\underline{x}, M(\lambda + i\varepsilon)\underline{x})_{\mathbb{C}^n}). \tag{5.21}$$

The polarization identity for $(\underline{x}, M(z)\underline{y})_{\mathbb{C}^n}$ then yields for all $\underline{x}, \underline{y} \in \mathbb{C}^n$,

$$\begin{aligned} (\underline{x}, M(z)\underline{y})_{\mathbb{C}^n} = &C(\underline{x},\underline{y}) + D(\underline{x},\underline{y})z \\ &+ \int_{\mathbb{R}} d\Omega(\underline{x},\underline{y})(\lambda)((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}), \end{aligned} \tag{5.22}$$

where, in obvious notation,

$$C(\underline{x},\underline{y}) = \frac{1}{4}(c_{\underline{x}+\underline{y}} - c_{\underline{x}-\underline{y}} + ic_{\underline{x}-i\underline{y}} - ic_{\underline{x}+i\underline{y}}), \tag{5.23}$$

$$D(\underline{x},\underline{y}) = \frac{1}{4}(d_{\underline{x}+\underline{y}} - d_{\underline{x}-\underline{y}} + id_{\underline{x}-i\underline{y}} - id_{\underline{x}+i\underline{y}}), \tag{5.24}$$

$$\begin{aligned}
&\frac{1}{2}\Omega(\underline{x},\underline{y})(\{\lambda_1\}) + \frac{1}{2}\Omega(\underline{x},\underline{y})(\{\lambda_2\}) + \Omega(\underline{x},\underline{y})((\lambda_1,\lambda_2)) \\
&\quad = \frac{1}{4}\bigg(\frac{1}{2}\omega_{\underline{x}+\underline{y}}(\{\lambda_1\}) - \frac{1}{2}\omega_{\underline{x}-\underline{y}}(\{\lambda_1\}) + \frac{i}{2}\omega_{\underline{x}-i\underline{y}}(\{\lambda_1\}) - \frac{i}{2}\omega_{\underline{x}+i\underline{y}}(\{\lambda_1\}) \\
&\qquad + \frac{1}{2}\omega_{\underline{x}+\underline{y}}(\{\lambda_2\}) - \frac{1}{2}\omega_{\underline{x}-\underline{y}}(\{\lambda_2\}) + \frac{i}{2}\omega_{\underline{x}-i\underline{y}}(\{\lambda_2\}) - \frac{i}{2}\omega_{\underline{x}+i\underline{y}}(\{\lambda_2\}) \\
&\qquad + \omega_{\underline{x}+\underline{y}}((\lambda_1,\lambda_2)) - \omega_{\underline{x}-\underline{y}}((\lambda_1,\lambda_2)) + i\omega_{\underline{x}-i\underline{y}}((\lambda_1,\lambda_2)) - i\omega_{\underline{x}+i\underline{y}}((\lambda_1,\lambda_2))\bigg).
\end{aligned} \tag{5.25}$$

Since $C(\underline{x},\underline{y})$ and $D(\underline{x},\underline{y})$ are symmetric sesquilinear forms and $D(\underline{x},\underline{x}) \geq 0$ for all $\underline{x} \in \mathbb{C}^n$, one infers

$$C(\underline{x},\underline{y}) = (\underline{x}, C\underline{y})_{\mathbb{C}^n}, \quad D(\underline{x},\underline{y}) = (\underline{x}, D\underline{y})_{\mathbb{C}^n} \tag{5.26}$$

for some

$$C = C^* \in M_n(\mathbb{C}), \quad 0 \leq D \in M_n(\mathbb{C}). \tag{5.27}$$

Similarly, using the obvious fact that $\mathrm{Im}((\underline{x}, M(z)\underline{x})_{\mathbb{C}^n}) = (\underline{x}, \mathrm{Im}(M(z))\underline{x})_{\mathbb{C}^n}$, $\underline{x} \in \mathbb{C}^n$, (5.21) then becomes

$$(5.22) = (\underline{x}, \pi^{-1} \lim_{\varepsilon\downarrow 0} \int_{\lambda_1}^{\lambda_2} d\lambda\, \mathrm{Im}(M(\lambda+i\varepsilon))\underline{y})_{\mathbb{C}^n}. \tag{5.28}$$

Arbitrariness of $\underline{x},\underline{y} \in \mathbb{C}^n$ then yields the representation (5.14) for $M(z)$ and the Stieltjes inversion formula (5.15). That $C = \mathrm{Re}(M(i))$ and $D = \lim_{\eta\uparrow\infty} M(i\eta)/(i\eta)$ is clear from the corresponding properties in (5.20).

(iii). Let $X_0 \subseteq \mathbb{R}$ be the fixed subset in (iii). Then by hypothesis, $D = 0$, $\Omega = 0$ using (5.14), (5.15) and $\mathrm{Im}(M(\lambda + i0)) = 0$ for $\lambda \in X_0$ by Lemma 5.1(ii). Thus $M(z) = C$ is constant with vanishing diagonal elements.

(vi). Studying $(\underline{x}, \mathrm{Im}(M(\lambda+i\varepsilon))\underline{x})_{\mathbb{C}^n}$, $\underline{x} \in \mathbb{C}^n$, one can follow the argument in [135], Theorem 1.6(iv) step by step.

(vii). First-order poles with nonpositive residues at isolated singularities of $M(z)$ on the real axis follows from polarization, (5.17), and Theorem 2.2(vi). □

In the scalar case described in Theorem 2.2, isolated zeros of $m(z)$ are necessarily simple and located on $\mathbb{R}$. This can of course be inferred from the fact that $-1/m(z)$ is a Herglotz function whenever $m(z)$ is one (cf. (2.10)) and hence isolated poles of $1/m(z)$ are necessarily simple. This reformulation concerning isolated simple real zeros of $m(z)$ extends to the matrix case since we will show later on (cf. Theorem 6.4(i)) that if $M(z)$ is invertible on $\mathbb{C}_+$, then $-M(z)^{-1}$ is a Herglotz matrix whenever $M(z)$ is one. Hence isolated poles of $M(z)^{-1}$ on $\mathbb{R}$ are necessarily simple.

It should be remarked at this point that Theorem 5.4(iv) as well as Theorem 5.5(iii) below, are well-known to extend to infinite-dimensional situations under appropriate hypotheses on $M(z)$. We will return to this circle of ideas elsewhere.

Due to (5.6), Theorem 2.3(i)–(vi) and Theorem 2.4(i) extend to the present matrix-valued context with only minor modifications. For later reference we summarize a few of these extensions below.

Theorem 5.5. *Let $M(z) \in M_n(\mathbb{C})$ be a matrix-valued Herglotz function with representation* (5.14)*. Then* *(i). For all* $\lambda \in \mathbb{R}$,

$$\lim_{\varepsilon \downarrow 0} \varepsilon \mathrm{Re}(M(\lambda + i\varepsilon)) = 0, \tag{5.29}$$

$$\Omega(\{\lambda\}) = \lim_{\varepsilon \downarrow 0} \varepsilon \mathrm{Im}(M(\lambda + i\varepsilon)) = -i \lim_{\varepsilon \downarrow 0} \varepsilon M(\lambda + i\varepsilon). \tag{5.30}$$

(ii). Let $L > 0$ *and suppose* $0 \leq \mathrm{Im}(M(z)) \leq L I_n$ *for all* $z \in \mathbb{C}_+$. *Then* $D = 0$, Ω *is purely absolutely continuous,* $\Omega = \Omega_{ac}$, *and*

$$0 \leq \frac{d\Omega(\lambda)}{d\lambda} = \pi^{-1} \lim_{\varepsilon \downarrow 0} \mathrm{Im}(M(\lambda + i\varepsilon)) \leq \pi^{-1} L I_n \text{ for a.e. } \lambda \in \mathbb{R}. \tag{5.31}$$

(iii). Assume $M(z)$ *is invertible for all* $z \in \mathbb{C}_+$. *Then there exist* $\Xi_{j,k} \in L^\infty(\mathbb{R})$, $1 \leq j, k \leq n$, $0 \leq \Xi \leq I_n$ *a.e., such that*

$$\ln(M(z)) = K + \int_{\mathbb{R}} d\lambda\, \Xi(\lambda)((\lambda - z)^{-1} - \lambda(1 + \lambda^2)^{-1}), \quad z \in \mathbb{C}_+, \tag{5.32}$$
$$K = \mathrm{Re}(\ln(M(i))),$$

where

$$\Xi(\lambda) = \pi^{-1} \lim_{\varepsilon \downarrow 0} \mathrm{Im}(\ln(M(\lambda + i\varepsilon))) \text{ for a.e. } \lambda \in \mathbb{R}. \tag{5.33}$$

Proof of (iii). We briefly sketch an approach by Carey [28] (designed for the infinite-dimensional context). Define $\ln(z)$ with a cut along $(-\infty, 0]$ such that $\ln(\lambda)$ is real-valued for $\lambda > 0$, that is, $0 < \arg(\ln(z)) < \pi$ for all $z \in \mathbb{C}_+$. Since by hypothesis $0 \notin \sigma(M(z))$, $z \in \mathbb{C}_+$, one can define $\ln(M(z))$ for $z \in \mathbb{C}_+$ by

$$\ln(M(z)) = \int_{-\infty}^{0} d\lambda((\lambda - M(z))^{-1} - \lambda(1 + \lambda^2)^{-1}). \tag{5.34}$$

Next, introducing $\ln(z; \eta) = \ln(z + i\eta)$ for $\eta > 0$, $\ln(\cdot; \eta)$ is analytic on $\mathbb{C}_+$. Denoting by $W(A)$ the numerical range of $A \in M_n(\mathbb{C})$ (i.e., $W(A) = \{(\underline{x}, A\underline{x}) \,|\, \underline{x} \in \mathbb{C}^n, \|\underline{x}\|_{\mathbb{C}^n} = 1\}$), a theorem by Kato [88] relating $W(A)$ and $W(f(A))$ for analytic functions f on closed domains conformally equivalent to $\overline{D}$ (the closure of the open unit disk $D \in \mathbb{C}$), applied to $\ln(z; \eta)$ for $z \in \mathbb{C}_+$, yields

$$W(\ln(M(z); \eta)) \subset \{\zeta \in \mathbb{C}_+ \,|\, 0 \leq \mathrm{Im}(\zeta) \leq \pi\}, \quad z \in \mathbb{C}_+, \tag{5.35}$$

that is,

$$0 \leq \mathrm{Im}(\ln(M(z); \eta)) \leq \pi I_n, \quad z \in \mathbb{C}_+. \tag{5.36}$$

Continuity of $\ln(A; \eta)$ with respect to η, $\lim_{\eta \downarrow 0} \ln(A; \eta) = \ln(A)$, for $A \in M_n(\mathbb{C})$ nonsingular, then yields

$$0 \leq \mathrm{Im}(\ln(M(z))) \leq \pi I_n, \quad z \in \mathbb{C}_+ \tag{5.37}$$

and one can apply part (ii) (as in Theorem 2.3). $\square$

Finally we state the matrix analogs of Lemmas 2.5 and 2.6, the proofs of which we omit since they are essentially identical to the scalar case.

Lemma 5.6. *Let* M *be a Herglotz matrix with representation* (5.14) *and* $(\lambda_1, \lambda_2) \subseteq \mathbb{R}$, $\lambda_1 < \lambda_2$. *Then* M *can be analytically continued from* $\mathbb{C}_+$ *into a subset of* $\mathbb{C}_-$ *through the interval* (λ_1, λ_2) *if and only if the associated measure* Ω *is purely absolutely continuous on* (λ_1, λ_2), $\omega\big|_{(\lambda_1, \lambda_2)} = \Omega\big|_{(\lambda_1, \lambda_2), ac}$, *and the density* $\Omega' \geq 0$

of Ω is real-analytic on (λ_1, λ_2). In this case, the analytic continuation of M into some domain $\mathcal{D}_- \subseteq \mathbb{C}_-$ is given by

$$M(z) = M(\overline{z})^* + 2\pi i \Omega'(z), \quad z \in \mathcal{D}_-, \tag{5.38}$$

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 and only if Ω has no support in (λ_1, λ_2).

Lemma 5.7 ([96]). *Let M be a Herglotz matrix and $(\lambda_1, \lambda_2) \subseteq \mathbb{R}$, $\lambda_1 < \lambda_2$. Suppose $\lim_{\varepsilon \to 0} \mathrm{Re}(M(\lambda + i\varepsilon)) = 0$ for a.e. $\lambda \in (\lambda_1, \lambda_2)$. Then M can be analytically continued from $\mathbb{C}_+$ into $\mathbb{C}_-$ through the interval (λ_1, λ_2) and*

$$M(z) = -M(\overline{z})^*. \tag{5.39}$$

In addition, $\mathrm{Im}(M(\lambda + i0)) > 0$, $\mathrm{Re}(M(\lambda + i0)) = 0$ *for all* $\lambda \in (\lambda_1, \lambda_2)$.

6. Support Theorems in the Matrix Case

The principal aim of this section is to prove a support theorem for Ω_{ac} in connection with the matrix analog of the Aronszajn-Donoghue theory (cf. Theorem 3.2(i),(ii)).

Supports S_Ω, topological supports S_Ω^{cl}, and minimal supports (with respect to Lebesgue measure on $\mathbb{R}$) of matrix-valued measures such as Ω in (5.3), (5.3) are defined as in the beginning of Section 3. Because of (5.5), in discussing supports of the matrix measure Ω, we will occasionally replace Ω by the (scalar) trace measure $\omega^{tr} = \mathrm{tr}_{\mathbb{C}^n}(\Omega)$. For pure point measures, $\Omega = \Omega_{pp}$, we again consider the smallest support. If a pure point measure $\Omega = \Omega_{pp}$ contains no finite accumulation points in its support we call it a discrete point measure and denote it by Ω_d.

In order to capture spectral multiplicities in the matrix-valued case in connection with applications to differential and difference operators we introduce the sets ($1 \leq r \leq n$)

$$S_{\Omega_{ac},r} = \{\lambda \in \mathbb{R} \,|\, \lim_{\varepsilon \downarrow 0} M(\lambda + i\varepsilon) \text{ exists finitely}, \operatorname{rank}(\mathrm{Im}(M(\lambda + i0))) = r\}, \tag{6.1}$$

$$S_{\Omega_{ac}} = \bigcup_{r=1}^{n} S_{\Omega_{ac},r}, \tag{6.2}$$

$$S_{\Omega_{pp},r} = \{\lambda \in \mathbb{R} \,|\, \operatorname{rank}(\lim_{\varepsilon \downarrow 0} \varepsilon M(\lambda + i\varepsilon)) = r\}, \quad 1 \leq r \leq n, \tag{6.3}$$

$$S_{\Omega_{pp}} = \bigcup_{r=1}^{n} S_{\Omega_{pp},r}, \tag{6.4}$$

$$S_{\Omega_s} = \{\lambda \in \mathbb{R} \,|\, \lim_{\varepsilon \downarrow 0} \mathrm{Im}(\mathrm{tr}_{\mathbb{C}^n}(M(\lambda + i\varepsilon))) = +\infty\}, \tag{6.5}$$

$$S_{\Omega_{sc}} = \{\lambda \in S_{\Omega_s} \,|\, \lim_{\varepsilon \downarrow 0} \varepsilon \, \mathrm{tr}_{\mathbb{C}^n}(M(\lambda + i\varepsilon)) = 0\}, \tag{6.6}$$

$$S_\Omega = S_{\Omega_{ac}} \cup S_{\Omega_s}. \tag{6.7}$$

(Here existence of matrix limits are of course understood for each individual matrix element.) Thus, $S_{\Omega_{ac},r}$, $S_{\Omega_{pp},r'}$, $S_{\Omega_{sc}}$ are all disjoint for any $1 \leq r, r' \leq n$.

As in (3.9) we define the equivalence classes $\mathcal{E}(\Omega_{ac})$ and $\mathcal{E}_r(\Omega_{ac})$ of $S_{\Omega_{ac}}$ and $S_{\Omega_{ac},r}$, $1 \leq r \leq n$ with respect to the equivalence relation (3.1) (with ν representing Lebesgue measure on $\mathbb{R}$ and $\mu = \Omega_{ac}$).

The following result is analogous to Theorem 3.1 in the scalar case and can be reduced to it by studying the trace measure ω^{tr} of Ω.

Theorem 6.1. *Let M be a matrix-valued Herglotz function with representations* (5.14) *and* (5.32)*. Then*
(i). $S_{\Omega_{ac}}$ is a minimal support of Ω_{ac}.
(ii). $S_{\Omega_{sc}}$ is a minimal support of Ω_{sc}.
(iii). $S_{\Omega_{pp}}$ is the smallest support of Ω_{pp}.
(iv). S_{Ω} is a minimal support of Ω.
(v). If in addition $M(z)$ is invertible for all $z \in \mathbb{C}_+$, then

$$\widetilde{S}_{ac} = \{\lambda \in S_{\Omega_{ac}} \mid \ln(M(\lambda + i0)) \text{ exists finitely and } 0 < \operatorname{tr}(\Xi(\lambda)) < n\} \tag{6.8}$$

is a minimal support of Ω_{ac}.

Proof of (v). By definition, $\widetilde{S}_{ac} \backslash S_{\Omega_{ac}} = \emptyset$. Next, suppose $\operatorname{tr}(\Xi(\lambda))$ equals 0 or n. Then one concludes from $0 \leq \Xi(\lambda) \leq I_n$ for a.e. $\lambda \in \mathbb{R}$ (cf. Theorem 5.4 (iii)) that $\operatorname{Im}(\ln(M(\lambda + i0))) = 0$ or $\operatorname{Im}(\ln(-M(\lambda + i0))) = 0$, that is, $\ln(M(\lambda + i0))$ or $\ln(-M(\lambda + i0))$ is self-adjoint. Taking exponentials, $M(\lambda + i0)$ is self-adjoint and hence

$$\operatorname{Im}(M(\lambda + i0)) = 0 \text{ for } \lambda \in \{\nu \in \mathbb{R} \,|\, \operatorname{tr}(\Xi(\nu)) \in \{0, n\}\}. \tag{6.9}$$

Thus, abbreviating Lebesgue measure on $\mathbb{R}$ by $|\cdot|$, one infers

$$\begin{aligned}
|S_{\Omega_{ac}} \backslash \widetilde{S}_{ac}| &= |\{\lambda \in S_{\Omega_{ac}} \,|\, \text{either } \operatorname{Im}(\ln(M(\lambda + i0))_{j,j}) \text{ does not exist finitely} \\
&\qquad \text{for some } 1 \leq j \leq n, \text{ or } \operatorname{tr}(\Xi(\lambda)) \in \{0, n\}\}| \\
&= |\{\lambda \in S_{\Omega_{ac}} \,|\, \operatorname{Im}(\ln(M(\lambda + i0))_{j,j}) \text{ does not exist finitely for some } 1 \leq j \leq n\}| \\
&= 0
\end{aligned} \tag{6.10}$$

by (6.9), the fact that $\lambda \in S_{\Omega_{ac}}$ implies $\operatorname{Im}(M(\lambda + i0)) > 0$, and Theorem 5.4 (ii) (applied to $\ln(M(z))$). Thus, $|\widetilde{S}_{ac} \triangle S_{\Omega_{ac}}| = 0$ and since Ω_{ac} is absolutely continuous with respect to Lebesgue measure $|\cdot|$, also $\Omega_{ac}(\widetilde{S}_{ac} \triangle S_{\Omega_{ac}}) = 0$. Consequently, $\widetilde{S}_{ac}$ and $S_{\Omega_{ac}}$ are equivalent minimal supports for Ω_{ac}, $\widetilde{S}_{ac} \sim S_{\Omega_{ac}}$. □

In order to prove the analog of Theorem 3.2(i) in the matrix-valued case, that is, the stability of the minimal support $S_{\Omega_{ac}}$ with respect to linear fractional transformations (generalizing (2.11) to the matrix case as in (6.22)), we need to introduce a bit of preparatory material.

Define

$$J_{2n} = \begin{pmatrix} 0 & -I_n \\ I_n & 0 \end{pmatrix}, \tag{6.11}$$

$$\mathcal{A}_{2n} = \{A \in M_{2n}(\mathbb{C}) \,|\, A^* J_{2n} A = J_{2n}\}. \tag{6.12}$$

Representing $A \in M_{2n}(\mathbb{C})$ by

$$A = \begin{pmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{pmatrix}, \quad A_{p,q} \in M_n(\mathbb{C}), \quad 1 \leq p, q \leq 2, \tag{6.13}$$

the condition $A^* J_{2n} A = J_{2n}$ in (6.12) explicitly reads

$$\begin{aligned}
&A_{1,1}^* A_{2,1} = A_{2,1}^* A_{1,1}, \quad A_{2,2}^* A_{1,2} = A_{1,2}^* A_{2,2}, \\
&A_{2,2}^* A_{1,1} - A_{1,2}^* A_{2,1} = I_n = A_{1,1}^* A_{2,2} - A_{2,1}^* A_{1,2},
\end{aligned} \tag{6.14}$$

or equivalently,

$$\begin{pmatrix} A_{2,2}^* & -A_{1,2}^* \\ -A_{2,1}^* & A_{1,1}^* \end{pmatrix} \begin{pmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{pmatrix} = I_{2n}. \tag{6.15}$$

Since left inverses in $M_{2n}(\mathbb{C})$ are also right inverses, (6.15) implies

$$\begin{pmatrix} A_{1,1} & A_{1,2} \\ A_{2,1} & A_{2,2} \end{pmatrix} \begin{pmatrix} A_{2,2}^* & -A_{1,2}^* \\ -A_{2,1}^* & A_{1,1}^* \end{pmatrix} = I_{2n}, \tag{6.16}$$

that is,

$$\begin{aligned} &A_{1,1}A_{1,2}^* = A_{1,2}A_{1,1}^*, \quad A_{2,2}A_{2,1}^* = A_{2,1}A_{2,2}^*, \\ &A_{2,2}A_{1,1}^* - A_{2,1}A_{1,2}^* = I_n = A_{1,1}A_{2,2}^* - A_{1,2}A_{2,1}^*, \end{aligned} \tag{6.17}$$

or equivalently,

$$AJ_{2n}A^* = J_{2n}. \tag{6.18}$$

In particular,

$$A \in \mathcal{A}_{2n} \text{ if and only if } A^{-1} \in \mathcal{A}_{2n}. \tag{6.19}$$

Next, let $A = (A_{p,q})_{1\le p,q\le 2} \in \mathcal{A}_{2n}$ and suppose $M \in M_n(\mathbb{C})$ is chosen such that $\ker(A_{1,1} + A_{1,2}M) = \{0\}$, that is $(A_{1,1} + A_{1,2}M)$ is invertible in $\mathbb{C}^n$. Define (cf., e.g., [102])

$$M_A(M) = (A_{2,1} + A_{2,2}M)(A_{1,1} + A_{1,2}M)^{-1} \tag{6.20}$$

to observe

$$\begin{aligned} M_{I_{2n}}(M) &= M, \\ M_A(M_B(M)) &= M_{AB}(M), \\ M_A(M) &= M_{AB^{-1}}(M_B(M)), \end{aligned} \tag{6.21}$$

whenever $M_A(M)$ and $M_B(M)$ exist.

We are particularly interested in the case where M in (6.20) equals an $n \times n$ Herglotz matrix $M(z)$. In this case the existence of $(A_{1,1} + A_{1,2}M(z_0))^{-1}$ for some $z_0 \in \mathbb{C}_+$ and analyticity of $M(z)$ on $\mathbb{C}_+$ proves that $(A_{1,1} + A_{1,2}M(z))^{-1}$ is meromorphic on $\mathbb{C}_+$. However, since later on we are interested in analyticity of $M_A(M(z))$ for all $z \in \mathbb{C}_+$, we will usually assume that $\ker(A_{1,1} + A_{1,2}M(z)) = \{0\}$ for all $z \in \mathbb{C}_+$. Moreover, in a slight abuse of notation, we shall abbreviate $M_A(M(z))$ by

$$M_A(z) = (A_{2,1} + A_{2,2}M(z))(A_{1,1} + A_{1,2}M(z))^{-1}, \quad A \in \mathcal{A}_{2n}, \quad z \in \mathbb{C}_+ \tag{6.22}$$

from now on.

We start with a series of results concerning linear fractional transformations of the type (6.22).

Lemma 6.2. *Suppose* $A = (A_{p,q})_{1\le p,q\le 2} \in \mathcal{A}_{2n}$ *and* $M \in M_n(\mathbb{C})$ *with* $\mathrm{Im}(M) \ge 0$. *Then*

$$\ker(A_{1,1} + A_{1,2}M) \subseteq \ker(\mathrm{Im}(M)). \tag{6.23}$$

In particular,

$$\mathrm{Im}(M) > 0 \text{ implies } \ker(A_{1,1} + A_{1,2}M) = \{0\}. \tag{6.24}$$

Proof. Suppose the existence of an $\underline{x}_0 \in \mathbb{C}^n\backslash\{0\}$ such that

$$(A_{1,1} + A_{1,2}M)\underline{x}_0 = 0. \tag{6.25}$$

Then

$$\begin{aligned}
&(\underline{x}_0, \mathrm{Im}(M)\underline{x}_0)_{\mathbb{C}^n} = (2i)^{-1}\big((\underline{x}_0, M\underline{x}_0)_{\mathbb{C}^n} - (M\underline{x}_0, \underline{x}_0)_{\mathbb{C}^n}\big) \\
&= (2i)^{-1}\big((\underline{x}_0, (A_{1,1}^*A_{2,2} - A_{2,1}^*A_{1,2})M\underline{x}_0)_{\mathbb{C}^n} - ((A_{1,1}^*A_{2,2} - A_{2,1}^*A_{1,2})M\underline{x}_0, \underline{x}_0)_{\mathbb{C}^n}\big) \\
&= (2i)^{-1}\big((A_{1,1}\underline{x}_0, A_{2,2}M\underline{x}_0)_{\mathbb{C}^n} + (\underline{x}_0, A_{2,1}^*A_{1,1}\underline{x}_0)_{\mathbb{C}^n} - (A_{2,2}M\underline{x}_0, A_{1,1}\underline{x}_0)_{\mathbb{C}^n} \\
&\qquad - (\underline{x}_0, A_{1,1}^*A_{2,1}\underline{x}_0)_{\mathbb{C}^n}\big) \\
&= (2i)^{-1}\big(-(A_{1,2}M\underline{x}_0, A_{2,2}M\underline{x}_0)_{\mathbb{C}^n} + (A_{2,2}M\underline{x}_0, A_{1,2}M\underline{x}_0)_{\mathbb{C}^n}\big) \\
&= (2i)^{-1}(M\underline{x}_0, (A_{2,2}^*A_{1,2} - A_{1,2}^*A_{2,2})M\underline{x}_0)_{\mathbb{C}^n} = 0,
\end{aligned} \tag{6.26}$$

where we repeatedly used (6.14) and (6.25). Since $\mathrm{Im}(M) \geq 0$ by hypothesis, (6.26) yields $\mathrm{Im}(M)\underline{x}_0 = 0$ and hence (6.23). ☐

Lemma 6.3. *Suppose* $A = (A_{p,q})_{1\leq p,q\leq 2} \in \mathcal{A}_{2n}$, $M \in M_n(\mathbb{C})$, *and* $\ker(A_{1,1} + A_{1,2}M) = \{0\}$. *Define*

$$M_A = (A_{2,1} + A_{2,2}M)(A_{1,1} + A_{1,2}M)^{-1}. \tag{6.27}$$

Then
(i).

$$\mathrm{Im}(M_A) = ((A_{1,1} + A_{1,2}M)^{-1})^*\mathrm{Im}(M)(A_{1,1} + A_{1,2}M)^{-1}. \tag{6.28}$$

(ii).

$$(A_{2,2}^* - A_{1,2}^*M_A)(A_{1,1} + A_{1,2}M) = I_n, \tag{6.29}$$

$$\ker(A_{2,2}^* - A_{1,2}^*M_A) = \{0\}. \tag{6.30}$$

(iii).

$$M = -(A_{2,1}^* - A_{1,1}^*M_A)(A_{2,2}^* - A_{1,2}^*M_A)^{-1}, \tag{6.31}$$

$$\mathrm{Im}(M) = ((A_{2,2}^* - A_{1,2}^*M_A)^{-1})^*\mathrm{Im}(M_A)(A_{2,2}^* - A_{1,2}^*M_A)^{-1}. \tag{6.32}$$

Proof. (i) is a straightforward consequence of (6.27) and (6.14). (6.29) is a simple consequence of (6.27) and (6.30) follows from (6.29). (iii) is readily derived from (6.14) and (6.27). ☐

Applying Lemmas 6.2 and 6.3 to $M_A(z)$ in (6.22) then yields the following result.

Theorem 6.4. *Assume* $A = (A_{p,q})_{1\leq p,q\leq 2} \in \mathcal{A}_{2n}$, *let* $M(z)$ *be an* $n\times n$ *Herglotz matrix, and suppose* $\ker(A_{1,1} + A_{1,2}M(z)) = \{0\}$ *for all* $z \in \mathbb{C}_+$. *Define* $M_A(z)$, $z \in \mathbb{C}_+$ *as in* (6.22). *Then*
(i). $M_A(z)$ *is an* $n\times n$ *Herglotz matrix and*

$$\mathrm{Im}(M_A(z)) = ((A_{1,1} + A_{1,2}M(z))^{-1})^*\mathrm{Im}(M(z))(A_{1,1} + A_{1,2}M(z))^{-1} \geq 0, \quad z \in \mathbb{C}_+. \tag{6.33}$$

(ii). For all $z \in \mathbb{C}_+$,

$$(A_{2,2}^* - A_{1,2}^*M_A(z))(A_{1,1} + A_{1,2}M(z)) = I_n, \tag{6.34}$$

$$\ker(A_{2,2}^* - A_{1,2}^*M_A(z)) = \{0\}, \tag{6.35}$$

$$M(z) = -(A_{2,1}^* - A_{1,1}^*M_A(z))(A_{2,2}^* - A_{1,2}^*M_A(z))^{-1}, \tag{6.36}$$

$$\operatorname{Im}(M(z)) = ((A_{2,2}^* - A_{1,2}^* M_A(z))^{-1})^* \operatorname{Im}(M_A(z))(A_{2,2}^* - A_{1,2}^* M_A(z))^{-1}. \quad (6.37)$$

Proof. Assertions (6.33)–(6.37) are clear from Lemmas 6.2 and 6.3. Since $M(z)^* = M(\overline{z})$ clearly implies $M_A(z)^* = M_A(\overline{z})$ by (6.14), $M_A(z)$ is an $n \times n$ Herglotz matrix. □

We note in connection with Lemma 5.3 and Theorem 6.4 that

$$\begin{aligned} &\operatorname{Im}(M(z_0)) > 0 \text{ for some } z_0 \in \mathbb{C}_+ \\ &\text{implies } \ker(A_{1,1} + A_{1,2}M(z)) = \{0\} \text{ for all } z \in \mathbb{C}_+ \end{aligned} \quad (6.38)$$

by (6.24).

Remark 6.5. The condition $A \in \mathcal{A}_{2n}$ in the definition (6.22) of $M_A(z)$ for $M_A(z)$ to be a Herglotz matrix (assuming $M(z)$ to be a Herglotz matrix) is not a necessary one. As discussed in detail by Krein and Shmulyan [102], the condition $A \in \mathcal{A}_{2n}$ in Theorem 6.4 can be replaced by the pair of conditions

$$iA^* J_{2n} A \geq icJ_{2n}, \quad iAJ_{2n}A^* \geq icJ_{2n} \quad (6.39)$$

for some $c > 0$. In a sense, by using the condition $A \in \mathcal{A}_{2n}$, we chose equality in (6.39) (and $c = 1$). From the point of view of applications of matrix Herglotz functions to spectral theory of matrix Schrödinger and Jacobi operators and more generally, even-order Hamiltonian systems, with various boundary conditions involved, our restrictive hypothesis (6.12) is sufficiently general to cover all such cases. Pertinent references to spectral theory for even-order Hamiltonian systems are, for instance, [14], Ch. 9, [30], [75]–[80], [96]–[98], [99], Chs. 7, 8, [116], [120], [129]–[131] and the literature cited therein.

Finally, we turn to $\mathcal{E}(\Omega_{A,ac})$ and $\mathcal{E}_r(\Omega_{A,ac})$ the equivalence classes of $S_{\Omega_{A,ac}}$ and $S_{\Omega_{A,ac,r}}$, $1 \leq r \leq n$ associated with $M_A(z)$, $A \in \mathcal{A}_{2n}$ (cf. (3.1) and the paragraph following Theorem 6.1). We recall that $\mathcal{E}(\Omega_{ac})$ and $\mathcal{E}_r(\Omega_{ac})$ are the corresponding equivalence classes of $S_{\Omega_{ac}}$ and $S_{\Omega_{ac},r}$, $1 \leq r \leq n$ associated with $M(z)$ (cf. (6.1), (6.2)). We also recall (cf. (6.22))

$$M_A(z) = (A_{2,1} + A_{2,2}M(z))(A_{1,1} + A_{1,2}M(z))^{-1}, \quad A \in \mathcal{A}_{2n},\ z \in \mathbb{C}_+ \quad (6.40)$$

and its general version

$$\begin{aligned} M_A(z) = ((AB^{-1})_{2,1} + (AB^{-1})_{2,2}M_B(z))((AB^{-1})_{1,1} + (AB^{-1})_{1,2}M_B(z))^{-1}&, \\ A, B \in \mathcal{A}_{2n},\ z \in \mathbb{C}_+&. \quad (6.41) \end{aligned}$$

Our principal result on the absolutely continuous part of Ω_A, the matrix analog of Theorem 3.2 (i)–(iii), then reads as follows.

Theorem 6.6. *Let $M(z)$ and $M_A(z)$, $A = (A_{p,q})_{1 \leq p,q \leq 2} \in \mathcal{A}_{2n}$ be Herglotz matrices related by* (6.40) *assuming* $\ker(A_{1,1} + A_{1,2}M(z)) = \{0\}$ *for all $z \in \mathbb{C}_+$. Let Ω and Ω_A be the measures associated with $M(z)$ and $M_A(z)$, respectively. Then*
(i). For all $A \in \mathcal{A}_{2n}$,

$$\mathcal{E}_r(\Omega_{A,ac}) = \mathcal{E}_r(\Omega_{ac}), \quad 1 \leq r \leq n, \quad (6.42)$$

$$\mathcal{E}(\Omega_{A,ac}) = \mathcal{E}(\Omega_{ac}), \quad (6.43)$$

that is, $\mathcal{E}_r(\Omega_{A,ac})$, $1 \leq r \leq n$ and $\mathcal{E}(\Omega_{A,ac})$ are independent of $A \in \mathcal{A}_{2n}$ (and hence denoted by $\mathcal{E}_{ac,r}$, $1 \leq r \leq n$ and $\mathcal{E}_{ac}$ below) and $\Omega_{A,ac} \sim \Omega_{ac}$ for all $A \in \mathcal{A}_{2n}$.
(ii). Suppose Ω_B is a discrete point measure, $\Omega_B = \Omega_{B,d}$, for some $B \in \mathcal{A}_{2n}$. Then $\Omega_A = \Omega_{A,d}$ is a discrete point measure for all $A \in \mathcal{A}_{2n}$.

(iii). Define

$$S = \{\lambda \in \mathbb{R} \,|\, \textit{there is no } A \in \mathcal{A}_{2n} \textit{ for which } \mathrm{Im}(M_A(\lambda + i0)) \textit{ exists and equals } 0\}. \tag{6.44}$$

Then $S \in \mathcal{E}_{ac}$.

Proof. (i). Define

$$\widehat{S}_{A,r} = S_{\Omega_{A,ac,r}} \cap \{\lambda \in \mathbb{R} \,|\, M(\lambda + i0) \text{ exists finitely}\}. \tag{6.45}$$

Then Theorem 5.4(ii) yields

$$|S_{\Omega_{A,ac,r}} \backslash \widehat{S}_{A,r}| = 0, \tag{6.46}$$

where $|\cdot|$ abbreviates Lebesgue measure on $\mathbb{R}$. Since by (6.34),

$$(A_{1,1} + A_{1,2}M(\lambda + i0))^{-1} = A_{2,2}^* - A_{1,2}^* M_A(\lambda + i0) \text{ exists for } \lambda \in \widehat{S}_{A,r}, \tag{6.47}$$

$(A_{1,1} + A_{1,2}M(\lambda + i0))^{-1} : \mathbb{C}^n \to \mathbb{C}^n$ is a bijection for $\lambda \in \widehat{S}_{A,r}$ and (6.33) yields

$$\begin{aligned} &\mathrm{Im}(M_A(\lambda + i0)) \\ &\quad = ((A_{1,1} + A_{1,2}M(\lambda + i0))^{-1})^* \mathrm{Im}(M(\lambda + i0))(A_{1,1} + A_{1,2}M(\lambda + i0))^{-1}, \\ &\qquad\qquad \lambda \in \widehat{S}_{A,r} \end{aligned} \tag{6.48}$$

and hence

$$\mathrm{rank}(\mathrm{Im}(M_A(\lambda + i0))) = \mathrm{rank}(\mathrm{Im}(M(\lambda + i0))), \quad \lambda \in \widehat{S}_{A,r}. \tag{6.49}$$

Thus,

$$\widehat{S}_{A,r} \subseteq S_{\Omega_{ac},r}. \tag{6.50}$$

Similarly, defining

$$\widehat{S}_r = S_{\Omega_{ac},r} \cap \{\lambda \in \mathbb{R} \,|\, M_A(\lambda + i0) \text{ exists finitely}\}, \tag{6.51}$$

then

$$|S_{\Omega_{ac},r} \backslash \widehat{S}_r| = 0. \tag{6.52}$$

By (6.34) we conclude the existence of

$$(A_{2,2}^* - A_{1,2}^* M_A(\lambda + i0))^{-1} = (A_{1,1} + A_{1,2}M(\lambda + i0)), \quad \lambda \in \widehat{S}_r \tag{6.53}$$

and hence $(A_{2,2}^* - A_{1,2}^* M_A(\lambda + i0))^{-1} : \mathbb{C}^n \to \mathbb{C}^n$ is a bijection for $\lambda \in \widehat{S}_r$. Thus (6.37) yields

$$\begin{aligned} &\mathrm{Im}(M(\lambda + i0)) \\ &\quad = ((A_{2,2}^* - A_{1,2}^* M_A(\lambda + i0))^{-1})^* \mathrm{Im}(M_A(\lambda + i0))(A_{2,2}^* - A_{1,2}^* M_A(\lambda + i0))^{-1}, \\ &\qquad\qquad \lambda \in \widehat{S}_r \end{aligned} \tag{6.54}$$

and consequently,

$$\mathrm{rank}(\mathrm{Im}(M(\lambda + i0))) = \mathrm{rank}(\mathrm{Im}(M_A(\lambda + i0))), \quad \lambda \in \widehat{S}_r. \tag{6.55}$$

Thus,

$$\widehat{S}_r \subseteq S_{\Omega_{A,ac},r}. \tag{6.56}$$

By (6.46), (6.50), (6.52), and (6.56),

$$|S_{\Omega_{A,ac},r} \triangle S_{\Omega_{ac},r}| = 0. \tag{6.57}$$

Since $\Omega_{A,ac}$ and Ω_{ac} are absolutely continuous with respect to Lebesgue measure on $\mathbb{R}$, (6.57) yields

$$\Omega_{A,ac}(S_{\Omega_{A,ac},r}\triangle S_{\Omega_{ac},r}) = \Omega_{ac}(S_{\Omega_{A,ac},r}\triangle S_{\Omega_{ac},r}) = 0 \tag{6.58}$$

proving (6.42). Equality (6.43) is then obvious from (6.42) and (6.2).

(ii). Part (ii) follows from (6.41) (cf. (6.21)) and the fact that $\Omega_A = \Omega_{A,d}$ if and only if $M_A(z)$ is meromorphic on $\mathbb{C}$.

(iii). We follow the proof of Corollary 1 in [64] in the scalar case $n = 1$. Since by hypothesis $\mathrm{Im}(M(\lambda + i0)) > 0$ for all $\lambda \in S_{\Omega_{ac}}$ one concludes from (6.23) that $\ker(A_{1,1} + A_{1,2}M(\lambda+i0)) = \ker(\mathrm{Im}(M(\lambda+i0))) = \{0\}$ and hence $\mathrm{Im}(M_A(\lambda+i0)) > 0$ for a.e. $\lambda \in S_{\Omega_{ac}}$ and all $A \in \mathcal{A}_{2n}$ by (6.33). Thus, one computes

$$|S_{\Omega_{ac}}\backslash S| = |\{\lambda \in S_{\Omega_{ac}} \,|\, \text{there is an } A_\lambda \in \mathcal{A}_{2n} \text{ s.t. } \mathrm{Im}(M_{A_\lambda}(\lambda + i0)) = 0\}| = 0. \tag{6.59}$$

Similarly,

$$\begin{aligned} |S\backslash S_{\Omega_{ac}}| = |\{\lambda \in \mathbb{R} \,|\, &\text{there is no } A \in \mathcal{A}_{2n} \text{ s.t. } \mathrm{Im}(M_A(\lambda + i0)) = 0 \text{ exists}\\ &\text{and either } M(\lambda + i0) \text{ does not exist, or } M(\lambda + i0)_{j,j} \text{ exists}\\ &\text{and equals } \infty \text{ for some } 1 \le j \le n\}|\\ \le |\{\lambda \in \mathbb{R} \,|\, &\text{either } M(\lambda + i0) \text{ does not exist, or } M(\lambda + i0)_{j,j} \text{ exists}\\ &\text{and equals } \infty \text{ for some } 1 \le j \le n\}| = 0 \end{aligned} \tag{6.60}$$

by Theorem 5.4 (ii). Thus $|S_{\Omega_{ac}}\triangle S| = 0$. Since $\Omega_{ac} \ll |\cdot|$, one infers $\Omega_{ac}(S_{\Omega_{ac}}\triangle S) = 0$ and hence $S \sim S_{\Omega_{ac}}$, or equivalently, $S \in \mathcal{E}_{ac}$. ☐

Remark 6.7. One might ask whether the first part of Theorem 3.2 (iv) extends to the matrix-valued situation. However, the simple counter example

$$M_1(z) = \begin{pmatrix} m(z) & 0 \\ 0 & -m(z)^{-1} \end{pmatrix}, \quad M_2(z) = -M_1(z)^{-1} = \begin{pmatrix} -m(z)^{-1} & 0 \\ 0 & m(z) \end{pmatrix}, \tag{6.61}$$

with $m(z)$ a scalar Herglotz function with representation (2.15) and $\omega_{pp} \neq 0$ or $\omega_{sc} \neq 0$, immediately destroys such hopes since the measures Ω_1 and Ω_2 corresponding to $M_1(z)$ and $M_2(z)$ are clearly equivalent.

Remark 6.8. Theorem 6.6(i) is quite familiar in the context of finite-rank perturbations of the resolvent of a self-adjoint operator in a (complex, separable) Hilbert space. For instance, the absolutely continuous (ac) parts of self-adjoint extensions of a densely defined symmetric operator with deficiency indices (n, n) are all unitarily equivalent. In particular, their absolutely continuous spectra and the multiplicity functions (associated with the ac spectra) coincide, which is essentially (6.42) and (6.43). However, even-order Hamiltonian systems do not necessarily have such an underlying Hilbert space formulation (cf., e.g., [75]–[80], [97], [98], [120] and the literature cited therein) and in these cases Theorem 6.6(i) appears to be an ideal tool for identifying ac spectra associated with Ω_A.

As in the scalar case, the relationship between $\mathrm{Im}(\ln(M_A(z)))$ (respectively, $\Xi_A(\lambda)$) and $\mathrm{Im}(\ln(M(z)))$ (respectively, $\Xi(\lambda)$), analogous to (6.40), in general, is quite involved. The special case $A = J_{2n}$, that is,

$$M_A(z) = -M(z)^{-1}, \tag{6.62}$$

however, is particularly simple and leads to the analog of (3.25),

$$\Xi_{J_{2n}}(\lambda) = I_n - \Xi(\lambda) \text{ for a.e. } \lambda \in \mathbb{R}. \tag{6.63}$$

The analog of Lemma 3.3 in the present matrix-valued context appears to be more involved.

7. Applications of Matrix-Valued Herglotz Functions

In this section we extend some of the applications of scalar Herglotz functions in Section 4 to the matrix-valued context. In particular, we will study self-adjoint finite-rank perturbations of self-adjoint operators, Friedrichs and Krein extensions of densely defined symmetric operators bounded from below with finite deficiency indices, and a class of Hamiltonian systems on a half-line. Throughout this section we closely follow the setup in Section 4. In particular, we omit proofs whenever they parallel the corresponding scalar situation and focus on those arguments which require new elements when compared to Section 4.

Before we enter a discussion of these three cases, we briefly digress into the definition of L^2-spaces with underlying matrix-valued measures (see, e.g., [46], Sect. XIII.5, [119], Ch. VI). Suppose $\Omega = (\Omega_{j,k})_{1\leq j,k\leq n}$ generates a matrix-valued measure on an interval $\Lambda \subseteq \mathbb{R}$ as in (5.3)–(5.6) with $\omega^{tr} = \sum_{j=1}^n \Omega_{j,j}$, the corresponding scalar trace measure. Let $\underline{\hat f} = (\hat f_1, \dots, \hat f_n)^t \in C_0(\Lambda)^n$, where "t" abbreviates transpose and $C_0(\Lambda)$ denotes the set of complex-valued continuous functions of compact support contained in Λ. On $C_0(\Lambda)^n$ we define the inner product,

$$(\underline{\hat f}, \underline{\hat g})_0 = \sum_{j,k=1}^n \int_\Lambda d\Omega_{j,k}(\lambda) \hat f_j(\lambda) \hat g_k(\lambda), \quad \underline{\hat f}, \underline{\hat g} \in C_0(\Lambda)^n. \tag{7.1}$$

The Hilbert space $L^2(\Lambda; d\Omega)$ is then defined as the completion of $C_0(\Lambda)^n$ with respect to the norm $\|\cdot\|_0$ induced by (7.1). A perhaps more useful, though equivalent, characterization of $L^2(\Lambda; d\Omega)$ can be obtained as follows. Introduce the density matrix ρ,

$$\rho(\lambda) = \big(\rho_{j,k}(\lambda)\big)_{1\leq j,k\leq n}, \quad \rho_{j,k}(\lambda) = \frac{d\Omega_{j,k}}{d\omega^{tr}}(\lambda), \quad j,k = 1, \dots, n. \tag{7.2}$$

Consider all complex-valued $\hat f_j : \Lambda \to \mathbb{C}$ such that $\sum_{j,k=1}^n \overline{\hat f_j(\lambda)} \rho_{j,k}(\lambda) \hat f_k(\lambda) \geq 0$ is ω^{tr} integrable over Λ and define $\widehat{\mathcal{H}}(\Lambda)$ as the set of equivalence classes $\underline{\hat f} = (\hat f_1, \dots, \hat f_n)^t$ modulo Ω-null functions. (Here $\underline{\hat g} = (\hat g_1, \dots, \hat g_n)^t$ is defined to be an Ω-null function if $\int_\Lambda d\omega^{tr}(\lambda)(\sum_{j,k=1}^n \overline{g_j(\lambda)} \rho_{j,k}(\lambda) g_k(\lambda)) = 0$.) This space is complete with respect to the norm induced by the scalar product

$$(\underline{\hat f}, \underline{\hat g})_{\widehat{\mathcal{H}}(\Lambda)} = \int_\Lambda d\omega^{tr}(\lambda) \bigg(\sum_{j,k=1}^n \overline{f_j(\lambda)} \rho_{j,k}(\lambda) g_k(\lambda) \bigg), \quad \underline{\hat f}, \underline{\hat g} \in \widehat{\mathcal{H}}(\Lambda) \tag{7.3}$$

and coincides with $L^2(\Lambda; d\Omega)$,

$$\widehat{\mathcal{H}}(\Lambda) = L^2(\Lambda; d\Omega). \tag{7.4}$$

Now we turn to self-adjoint finite-rank perturbations of self-adjoint operators. Let $\mathcal{H}$ be a separable complex Hilbert space with scalar product $(\cdot,\cdot)_{\mathcal{H}}$, H_0 a self-adjoint operator in $\mathcal{H}$ (which may or may not be bounded), and $\{f_1, \dots, f_n\} \subset \mathcal{H}$ an orthogonal generating basis for H_0 (i.e., $(f_j, f_k)_{\mathcal{H}} = \delta_{j,k}$, $j,k = 1, \dots, n$ and $\mathcal{H} =$

$\overline{\text{linspan}\{(H_0 - z)^{-1} f_j \in \mathcal{H} \,|\, j = 1, \dots, n,\, z \in \mathbb{C}\backslash\mathbb{R}\}} = \overline{\text{linspan}\{E_0(\lambda) f_j \in \mathcal{H} \,|\, j = 1, \dots, n,\, \lambda \in \mathbb{R}\}}$, $E_0(\cdot)$ the family of orthogonal spectral projections of H_0). Introducing the self-adjoint diagonal matrix

$$\alpha = \big(\alpha_j \delta_{j,k}\big)_{1 \le j,k \le n}, \quad \alpha_j \in \mathbb{R},\ j = 1, \dots, n, \tag{7.5}$$

we use the notation

$$\underline{c} = (c_1, \dots, c_n)^t \in \mathbb{C}^n, \quad \alpha \underline{c} = (\alpha_1 c_1, \dots, \alpha_n c_n)^t, \text{ etc.} \tag{7.6}$$

Moreover, we define

$$K : \mathbb{C}^n \to \mathcal{H}, \quad \underline{c} \to \sum_{j=1}^n c_j f_j, \tag{7.7}$$

$$K^* : \mathcal{H} \to \mathbb{C}^n, \quad f \to ((f_1, f)_{\mathcal{H}}, \dots, (f_n, f)_{\mathcal{H}})^t \tag{7.8}$$

and note that

$$K \alpha K^* = \sum_{j=1}^n \alpha_j (f_j, \cdot)_{\mathcal{H}} f_j. \tag{7.9}$$

After these preliminaries we can define the self-adjoint finite-rank perturbation of H_0 by

$$H_\alpha = H_0 + K \alpha K^* = H_0 + \sum_{j=1}^n \alpha_j (f_j, \cdot)_{\mathcal{H}} f_j, \tag{7.10}$$

with $\mathcal{D}(H_\alpha) = \mathcal{D}(H_0)$, $\alpha_j \in \mathbb{R}$, $j = 1, \dots, n$. Denoting by $E_\alpha(\lambda)$, $\lambda \in \mathbb{R}$ the family of orthogonal spectral projections of H_α one introduces

$$\begin{aligned} &\Omega_\alpha(\lambda) = \big(\Omega_{\alpha,j,k}(\lambda)\big)_{1 \le j,k \le n}, \quad d\Omega_{\alpha,j,k}(\lambda) = (f_j, dE_\alpha(\lambda) f_k)_{\mathcal{H}}, \\ &\int_{\mathbb{R}} d\Omega_{\alpha,j,k}(\lambda) = (f_j, f_k)_{\mathcal{H}} = \delta_{j,k}, \quad j,k = 1, \dots, n. \end{aligned} \tag{7.11}$$

By the canonical representation of self-adjoint operators with finite spectral multiplicity (cf., e.g., [119], Sect. 20), H_α in $\mathcal{H}$ is unitarily equivalent to $\widehat{H}_\alpha$ in $\widehat{\mathcal{H}}_\alpha = L^2(\mathbb{R}; d\Omega_\alpha)$, where

$$(\widehat{H}_\alpha \underline{\hat{g}})(\lambda) = \lambda \underline{\hat{g}}(\lambda), \quad \underline{\hat{g}} \in \mathcal{D}(\widehat{H}_\alpha) = L^2(\mathbb{R}; (1 + \lambda^2) d\Omega_\alpha), \tag{7.12}$$

$$H_\alpha = U_\alpha \widehat{H}_\alpha U_\alpha^{-1}, \quad \mathcal{H} = U_\alpha L^2(\mathbb{R}; d\Omega_\alpha), \tag{7.13}$$

with U_α unitary,

$$\begin{aligned} &U_\alpha : \widehat{\mathcal{H}}_\alpha = L^2(\mathbb{R}; d\Omega_\alpha) \to \mathcal{H}, \\ &\underline{\hat{g}} \to (U_\alpha \underline{\hat{g}}) = \operatorname*{s-lim}_{N \to \infty} \sum_{j=1}^n \int_{-N}^N d(E_\alpha(\lambda) f_j) \hat{g}_j(\lambda), \quad \underline{\hat{g}} = (\hat{g}_1, \dots, \hat{g}_n)^t \in L^2(\mathbb{R}; d\Omega). \end{aligned} \tag{7.14}$$

Moreover,

$$f_j = U_\alpha \underline{\hat{f}}_j, \quad \underline{\hat{f}}_j(\lambda) = (\delta_{j,1}, \dots, \delta_{j,n})^t, \quad \lambda \in \mathbb{R}. \tag{7.15}$$

The family of spectral projections $\widehat{E}_\alpha(\lambda)$, $\lambda \in \mathbb{R}$ of $\widehat{H}_\alpha$ is then given by

$$(\widehat{E}_\alpha(\lambda) \underline{\hat{g}})(\mu) = \theta(\lambda - \mu) \underline{\hat{g}}(\mu) \text{ for } \Omega_\alpha\text{–a.e. } \mu \in \mathbb{R},\ \underline{\hat{g}} \in L^2(\mathbb{R}; d\Omega_\alpha). \tag{7.16}$$

Introducing the matrix-valued Herglotz function

$$M_\alpha(z) = \big((\underline{e}_j, K^*(H_\alpha - z)^{-1} K \underline{e}_k)_{\mathbb{C}^n}\big)_{1 \le j,k \le n} = \big((f_j, (H_\alpha - z)^{-1} f_k)_{\mathcal{H}}\big)_{1 \le j,k \le n}$$

$$= \int_{\mathbb{R}} \frac{d\Omega_\alpha}{\lambda - z}, \quad z \in \mathbb{C}_+, \tag{7.17}$$

with

$$\underline{e}_j = (\delta_{j,1}, \dots, \delta_{j,n})^t \in \mathbb{C}^n, \quad j = 1, \dots, n, \tag{7.18}$$

one verifies

$$M_\beta(z) = M_\alpha(z)(I_n + (\beta - \alpha) M_\alpha(z))^{-1}, \tag{7.19}$$
$$\alpha = \big(\alpha_j \delta_{j,k}\big)_{1 \le j,k \le n}, \ \beta = \big(\beta_j \delta_{j,k}\big)_{1 \le j,k \le n}, \ \alpha_j, \beta_j \in \mathbb{R}, \ j = 1, \dots, n.$$

A comparison of (7.19) and (6.40) suggests the introduction of

$$A(\alpha, \beta) = \begin{pmatrix} I_n & \beta - \alpha \\ 0 & I_n \end{pmatrix} \in \mathcal{A}_{2n}, \tag{7.20}$$
$$\alpha = \big(\alpha_j \delta_{j,k}\big)_{1 \le j,k \le n}, \ \beta = \big(\beta_j \delta_{j,k}\big)_{1 \le j,k \le n}, \ \alpha_j, \beta_j \in \mathbb{R}, \ j = 1, \dots, n.$$

In particular, Theorem 6.6 applies (with $A_{1,1}(\alpha,\beta) = A_{2,2}(\alpha,\beta) = I_n$, $A_{1,2}(\alpha,\beta) = \beta - \alpha$, $A_{2,1}(\alpha,\beta) = 0$).

If $\{f_1, \dots, f_n\}$ is not a generating basis for H_0, then $\mathcal{H}$ decomposes into $\mathcal{H} = \mathcal{H}^n \oplus \mathcal{H}^{n,\perp}$, with $\mathcal{H}^n = \overline{\operatorname{linspan}\{(H_0 - z)^{-1} f_j \,|\, z \in \mathbb{C}, \, j = 1, \dots, n\}}$ separable and $\mathcal{H}^n$, $\mathcal{H}^{n,\perp}$ reducing subspaces for all H_α. The part H_α^n of H_α in $\mathcal{H}^n$ then plays the role analogous to H_α^1 in the context of (4.11)–(4.16).

Introducing the following set of Herglotz matrices

$$\mathcal{N}_1^{n\times n} = \{M : \mathbb{C}_+ \to M_n(\mathbb{C}) \text{ Herglotz} \,|\, M(z) = \textstyle\int_{\mathbb{R}} d\Omega(\lambda)(\lambda - z)^{-1},$$
$$\text{for all } \underline{c} \in \mathbb{C}^n, \ \textstyle\int_{\mathbb{R}} (\underline{c}, d\Omega(\lambda)\underline{c})_{\mathbb{C}^n} < \infty\}, \tag{7.21}$$

we now turn to a realization theorem for Herglotz matrices of the type (7.17) and state the analog of Theorem 4.1.

Theorem 7.1.
(i). Any $M \in \mathcal{N}_1^{n\times n}$ with associated measure Ω can be realized in the form

$$M(z) = \big((\underline{e}_j, K^*(H - z)^{-1} K \underline{e}_k)_{\mathbb{C}^n}\big)_{1 \le j,k \le n}$$
$$= \big((f_j, (H - z)^{-1} f_k)_{\mathcal{H}}\big)_{1 \le j,k \le n}, \quad z \in \mathbb{C}_+, \tag{7.22}$$

where H denotes a self-adjoint operator in some separable complex Hilbert space $\mathcal{H}$, $\{f_1, \dots, f_n\} \subset \mathcal{H}$, $(f_j, f_k)_{\mathcal{H}} = \delta_{j,k}$, $j, k = 1, \dots, n$ and

$$\int_{\mathbb{R}} d\Omega(\lambda) = \big(\|f_j\|_{\mathcal{H}}^2 \delta_{j,k}\big)_{1 \le j,k \le n}. \tag{7.23}$$

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

$$M_\ell(z) = \big((\underline{e}_j, K^*(H_\ell - z)^{-1} K \underline{e}_k)_{\mathbb{C}^n}\big)_{1 \le j,k \le n}$$
$$= \big((f_j, (H_\ell - z)^{-1} f_k)_{\mathcal{H}}\big)_{1 \le j,k \le n}, \quad \ell = 1, 2, \ z \in \mathbb{C}_+, \tag{7.24}$$

where H_ℓ, $\ell = 1, 2$ are self-adjoint finite-rank perturbations of one and the same self-adjoint operator H_0 in some complex Hilbert space $\mathcal{H}$ (which may be chosen separable) with $\{f_1, \dots, f_n\} \subset \mathcal{H}$, $(f_j, f_k)_{\mathcal{H}} = \delta_{j,k}$, $j, k = 1, \dots, n$, that is,

$$H_\ell = H_0 + K \alpha_\ell K^* = H_0 + \sum_{j=1}^n \alpha_{\ell,j} (f_j, \cdot)_{\mathcal{H}} f_j \tag{7.25}$$

for some $\alpha_\ell = \big(\alpha_{\ell,j}\delta_{j,k}\big)_{1\leq j,k\leq n}$, $\alpha_{\ell,j} \in \mathbb{R}$, $j = 1,\dots,n$, $\ell = 1,2$, *if and only if the following conditions hold:*

$$\int_{\mathbb{R}} d\Omega_1(\lambda) = \int_{\mathbb{R}} d\Omega_2(\lambda) = \big(\|f_j\|_{\mathcal{H}}^2\delta_{j,k}\big)_{1\leq j,k\leq n}, \tag{7.26}$$

and for all $z \in \mathbb{C}_+$,

$$M_2(z) = M_1(z)\big(I_n + \big(\|f_j\|_{\mathcal{H}}^{-2}\delta_{j,k}\big)_{1\leq j,k\leq n}(\alpha_2 - \alpha_1)M_1(z)\big)^{-1}. \tag{7.27}$$

Since the proof parallels that of Theorem 4.1 step by step we omit further details.

It is possible to extend this formalism to more general classes of (possibly unbounded) symmetric finite-rank (form) perturbations of $|H_0|$, see, for instance, [5] and the references therein.

Next we turn to a characterization of Friedrichs and Krein extensions of densely defined operators bounded from below with deficiency indices (n,n) (see also [9], [35], [37], [38], [42], [100], [137], [140]–[142]).

We start by describing a canonical representation of densely defined closed symmetric operators with deficiency indices (n,n) as discussed in [119] (in close analogy to the scalar case treated in detail by Donoghue [42]). Let $\mathcal{H}$ be a separable complex Hilbert space, H a closed densely defined symmetric operator with domain $\mathcal{D}(H)$ and deficiency indices (n,n). Let

$$U_\alpha : \ker(H^*-i) \to \ker(H^*+i) \tag{7.28}$$

be a linear isometric isomorpism and parametrize all self-adjoint extensions H_α of H according to von Neumann's formula by

$$\begin{aligned} &H_\alpha(g + (1+U_\alpha)u_+) = Hg + i(1-U_\alpha)u_+, \\ &\mathcal{D}(H_\alpha) = \{(g + (1+U_\alpha)u_+) \in \mathcal{D}(H^*) \,|\, g \in \mathcal{D}(H),\, u_+ \in \ker(H^*-i)\}. \end{aligned} \tag{7.29}$$

In order to resemble the notation employed in Section 4, we think of 2α as a self-adjoint matrix representing $U_\alpha = e^{2i\alpha} \in U(n)$ with respect to fixed bases in $\ker(H^* \mp i)$. (Here $U(n)$ denotes the set of unitary $n\times n$ matrices with entries in $\mathbb{C}$.) Next, we assume that $\{u_{+,j}\}_{1\leq j\leq n}$ is a generating basis for H_α for some (and hence for all) $e^{2i\alpha} \in U(n)$. Let $E_\alpha(\cdot)$ be the corresponding family of orthogonal spectral projections of H_α and define

$$\begin{aligned} &d\Upsilon_\alpha(\lambda) = \big(d\Upsilon_{\alpha,j,k}(\lambda)\big)_{1\leq j,k\leq n}, \quad d\Upsilon_{\alpha,j,k}(\lambda) = (u_{+,j}, dE_\alpha(\lambda)u_{+,k})_{\mathcal{H}}, \\ &\int_{\mathbb{R}} d\Upsilon_{\alpha,j,k}(\lambda) = (u_{+,j}, u_{+,k})_{\mathcal{H}} = \delta_{j,k},, \quad j,k = 1,\dots,n, \ e^{2i\alpha} \in U(n). \end{aligned} \tag{7.30}$$

Then H_α is unitarily equivalent to multiplication by λ in $L^2(\mathbb{R}; d\Upsilon_\alpha)$ and $u_{+,j}$ can be mapped into the vector $(\delta_{j,1},\dots,\delta_{j,n})^t$. However, it is more convenient to define

$$d\Omega_\alpha(\lambda) = (1+\lambda^2)d\Upsilon_\alpha(\lambda), \tag{7.31}$$

such that

$$\int_{\mathbb{R}} \frac{d\Omega_\alpha(\lambda)}{1+\lambda^2} = I_n, \quad \int_{\mathbb{R}} (\underline{c}, d\Omega_\alpha(\lambda)\underline{c})_{\mathbb{C}^n} = \infty \text{ for all } \underline{c} \in \mathbb{C}^n\backslash\{0\}, \ e^{2i\alpha} \in U(n) \tag{7.32}$$

(by (7.30) and the fact that $u_{+,j} \notin \mathcal{D}(H_\alpha)$). Thus, H_α is unitarily equivalent to $\widehat{H}_\alpha$ in $\widehat{\mathcal{H}}_\alpha = L^2(\mathbb{R}; d\Omega_\alpha)$, where

$$(\widehat{H}_\alpha\underline{\hat g})(\lambda) = \lambda\underline{\hat g}(\lambda), \quad \underline{\hat g} \in \mathcal{D}(\widehat{H}_\alpha) = L^2(\mathbb{R}; (1+\lambda^2)d\Omega_\alpha), \tag{7.33}$$

$$H_\alpha = U_\alpha \widehat{H}_\alpha U_\alpha^{-1}, \quad \mathcal{H} = U_\alpha L^2(\mathbb{R}; d\Omega_\alpha), \tag{7.34}$$

with U_α unitary,

$$\begin{aligned} &U_\alpha : \widehat{\mathcal{H}}_\alpha = L^2(\mathbb{R}; d\Omega_\alpha) \to \mathcal{H}, \\ &\underline{\hat{g}} \to U_\alpha \underline{\hat{g}} = \operatorname*{s-lim}_{N\to\infty} \sum_{j=1}^n \int_{-N}^N d(E_\alpha(\lambda)u_{+,j})(\lambda - i)\hat{g}_j(\lambda), \\ &\qquad\qquad \underline{\hat{g}} = (\hat{g}_1, \dots, \hat{g}_n)^t \in L^2(\mathbb{R}; d\Omega_\alpha). \end{aligned} \tag{7.35}$$

Moreover,

$$u_{+,j} = U_\alpha \underline{\hat{u}}_{+,j}, \quad \underline{\hat{u}}_{+,j}(\lambda) = (\lambda - i)^{-1} \underline{e}_j, \ j = 1, \dots, n \tag{7.36}$$

and

$$\begin{aligned} &(\widehat{H}(\alpha)\underline{\hat{g}})(\lambda) = \lambda \underline{\hat{g}}(\lambda), \\ &\underline{\hat{g}} \in \mathcal{D}(\widehat{H}(\alpha)) = \{\underline{\hat{h}} \in \mathcal{D}(\widehat{H}_\alpha) \,|\, \textstyle\int_{\mathbb{R}} (\underline{e}_j, d\Omega_\alpha(\lambda)\underline{\hat{h}}(\lambda))_{\mathbb{C}^n} = 0, \, j = 1, \dots, n\}, \end{aligned} \tag{7.37}$$

where $\underline{e}_j$ has been defined in (7.18) and

$$H = U_\alpha \widehat{H}(\alpha) U_\alpha^{-1}. \tag{7.38}$$

Thus $\widehat{H}(\alpha)$ in $L^2(\mathbb{R}; d\omega_\alpha)$ is a canonical representation for a densely defined closed symmetric operator H with deficiency indices (n, n) in a separable Hilbert space $\mathcal{H}$ and a generating basis $\{u_{+,j} \in \ker(H^* - i)\}_{1 \le j \le n}$. We shall prove in Theorem 7.2 below that $\widehat{H}(\alpha)$ in $L^2(\mathbb{R}; d\Omega_\alpha)$ is actually a model for all such operators. Moreover, since

$$\begin{aligned} ((H - \overline{z})g, U_\alpha(\cdot - z)^{-1}\underline{e}_j)_{\mathcal{H}} = \int_{\mathbb{R}} (\lambda - z)((\underline{U_\alpha^{-1} g})(\lambda), d\Omega_\alpha(\lambda)\underline{e}_j)_{\mathbb{C}^n} (\lambda - z)^{-1} = 0, \\ g \in \mathcal{D}(H), \ z \in \mathbb{C}\backslash\mathbb{R}, \end{aligned} \tag{7.39}$$

by (7.37), one infers that $U_\alpha(\cdot - z)^{-1}\underline{e}_j \in \mathcal{D}(H^*)$. Since $\mathcal{D}(H)$ is dense in $\mathcal{H}$, one concludes

$$\ker(\widehat{H}(\alpha)^* - z) = \{c_j(\cdot - z)^{-1}\underline{e}_j \,|\, c_j \in \mathbb{C}, \ j = 1, \dots, n\}, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{7.40}$$

where

$$H^* = U_\alpha \widehat{H}(\alpha)^* U_\alpha^{-1}. \tag{7.41}$$

If $\{u_{+,j} \in \ker(H^* - i)\}_{1 \le j \le n}$ is not a generating basis for H_α then, in close analogy to Section 4, $\mathcal{H}$ (not necessarily assumed to be separable at this point) decomposes into two orthogonal subspaces $\mathcal{H}^0$ and $\mathcal{H}^{0,\perp}$,

$$\mathcal{H} = \mathcal{H}^0 \oplus \mathcal{H}^{0,\perp}, \tag{7.42}$$

with $\mathcal{H}^0$ separable, each of which is a reducing subspace for all H_α, $e^{2i\alpha} \in U(n)$ and

$$\begin{aligned} \mathcal{H}^0 = &\overline{\operatorname{linspan}\{(H_\alpha - z)^{-1}u_{+,j} \in \mathcal{H} \,|\, z \in \mathbb{C}\backslash\mathbb{R}, \ j = 1, \dots, n\}} \\ &\text{is independent of } \alpha \in U(n), \end{aligned} \tag{7.43}$$

$$(H_\alpha - z)^{-1} = (H_\beta - z)^{-1} \text{ on } \mathcal{H}^{0,\perp} \text{ for all } e^{2i\alpha}, e^{2i\beta} \in U(n), \ z \in \mathbb{C}_+. \tag{7.44}$$

In particular, the part $H^{0,\perp}$ of H in $\mathcal{H}^{0,\perp}$ is then self-adjoint,

$$H = H^0 \oplus H^{0,\perp}, \quad H_\alpha = H_\alpha^0 \oplus H^{0,\perp}, \quad e^{2i\alpha} \in U(n), \tag{7.45}$$

$$\operatorname{ran}(H^{0,\perp} - z) = \mathcal{H}^{0,\perp}, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{7.46}$$

$$u_+ = u_+^0 \oplus 0, \tag{7.47}$$

with H^0 a densely defined closed symmetric operator in $\mathcal{H}^0$ and deficiency indices (n,n). One then computes

$$\begin{aligned} &z(u_{+,j}, u_{+,k})_{\mathcal{H}} + (1+z^2)(u_{+,j}, (H_\alpha - z)^{-1}u_{+,k})_{\mathcal{H}} \\ &= z(u^0_{+,j}, u^0_{+,k})_{\mathcal{H}^0} + (1+z^2)(u^0_{+,j}, (H^0_\alpha - z)^{-1}u^0_{+,k})_{\mathcal{H}^0}, \\ &\qquad\qquad j,k = 1,\dots,n, \ e^{2i\alpha} \in U(n) \end{aligned} \tag{7.48}$$

and hence α-dependent spectral properties of H_α in $\mathcal{H}$ are again effectively reduced to those of H^0_α in $\mathcal{H}^0$, where H^0_α are self-adjoint operators with a generating basis $\{u^0_{+,j} \in \ker((H^0)^* - i)\}_{1\le j\le n}$. We shall call the densely defined closed symmetric operator H with deficiency indices (n,n) *prime* if $\mathcal{H}^{0,\perp} = \{0\}$ in (7.42).

Next we show the model character of $(\widehat{\mathcal{H}}_\alpha, \widehat{H}(\alpha), \widehat{H}_\alpha)$ following the approach outlined in Theorem 4.2.

Theorem 7.2. *Let H be a densely defined closed prime symmetric operator with deficiency indices (n,n) and normalized deficiency vectors $u_{\pm,j} \in \ker(H^* \mp i)$, $\|u_{\pm,j}\|_{\mathcal{H}} = 1$, $j = 1,\dots,n$ in some separable complex Hilbert space $\mathcal{H}$. Let H_α be a self-adjoint extension of H with generating orthonormal basis $\{u_{+,j} \in \ker(H^* - i) \,|\, j = 1,\dots,n\}$. Then the pair (H, H_α) in $\mathcal{H}$ is unitarily equivalent to the pair $(\widehat{H}(\alpha), \widehat{H}_\alpha)$ in $\widehat{\mathcal{H}}$ defined in* (7.37) *and* (7.33) *with unitary operator U_α defined in* (7.35) *(cf.* (7.38) *and* (7.34)*). Conversely, given a matrix-valued measure $d\widetilde{\Omega}$ satisfying*

$$\int_{\mathbb{R}} \frac{d\widetilde{\Omega}(\lambda)}{1+\lambda^2} = I_n, \quad \int_{\mathbb{R}} (\underline{c}, d\widetilde{\Omega}(\lambda)\underline{c})_{\mathbb{C}^n} = \infty \text{ for all } \underline{c} \in \mathbb{C}^n\backslash\{0\}, \tag{7.49}$$

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

$$(\widetilde{H}\underline{\widetilde{g}})(\lambda) = \lambda\underline{\widetilde{g}}(\lambda), \quad \underline{\widetilde{g}} \in \mathcal{D}(\widetilde{H}) = L^2(\mathbb{R}; (1+\lambda^2)d\widetilde{\Omega}) \tag{7.50}$$

and the linear operator H in $\widetilde{\mathcal{H}}$,

$$\mathcal{D}(H) = \{\underline{\widetilde{g}} \in \mathcal{D}(\widetilde{H}) \,|\, \int_{\mathbb{R}} (\underline{e}_j, d\widetilde{\Omega}(\lambda)\underline{\widetilde{g}}(\lambda))_{\mathbb{C}^n} = 0, \, j = 1,\dots,n\}, \quad H = \widetilde{H}\big|_{\mathcal{D}(H)}. \tag{7.51}$$

Then H is a densely defined closed symmetric operator in $\widetilde{\mathcal{H}}$ with deficiency indices (n,n) and deficiency subspaces

$$\ker(H^* \mp i) = \{c_j(\lambda \mp i)^{-1}\underline{e}_j \,|\, c_j \in \mathbb{C}, \, j = 1,\dots,n\}. \tag{7.52}$$

Proof. Except for a few modifications one can follow the corresponding proof of Theorem 4.2 step by step. In particular, the first part goes through with the obvious changes indicated in (7.30)–(7.48). Hence we briefly turn to the proof of the second part of Theorem 7.2. Given (7.2)–(7.4), the scale of Hilbert spaces is still defined by $\widetilde{\mathcal{H}}_{2r} = L^2(\mathbb{R}; (1+\lambda^2)^r d\widetilde{\Omega})$, $r \in \mathbb{R}$, $\widetilde{\mathcal{H}}_0 = \widetilde{\mathcal{H}}$ and one considers again the unitary operator R,

$$R : \widetilde{\mathcal{H}}_2 \to \widetilde{\mathcal{H}}_{-2}, \quad \underline{\widetilde{f}} \to (1+\lambda^2)\underline{\widetilde{f}}. \tag{7.53}$$

We note that $\mathbb{C}^n \subset \widetilde{\mathcal{H}}_{-2}$. Again $\mathcal{D}(H)$ is well-defined, and as a restriction of the self-adjoint operator $\widetilde{H}$, H is clearly symmetric. By (7.53) and (7.51) one infers

$$\mathcal{D}(\widetilde{H}) = \widetilde{\mathcal{H}}_2 = \mathcal{D}(H) \oplus_{\tilde{\mathcal{H}}_2} R^{-1}\mathbb{C}^n, \tag{7.54}$$

which allows one to prove that $\mathcal{D}(H)$ is dense in $\widetilde{\mathcal{H}}$ as in the proof of Theorem 4.2. That H is a closed operator is also proved as in Section 4. Since $\widetilde{H}$ is self-adjoint, $\operatorname{ran}(\widetilde{H} - z) = \widetilde{\mathcal{H}}$ for all $z \in \mathbb{C}\backslash\mathbb{R}$, and $(\widetilde{H} \pm i) : \widetilde{\mathcal{H}}_2 \to \widetilde{\mathcal{H}}$ is unitary. Together with (7.54) this yields

$$\begin{aligned}
\widetilde{\mathcal{H}} &= (\widetilde{H} \pm i)\widetilde{\mathcal{H}}_2 = (\widetilde{H} \pm i)(\mathcal{D}(H) \oplus_{\tilde{\mathcal{H}}_2} R^{-1}\mathbb{C}) = (H \pm i)\mathcal{D}(H) \oplus_{\tilde{\mathcal{H}}} \left\{ \tfrac{\lambda \pm i}{1+\lambda^2} c \,\middle|\, c \in \mathbb{C} \right\} \\
&= \operatorname{ran}(H \pm i) \oplus_{\tilde{\mathcal{H}}} \{ c(\lambda \mp i)^{-1} \,|\, c \in \mathbb{C} \}
\end{aligned} \tag{7.55}$$

and hence (7.52). □

Introducing the Herglotz function

$$\begin{aligned}
M_\alpha(z) &= \int_{\mathbb{R}} d\Omega_\alpha(\lambda)((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}) && (7.56)\\
&= zI_n + (1+z^2)\big((u_{+,j}, (H_\alpha - z)^{-1} u_{+,k})_{\mathcal{H}}\big)_{1 \le j,k \le n} && (7.57)
\end{aligned}$$

(the last equality being a simple consequence of $\int_{\mathbb{R}} d\Omega_\alpha(\lambda)(1+\lambda^2)^{-1} = I_n$) one verifies,

$$\begin{aligned}
M_\beta(z) = (&-e^{-i\beta}(\sin(\beta)\cos(\alpha) - \cos(\beta)\sin(\alpha))e^{i\alpha} \\
&+ e^{-i\beta}(\cos(\beta)\cos(\alpha) + \sin(\beta)\sin(\alpha))e^{i\alpha} M_\alpha(z)) \\
&\times (e^{-i\beta}(\cos(\beta)\cos(\alpha) + \sin(\beta)\sin(\alpha))e^{i\alpha} \\
&+ e^{-i\beta}(\sin(\beta)\cos(\alpha) - \cos(\beta)\sin(\alpha))e^{i\alpha} M_\alpha(z))^{-1}, \\
&\exp(2i\alpha), \exp(2i\beta) \in U(n).
\end{aligned} \tag{7.58}$$

Since (7.58) does not seem to be a well-known result, we will provide its derivation, following [58], in Appendix B. A comparison of (7.58) and (6.40) suggests invoking

$$\begin{aligned}
&A(\alpha,\beta) = \big(A(\alpha,\beta)_{j,k}\big)_{1 \le j,k \le n} \in \mathcal{A}_{2n}, \\
&A(\alpha,\beta)_{1,1} = e^{-i\beta}(\cos(\beta)\cos(\alpha) + \sin(\beta)\sin(\alpha))e^{i\alpha}, \\
&A(\alpha,\beta)_{1,2} = e^{-i\beta}(\sin(\beta)\cos(\alpha) - \cos(\beta)\sin(\alpha))e^{i\alpha}, \\
&A(\alpha,\beta)_{2,1} = e^{-i\beta}(\cos(\beta)\sin(\alpha) - \sin(\beta)\cos(\alpha))e^{i\alpha}, \\
&A(\alpha,\beta)_{2,2} = e^{-i\beta}(\cos(\beta)\cos(\alpha) + \sin(\beta)\sin(\alpha))e^{i\alpha}, \\
&\qquad \exp(2i\alpha), \exp(2i\beta) \in U(n).
\end{aligned} \tag{7.59}$$

Moreover, Theorem 6.6 applies (with $A_{1,1}(\alpha,\beta) = A_{2,2}(\alpha,\beta) = e^{-i\beta}(\cos(\beta)\cos(\alpha) + \sin(\beta)\sin(\alpha))e^{i\alpha}$, $A_{1,2}(\alpha,\beta) = -A_{2,1}(\alpha,\beta) = e^{-i\beta}(\sin(\beta)\cos(\alpha) - \cos(\beta)\sin(\alpha))e^{i\alpha}$). Since by definition, $M_\alpha(i) = iI_n$, Lemma 5.3 yields $\operatorname{Im}(M_\alpha(z)) > 0$ for all $z \in \mathbb{C}_+$. In fact, Lemma B.4 yields an explicit lower bound for $\operatorname{Im}(z)\operatorname{Im}(M_\alpha(z))$.

Next, assuming that H is nonnegative, $H \geq 0$, we again intend to characterize the Friedrichs and Krein extensions, H_F and H_K, of H. In order to apply Krein's results [100] (see also [9], [140], [141]) in a slightly different form (see, e.g., [137], Sect. 4 for an efficient summary of Krein's results most relevant in our context) we start with the analog of Theorem 4.3.

Theorem 7.3.
(i). $H_\alpha = H_F$ *for some* $e^{2i\alpha} \in U(n)$ *if and only if for all* $R > 0$, $\int_R^\infty d\|E_\alpha(\lambda)u_+\|_{\mathcal{H}}^2 \lambda = \infty$ *for all* $0 \neq u_+ \in \ker(H^* - i)$, *or equivalently, if and only if* $\int_R^\infty (\underline{c}, d\Omega_\alpha(\lambda)\underline{c})_{\mathbb{C}^n} \lambda^{-1} = \infty$ *for all* $\underline{c} \in \mathbb{C}^n \backslash \{0\}$.
(ii). $H_\beta = H_K$ *for some* $e^{2i\beta} \in U(n)$ *if and only if for all* $R > 0$, $\int_0^R d\|E_\beta(\lambda)u_+\|_{\mathcal{H}}^2 \lambda^{-1} = \infty$ *for all* $0 \neq u_+ \in \ker(H^* - i)$, *or equivalently, if and only if* $\int_0^R (\underline{c}, d\Omega_\beta(\lambda)\underline{c})_{\mathbb{C}^n} \lambda^{-1} = \infty$ *for all* $\underline{c} \in \mathbb{C}^n \backslash \{0\}$.
(iii). $H_\gamma = H_F = H_K$ *for some* $e^{2i\gamma} \in U(n)$ *if and only if* $\int_R^\infty d\|E_\gamma(\lambda)u_+\|_{\mathcal{H}}^2 \lambda = \infty = \int_0^R d\|E_\gamma(\lambda)u_+\|_{\mathcal{H}}^2 \lambda^{-1}$ *for all* $R > 0$ *and all* $0 \neq u_+ \in \ker(H^* - i)$, *or equivalently, if and only if* $\int_R^\infty (\underline{c}, d\Omega_\gamma(\lambda)\underline{c})_{\mathbb{C}^n} \lambda^{-1} = \int_0^R (\underline{c}, d\Omega_\gamma(\lambda)\underline{c})_{\mathbb{C}^n} \lambda^{-1} = \infty$ *for all* $\underline{c} \in \mathbb{C}^n \backslash \{0\}$.

Proof. As in Section 4, in order to reduce the above statements (i)–(iii) to those in Krein [100] (as summarized in Skau [137]), it suffices to notice that $(\mu + 1)^{-1} - (\mu - i)^{-1} = O(\mu^{-2})$ as $\mu \uparrow \infty$ and $(\mu + 1)^{-1} - (\mu - i)^{-1} = O(1)$ as $\mu \downarrow 0$. □

Of course (4.69)–(4.71) remain valid in the present case of deficiency indices (n, n).

Applying Theorem 7.3 to H_α then yields the analog of Theorem 4.4 (i)–(iii).

Theorem 7.4. ([35], [37], [38], [101]).
(i). $H_\alpha = H_F$ *if and only if* $\lim_{\lambda \downarrow -\infty} (\underline{c}, M_\alpha(\lambda)\underline{c})_{\mathbb{C}^n} = -\infty$ *for all* $\underline{c} \in \mathbb{C}^n \backslash \{0\}$.
(ii). $H_\beta = H_K$ *if and only if* $\lim_{\lambda \uparrow 0} (\underline{c}, M_\beta(\lambda)\underline{c})_{\mathbb{C}^n} = \infty$ *for all* $\underline{c} \in \mathbb{C}^n \backslash \{0\}$.
(iii). $H_\gamma = H_F = H_K$ *if and only if for all* $\underline{c} \in \mathbb{C}^n \backslash \{0\}$, $\lim_{\lambda \downarrow -\infty} (\underline{c}, M_\gamma(\lambda)\underline{c})_{\mathbb{C}^n} = -\infty$ *and* $\lim_{\lambda \uparrow 0} (\underline{c}, M_\gamma(\lambda)\underline{c})_{\mathbb{C}^n} = \infty$.

Since the proof parallels the corresponding one in Section 4 step by step we omit further details.

If H_α and H_β are two distinct self-adjoint extensions of the symmetric operator H with deficiency indices (n, n), $n \geq 2$ considered in Theorem 7.2, then $\mathcal{D}(H_\alpha)$ and $\mathcal{D}(H_\beta)$ may have a nontrivial intersection, that is,

$$\mathcal{D}(H_\alpha) \cap \mathcal{D}(H_\beta) \underset{\neq}{\supset} \mathcal{D}(H), \quad e^{2i\alpha}, e^{2i\beta} \in U(n),\ U_\alpha \neq U_\beta. \tag{7.60}$$

Next, we characterize the case where the domain of a nonnegative self-adjoint extension $\widetilde{H}$ of H has only trivial intersection with that of H_F or H_K. These results go beyond those in [100] and appear to be new.

Theorem 7.5. *Suppose* $\widetilde{H} \geq 0$ *is a nonnegative self-adjoint extension of a densely defined nonnegative closed operator* $H \geq 0$ *with deficiency indices* (n, n). *We denote by* $\widetilde{E}(\lambda)$ *the family of spectral projections of* $\widetilde{H}$ *and by* $d\widetilde{\Omega}(\lambda)$ *the measure defined in* (7.30), (7.31). *Then*
(i). $\mathcal{D}(\widetilde{H}) \cap \mathcal{D}(H_F) = \mathcal{D}(H)$ *if and only if for all* $R > 0$, $\int_R^\infty d\|\widetilde{E}(\lambda)u_+\|_{\mathcal{H}}^2 \lambda < \infty$ *for all* $u_+ \in \ker(H^* - i)$, *or equivalently, if and only if* $\int_R^\infty (\underline{c}, d\widetilde{\Omega}(\lambda)\underline{c})_{\mathbb{C}^n} \lambda^{-1} < \infty$ *for all* $\underline{c} \in \mathbb{C}^n$.
(ii). $\mathcal{D}(\widetilde{H}) \cap \mathcal{D}(H_K) = \mathcal{D}(H)$ *if and only if for all* $R > 0$, $\int_0^R d\|\widetilde{E}(\lambda)u_+\|_{\mathcal{H}}^2 \lambda^{-1} < \infty$ *for all* $u_+ \in \ker(H^* - i)$, *or equivalently, if and only if* $\int_0^R (\underline{c}, d\widetilde{\Omega}(\lambda)\underline{c})_{\mathbb{C}^n} \lambda^{-1} < \infty$ *for all* $\underline{c} \in \mathbb{C}^n$.

(iii). $\mathcal{D}(\widetilde{H}) \cap \mathcal{D}(H_F) = \mathcal{D}(H) = \mathcal{D}(\widetilde{H}) \cap \mathcal{D}(H_K)$ *if and only if for all* $R > 0$, $\int_R^\infty d\|\widetilde{E}(\lambda)u_+\|_{\mathcal{H}}^2 \lambda + \int_0^R d\|\widetilde{E}(\lambda)u_+\|_{\mathcal{H}}^2 \lambda^{-1} < \infty$ *for all* $u_+ \in \ker(H^* - i)$*, or equivalently, if and only if* $\int_0^\infty (\underline{c}, d\widetilde{\Omega}(\lambda)\underline{c})_{\mathbb{C}^n} \lambda^{-1} < \infty$ *for all* $\underline{c} \in \mathbb{C}^n$.

Proof. It is sufficient to prove item (i) since the remaining proofs offer no new details. We use the terminology introduced in Appendix B and identify $A_1 = \widetilde{H}$, $A_2 = H_F$, $P_{1,2} = \widetilde{P}_F$, $\mathcal{U}_1 = \widetilde{\mathcal{U}}$, $\mathcal{U}_2 = \mathcal{U}_F$, etc. First we suppose that $\mathcal{D}(\widetilde{H}) \cap \mathcal{D}(H_F) = \mathcal{D}(H)$. Using von Neumann's parametrization of $\widetilde{H}$ and H_F in terms of the linear isometric isomorphisms $\widetilde{\mathcal{U}}$ and $\mathcal{U}_F$ from $\ker(H^* - i)$ onto $\ker(H^* + i)$, this assumption is equivalent to -1 not being an eigenvalue of U_F (the matrix representation of $\mathcal{U}_F$ in the orthogonal bases of $\ker(H^* \mp i)$ as discussed in Appendix B). By (B.23), this is equivalent to the existence of the inverse of $\widetilde{P}_F(i)$. In order to prove that $\int_R^\infty (\underline{c}, d\widetilde{\Omega}(\lambda)\underline{c})_{\mathbb{C}^n} \lambda^{-1} < \infty$ for all $\underline{c} \in \mathbb{C}^n$, it suffices to prove that the Herglotz matrix $\widetilde{M}(z)$ associated with the measure $d\widetilde{\Omega}(\lambda)$ corresponding to $\widetilde{H}$ has a limit as $z \to -\infty$. Using (B.30), one computes

$$\widetilde{M}(z) - \operatorname{Re}(\widetilde{P}_F(i)^{-1}) = (2iI_n - \widetilde{P}_F(-i)^{-1})(\widetilde{P}_F(-i)^{-1} - iI_n + M_F(z))^{-1}\widetilde{P}_F(-i)^{-1}. \tag{7.61}$$

Here $M_F(z)$ denotes the Herglotz matrix associated to H_F and we used the fact

$$\operatorname{Re}(\widetilde{P}_F(i)^{-1}) = iI_n + \widetilde{P}_F(i)^{-1} = -iI_n + \widetilde{P}_F(-i)^{-1}. \tag{7.62}$$

Next, recalling Theorem 7.4 (i), we will invoke that

$$\lim_{\lambda\downarrow-\infty} (\underline{c}, M_F(\lambda)\underline{c})_{\mathbb{C}^n} = -\infty \text{ for all } \underline{c} \in \mathbb{C}^n \backslash \{0\}. \tag{7.63}$$

Since $(\underline{c}, M_F(\lambda)\underline{c})_{\mathbb{C}^n}^{-1}$ converges monotonically to zero pointwise for any $\underline{c} \in \{\underline{d} \in \mathbb{C}^n \mid \|\underline{d}\|_{\mathbb{C}^n} = 1\}$, the compact unit sphere in $\mathbb{C}^n$, Dini's theorem yields in fact uniform convergence to zero. Consequently,

$$\widetilde{P}_F(-i)^{-1} - iI_n + M_F(\lambda) \leq \gamma(\lambda) I_n, \tag{7.64}$$

for λ sufficiently negative and some $\gamma(\lambda)$ with $\gamma(\lambda) \downarrow -\infty$ as $\lambda \downarrow -\infty$. In particular,

$$(\widetilde{P}_F(-i)^{-1} - iI_n + M_F(\lambda))^{-1} \to 0 \text{ as } \lambda \downarrow -\infty. \tag{7.65}$$

(7.61) and (7.65) then prove

$$\lim_{\lambda\downarrow-\infty} \widetilde{M}(\lambda) = \operatorname{Re}(\widetilde{P}_F(i)^{-1}). \tag{7.66}$$

Conversely, we suppose $\int_R^\infty (\underline{c}, d\widetilde{\Omega}(\lambda)\underline{c})_{\mathbb{C}^n} \lambda^{-1} < \infty$ for all $\underline{c} \in \mathbb{C}^n$ or equivalently, $\lim_{\lambda\downarrow-\infty} \widetilde{M}(\lambda) = \widetilde{M}(-\infty)$ exists. Similarly to (B.36), one derives

$$M_F(z) - \widetilde{M}(z) = (iI_n + \widetilde{M}(z))(I_n + i\widetilde{P}_F(i) - \widetilde{P}_F(i)\widetilde{M}(z))^{-1}\widetilde{P}_F(i)(-iI_n + \widetilde{M}(z)) \tag{7.67}$$

and hence

$$\begin{aligned}
&((-iI_n + \widetilde{M}(\lambda))^{-1}\underline{c}, (M_F(\lambda) - \widetilde{M}(\lambda))(-iI_n + \widetilde{M}(\lambda))^{-1}\underline{c})_{\mathbb{C}^n} \\
&= (\underline{c}, (I_n + i\widetilde{P}_F(i) - \widetilde{P}_F(i)\widetilde{M}(\lambda))^{-1}\widetilde{P}_F(i)\underline{c})_{\mathbb{C}^n}, \quad \lambda < 0, \ \underline{c} \in \mathbb{C}^n \backslash \{0\}.
\end{aligned} \tag{7.68}$$

By (7.63) and the existence of $\widetilde{M}(-\infty)$, the left-hand side of (7.68) tends to $-\infty$ as $\lambda \downarrow -\infty$. Consequently, $\ker(\widetilde{P}_F(i)) = \{0\}$, that is, $\widetilde{P}_F(i)$ is invertible. By (B.23), this is equivalent to -1 not being an eigenvalue of U_F implying $\mathcal{D}(\widetilde{H}) \cap \mathcal{D}(H_F) = \mathcal{D}(H)$. $\square$

Theorem 7.5 then yields the following result.

Theorem 7.6. *Suppose $\widetilde{H} \geq 0$ is a nonnegative self-adjoint extension of a densely defined nonnegative closed operator $H \geq 0$ with deficiency indices (n,n). We denote by $\widetilde{M}(z)$ the corresponding Herglotz matrix associated with the measure $d\widetilde{\Omega}(\lambda)$ defined in* (7.30), (7.31)*. Then*
(i). $\mathcal{D}(\widetilde{H}) \cap \mathcal{D}(H_F) = \mathcal{D}(H)$ if and only if $\lim_{\lambda\downarrow-\infty} |(\underline{c}, \widetilde{M}(\lambda)\underline{c})_{\mathbb{C}^n}| < \infty$ for all $\underline{c} \in \mathbb{C}^n$.
(ii). $\mathcal{D}(\widetilde{H}) \cap \mathcal{D}(H_K) = \mathcal{D}(H)$ if and only if $\lim_{\lambda\uparrow 0} |(\underline{c}, \widetilde{M}(\lambda)\underline{c})_{\mathbb{C}^n}| < \infty$ for all $\underline{c} \in \mathbb{C}^n$.
(iii). $\mathcal{D}(\widetilde{H}) \cap \mathcal{D}(H_F) = \mathcal{D}(H) = \mathcal{D}(\widetilde{H}) \cap \mathcal{D}(H_K)$ if and only if for all $\underline{c} \in \mathbb{C}^n$, $\lim_{\lambda\downarrow-\infty} |(\underline{c}, \widetilde{M}(\lambda)\underline{c})_{\mathbb{C}^n}| + \lim_{\lambda\uparrow 0} |(\underline{c}, \widetilde{M}(\lambda)\underline{c})_{\mathbb{C}^n}| < \infty$.

An analog of Theorem 4.4 (iv) can now be obtained as follows.

Theorem 7.7. *Let $\widetilde{H} \geq 0$ be a nonnegative self-adjoint extension of a densely defined nonnegative closed operator $H \geq 0$ with deficiency indices (n,n). We denote by $\widetilde{M}(z)$ the corresponding Herglotz matrix associated with the measure $d\widetilde{\Omega}(\lambda)$ defined in* (7.30), (7.31) *and identify $A_1 = \widetilde{H}$, $A_2 = H_F$ or H_K, $P_{1,2} = \widetilde{P}_F$ or $\widetilde{P}_K$, $\mathcal{U}_1 = \widetilde{\mathcal{U}}$, $\mathcal{U}_2 = \mathcal{U}_F$ or $\mathcal{U}_K$, etc., in Appendix* B*. Then*
(i). If $\mathcal{D}(\widetilde{H}) \cap \mathcal{D}(H_F) = \mathcal{D}(H)$ then

$$\lim_{\lambda\downarrow-\infty} \widetilde{M}(\lambda) = \operatorname{Re}(\widetilde{P}_F(i)^{-1}) = -\int_{\mathbb{R}} d\widetilde{\Omega}(\lambda)\lambda(1+\lambda^2)^{-1}. \tag{7.69}$$

(ii). If $\mathcal{D}(\widetilde{H}) \cap \mathcal{D}(H_K) = \mathcal{D}(H)$ then

$$\lim_{\lambda\uparrow 0} \widetilde{M}(\lambda) = \operatorname{Re}(\widetilde{P}_K(i)^{-1}) = \int_{\mathbb{R}} d\widetilde{\Omega}(\lambda)(\lambda^{-1} - \lambda(1+\lambda^2)^{-1}). \tag{7.70}$$

(iii). If $\mathcal{D}(\widetilde{H}) \cap \mathcal{D}(H_F) = \mathcal{D}(H) = \mathcal{D}(\widetilde{H}) \cap \mathcal{D}(H_K)$ then

$$\int_{\mathbb{R}} d\widetilde{\Omega}(\lambda)\lambda^{-1} = \operatorname{Re}(\widetilde{P}_K(i)^{-1} - \widetilde{P}_F(i)^{-1}). \tag{7.71}$$

Proof. Item (i) is clear from (7.56) and (7.66). Similarly, (ii) follows from (7.56) and

$$\lim_{\lambda\uparrow 0} \widetilde{M}(\lambda) = \operatorname{Re}(\widetilde{P}_K(i)^{-1}. \tag{7.72}$$

Finally, (iii) is obvious by taking the difference of (7.70) and (7.69). $\square$

Next, we turn to a realization theorem for Herglotz functions of the type (7.57). It will be convenient to introduce the following sets of Herglotz matrices,

$$\begin{aligned} \mathcal{N}_0^{n\times n} = \{M : \mathbb{C}_+ \to M_n(\mathbb{C}) \text{ Herglotz} \,|\, M(z) = \textstyle\int_{\mathbb{R}} d\Omega(\lambda)((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}),\\ \text{for all } \underline{c} \in \mathbb{C}^n\backslash\{0\},\ \textstyle\int_{\mathbb{R}} (\underline{c}, d\Omega(\lambda)\underline{c})_{\mathbb{C}^n} = \infty,\ \textstyle\int_{\mathbb{R}} (\underline{c}, d\Omega(\lambda)\underline{c})_{\mathbb{C}^n} (1+\lambda^2)^{-1} < \infty\}, \end{aligned} \tag{7.73}$$

$$\begin{aligned} \mathcal{N}_{0,F}^{n\times n} = \{M \in \mathcal{N}_0^{n\times n} \,|\, \operatorname{supp}(\omega^{tr}) \subseteq [0,\infty),\ \text{for all } \underline{c} \in \mathbb{C}^n\backslash\{0\},\\ \textstyle\int_R^\infty (\underline{c}, d\Omega(\lambda)\underline{c})_{\mathbb{C}^n} \lambda^{-1} = \infty \text{ for some } R > 0\}, \end{aligned} \tag{7.74}$$

$$\mathcal{N}_{0,K}^{n\times n} = \{M \in \mathcal{N}_0^{n\times n} \,|\, \operatorname{supp}(\omega^{tr}) \subseteq [0,\infty), \text{ for all } \underline{c} \in \mathbb{C}^n\backslash\{0\},$$
$$\int_0^R (\underline{c}, d\Omega(\lambda)\underline{c})_{\mathbb{C}^n}\, \lambda^{-1} = \infty \text{ for some } R > 0\}, \tag{7.75}$$
$$\mathcal{N}_{0,F,K}^{n\times n} = \{M \in \mathcal{N}_0^{n\times n} \,|\, \operatorname{supp}(\omega^{tr}) \subseteq [0,\infty), \text{ for all } \underline{c} \in \mathbb{C}^n\backslash\{0\},$$
$$\int_R^\infty (\underline{c}, d\Omega(\lambda)\underline{c})_{\mathbb{C}^n}\, \lambda^{-1} = \int_0^R (\underline{c}, d\Omega(\lambda)\underline{c})_{\mathbb{C}^n}\, \lambda^{-1} = \infty \text{ for some } R > 0\} \tag{7.76}$$
$$= \mathcal{N}_{0,F}^{n\times n} \cap \mathcal{N}_{0,K}^{n\times n}. \tag{7.77}$$
$$\mathcal{N}_{0,F^\perp}^{n\times n} = \{M \in \mathcal{N}_0^{n\times n} \,|\, \operatorname{supp}(\omega^{tr}) \subseteq [0,\infty), \text{ for all } \underline{c} \in \mathbb{C}^n,$$
$$\int_R^\infty (\underline{c}, d\Omega(\lambda)\underline{c})_{\mathbb{C}^n}\, \lambda^{-1} < \infty \text{ for some } R > 0\}, \tag{7.78}$$
$$\mathcal{N}_{0,K^\perp}^{n\times n} = \{M \in \mathcal{N}_0^{n\times n} \,|\, \operatorname{supp}(\omega^{tr}) \subseteq [0,\infty), \text{ for all } \underline{c} \in \mathbb{C}^n,$$
$$\int_0^R (\underline{c}, d\Omega(\lambda)\underline{c})_{\mathbb{C}^n}\, \lambda^{-1} < \infty \text{ for some } R > 0\}, \tag{7.79}$$
$$\mathcal{N}_{0,F^\perp,K^\perp}^{n\times n} = \{M \in \mathcal{N}_0^{n\times n} \,|\, \operatorname{supp}(\omega^{tr}) \subseteq [0,\infty), \text{ for all } \underline{c} \in \mathbb{C}^n,$$
$$\int_0^\infty (\underline{c}, d\Omega(\lambda)\underline{c})_{\mathbb{C}^n}\, \lambda^{-1} < \infty\} = \mathcal{N}_{0,F^\perp}^{n\times n} \cap \mathcal{N}_{0,K^\perp}^{n\times n}. \tag{7.80}$$

The sets in (7.74)–(7.79) are of course independent of $R > 0$. The analog of Theorem 4.6 then reads as follows.

Theorem 7.8.
(i). Any $\widetilde{M} \in \mathcal{N}_0^{n\times n}$ *can be realized in the form*

$$\begin{aligned}\widetilde{M}(z) &= z\big(\|u_{+,j}\|_{\widetilde{\mathcal{H}}}^2 \delta_{j,k}\big)_{1\le j,k\le n} \\ &\quad + (1+z^2)\big((u_{+,j}, (\widetilde{H}-z)^{-1}u_{+,k})_{\widetilde{\mathcal{H}}}\big)_{1\le j,k\le n}, \quad z \in \mathbb{C}_+,\end{aligned} \tag{7.81}$$

where $\widetilde{H}$ *denotes the self-adjoint extension of some densely defined closed symmetric operator* H *with deficiency indices* (n,n) *and deficiency subspace* $\{u_{+,j} \in \ker(H^*-i)\}_{1\le j,k\le n}$ *in some separable complex Hilbert space* $\widetilde{\mathcal{H}}$.
(ii). Any $\widetilde{M}_{F(resp.\ K)} \in \mathcal{N}_{0,F(resp.\ K)}^{n\times n}$ *can be realized in the form*

$$\begin{aligned}\widetilde{M}_{F(resp.\ K)}(z) &= z\big(\|u_{+,j}\|_{\widetilde{\mathcal{H}}}^2 \delta_{j,k}\big)_{1\le j,k\le n} \\ &\quad + (1+z^2)\big((u_+, (\widetilde{H}_{F(resp.\ K)}-z)^{-1}u_+)_{\widetilde{\mathcal{H}}}\big)_{1\le j,k\le n}, \quad z \in \mathbb{C}_+,\end{aligned} \tag{7.82}$$

where $\widetilde{H}_{F(resp.\ K)} \ge 0$ *denotes the Friedrichs (respectively, Krein) extension of some densely defined closed operator* $H \ge 0$ *with deficiency indices* (n,n) *and deficiency subspace* $\{u_{+,j} \in \ker(H^*-i)\}_{1\le j,k\le n}$ *in some separable complex Hilbert space* $\widetilde{\mathcal{H}}$.
(iii). Any $\widetilde{M}_{F,K} \in \mathcal{N}_{0,F,K}^{n\times n}$ *can be realized in the form*

$$\begin{aligned}\widetilde{M}_{F,K}(z) &= z\big(\|u_{+,j}\|_{\widetilde{\mathcal{H}}}^2 \delta_{j,k}\big)_{1\le j,k\le n} \\ &\quad + (1+z^2)\big((u_+, (\widetilde{H}_{F,K}-z)^{-1}u_+)_{\widetilde{\mathcal{H}}}\big)_{1\le j,k\le n}, \quad z \in \mathbb{C}_+,\end{aligned} \tag{7.83}$$

where $\widetilde{H}_{F,K} \ge 0$ *denotes the unique nonnegative self-adjoint extension of some densely defined closed operator* $H \ge 0$ *with deficiency indices* (n,n) *and deficiency subspace* $\{u_{+,j} \in \ker(H^*-i)\}_{1\le j,k\le n}$ *in some separable complex Hilbert space* $\widetilde{\mathcal{H}}$.

(iv). Any $\widetilde{M}_{F^\perp(resp.\ K^\perp)} \in \mathcal{N}^{n\times n}_{0,F^\perp(resp.\ K^\perp)}$ *can be realized in the form*

$$\begin{aligned}\widetilde{M}_{F^\perp(resp.\ K^\perp)}(z) &= z\big(\|u_{+,j}\|^2_{\widetilde{\mathcal{H}}}\delta_{j,k}\big)_{1\le j,k\le n} \\ &\quad + (1+z^2)\big((u_+, (\widetilde{H}_{F^\perp(resp.\ K^\perp)} - z)^{-1}u_+)_{\widetilde{\mathcal{H}}}\big)_{1\le j,k\le n}, \ z \in \mathbb{C}_+,\end{aligned} \tag{7.84}$$

where $\widetilde{H}_{F^\perp(resp.\ K^\perp)} \geq 0$ *denotes a nonnegative self-adjoint extension of some densely defined closed operator* $H \geq 0$ *with deficiency indices* (n,n) *and deficiency subspace* $\{u_{+,j} \in \ker(H^* - i)\}_{1\le j,k\le n}$ *in some separable complex Hilbert space* $\widetilde{\mathcal{H}}$ *such that* $\mathcal{D}(\widetilde{H}_{F^\perp} \cap \mathcal{D}(H_F) = \mathcal{D}(H)$ *(respectively,* $\mathcal{D}(\widetilde{H}_{K^\perp} \cap \mathcal{D}(H_K) = \mathcal{D}(H)$*).*
(v). Any $\widetilde{M}_{F^\perp,K^\perp} \in \mathcal{N}^{n\times n}_{0,F^\perp,K^\perp}$ *can be realized in the form*

$$\begin{aligned}\widetilde{M}_{F^\perp,K^\perp}(z) &= z\big(\|u_{+,j}\|^2_{\widetilde{\mathcal{H}}}\delta_{j,k}\big)_{1\le j,k\le n} \\ &\quad + (1+z^2)\big((u_+, (\widetilde{H}_{F^\perp,K^\perp} - z)^{-1}u_+)_{\widetilde{\mathcal{H}}}\big)_{1\le j,k\le n}, \quad z \in \mathbb{C}_+,\end{aligned} \tag{7.85}$$

where $\widetilde{H}_{F^\perp,K^\perp} \geq 0$ *denotes a nonnegative self-adjoint extension of some densely defined closed operator* $H \geq 0$ *with deficiency indices* (n,n) *and deficiency subspace* $\{u_{+,j} \in \ker(H^* - i)\}_{1\le j,k\le n}$ *in some separable complex Hilbert space* $\widetilde{\mathcal{H}}$ *such that* $\mathcal{D}(\widetilde{H}_{F^\perp} \cap \mathcal{D}(H_F) = \mathcal{D}(H) = \mathcal{D}(\widetilde{H}_{K^\perp} \cap \mathcal{D}(H_K)$*.*
In each case (i)–(v) one has

$$\int_{\mathbb{R}} d\widetilde{\Omega}(\lambda)(1+\lambda^2)^{-1} = \big(\|u_{+,j}\|^2_{\widetilde{\mathcal{H}}}\delta_{j,k}\big)_{1\le j,k\le n}, \tag{7.86}$$

where $\widetilde{\Omega}$ *denotes the measure in the Herglotz representation of* $\widetilde{M}(z)$*. Moreover,* H *may be chosen prime and* $\widetilde{\mathcal{H}}$ *separable.*

Proof. We use the notation established in Theorem 7.2. Define

$$u_{+,j}(\lambda) = (\lambda - i)^{-1}\underline{e}_j, \quad j = 1,\dots,n, \tag{7.87}$$

then

$$\begin{aligned}\|u_{+,j}\|^2_{\widetilde{\mathcal{H}}}\delta_{j,k} = (u_{+,j}, u_{+,k})_{\widetilde{\mathcal{H}}} &= \int_{\mathbb{R}} (\underline{e}_j, d\widetilde{\Omega}(\lambda)\underline{e}_k)_{\mathbb{C}^n}\,(1+\lambda^2)^{-1} \\ &= \int_{\mathbb{R}} d\widetilde{\Omega}_{j,k}(\lambda)(1+\lambda^2)^{-1}\end{aligned} \tag{7.88}$$

and

$$\begin{aligned}&z\|u_{+,j}\|^2_{\widetilde{\mathcal{H}}}\delta_{j,k} + (1+z^2)(u_{+,j}, (\widetilde{H} - z)^{-1}u_{+,k})_{\widetilde{\mathcal{H}}} \\ &= \int_{\mathbb{R}} (\underline{e}_j, d\widetilde{\Omega}(\lambda)\underline{e}_k)_{\mathbb{C}^n}\,(z(1+\lambda^2)^{-1} + (1+z^2)(\lambda - z)^{-1}(1+\lambda^2)^{-1}) \\ &= \int_{\mathbb{R}} d\widetilde{\Omega}_{j,k}(\lambda)((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}) = \widetilde{M}_{j,k}(z)\end{aligned} \tag{7.89}$$

proves (7.81) and hence part (i). Parts (ii) and (iii) then follow in the same manner from Theorems 7.2 and 7.3. Similarly, parts (iv) and (v) follow from Theorems 7.2 and 7.5. ∎

We also formulate the analog of Theorem 4.7.

Theorem 7.9. *Suppose $M_\ell \in \mathcal{N}_0^{n\times n}$ with corresponding measures Ω_ℓ in the Herglotz representation of M_ℓ, $\ell = 1,2$, and $M_1 \neq M_2$. Then M_1 and M_2 can be realized as*

$$\begin{aligned} M_\ell(z) = {} & z\big(\|u_{+,j}\|^2_{\mathcal{H}}\delta_{j,k}\big)_{1\leq j,k\leq n} \\ & + (1+z^2)\big((u_{+,j},(H_\ell - z)^{-1}u_{+,k})_{\mathcal{H}}\big)_{1\leq j,k\leq n}, \quad \ell=1,2,\ z\in\mathbb{C}_+, \end{aligned} \tag{7.90}$$

where H_ℓ, $\ell=1,2$ are distinct self-adjoint extensions of one and the same densely defined closed symmetric operator H (which may be chosen prime) with deficiency indices (n,n) and deficiency subspace $\{u_{+,j}\}_{1\leq j,k\leq n} \in \ker(H^*-i)$ in some complex Hilbert space $\mathcal{H}$ (which may be chosen separable) if and only if the following conditions hold:

$$\int_{\mathbb{R}} d\Omega_1(\lambda)(1+\lambda^2)^{-1} = \int_{\mathbb{R}} d\Omega_2(\lambda)(1+\lambda^2)^{-1} = \big(\|u_{+,j}\|^2_{\mathcal{H}}\delta_{j,k}\big)_{1\leq j,k\leq n}, \tag{7.91}$$

and for all $z\in\mathbb{C}_+$,

$$\begin{aligned} M_2(z) = {} & \big(-\big(\|u_{+,j}\|^2_{\mathcal{H}}\delta_{j,k}\big)_{1\leq j,k\leq n} e^{-i\alpha_2}(\sin(\alpha_2)\cos(\alpha_1)-\cos(\alpha_2)\sin(\alpha_1))e^{i\alpha_1} \\ & + \big(\|u_{+,j}\|^2_{\mathcal{H}}\delta_{j,k}\big)_{1\leq j,k\leq n} e^{-i\alpha_2}(\cos(\alpha_2)\cos(\alpha_1) \\ & + \sin(\alpha_2)\sin(\alpha_1))e^{i\alpha_1}\big(\|u_{+,j}\|^{-2}_{\mathcal{H}}\delta_{j,k}\big)_{1\leq j,k\leq n}M_1(z)\big) \\ & \times \big(e^{-i\alpha_2}(\cos(\alpha_2)\cos(\alpha_1)+\sin(\alpha_2)\sin(\alpha_1))e^{i\alpha_1} \\ & + e^{-i\alpha_2}(\sin(\alpha_2)\cos(\alpha_1)-\cos(\alpha_2)\sin(\alpha_1))e^{i\alpha_1}\big(\|u_{+,j}\|^{-2}_{\mathcal{H}}\delta_{j,k}\big)_{1\leq j,k\leq n}M_1(z)\big)^{-1}, \\ & \textit{for some } \alpha_\ell = \alpha_\ell^* \in M_n(\mathbb{C}),\ \ell=1,2. \end{aligned} \tag{7.92}$$

Proof. Assuming (7.90), (7.91) follows from

$$M_\ell(i) = i\big(\|u_{+,j}\|^2_{\mathcal{H}}\delta_{j,k}\big)_{1\leq j,k\leq n} = i\int_{\mathbb{R}} d\Omega(\lambda)(1+\lambda^2)^{-1}, \quad \ell=1,2, \tag{7.93}$$

and (7.92) is clear from (7.58) upon identifying $\alpha_1=\alpha$, $\alpha_2=\beta$, $(\|u_{+,j}\|^{-2}_{\mathcal{H}}\delta_{j,k})_{1\leq j,k\leq n}M_1(z) = M_\alpha(z)$, and $(\|u_{+,j}\|^{-2}_{\mathcal{H}}\delta_{j,k})_{1\leq j,k\leq n}M_2(z) = M_\beta(z)$. (Without loss of generality we may assume that $\{u_{+,j}\}_{1\leq j\leq n}$ is a generating basis for H_ℓ, $\ell=1,2$, since otherwise we may apply the reduction (7.48).) Conversely, assume (7.91) and (7.92). By Theorem 7.8 (i), we may realize $M_1(z)$ as

$$\begin{aligned} & \big(\|u_{+,j}\|^{-2}_{\mathcal{H}}\delta_{j,k}\big)_{1\leq j,k\leq n}M_1(z) = zI_n \\ & + (1+z^2)\big(\|u_{+,j}\|^{-2}_{\mathcal{H}}\delta_{j,k}\big)_{1\leq j,k\leq n}\big((u_{+,j},(H_1-z)^{-1}u_{+,k})\big)_{1\leq j,k\leq n}. \end{aligned} \tag{7.94}$$

By (7.48) we may assume that $\{u_{+,j}\}_{1\leq j\leq n}$ is a generating basis for H_1 and identify H_1 with H_α defined in (7.29). If H_β is another self-adjoint extension of H defined as in (7.29), distinct from H_α, introduce

$$M_\beta(z) = zI_n + (1+z^2)\big(\|u_{+,j}\|^{-2}_{\mathcal{H}}\delta_{j,k}\big)_{1\leq j,k\leq n}\big((u_{+,j},(H_\beta-z)^{-1}u_{+,k})\big)_{1\leq j,k\leq n}. \tag{7.95}$$

By (7.58) one obtains $(M_\alpha(z) = (\|u_{+,j}\|^{-2}_{\mathcal{H}}\delta_{j,k})_{1\leq j,k\leq n}M_1(z))$,

$$\begin{aligned} M_\beta(z) = {} & \big(-e^{-i\beta}(\sin(\beta)\cos(\alpha)-\cos(\beta)\sin(\alpha))e^{i\alpha} \\ & + e^{-i\beta}(\cos(\beta)\cos(\alpha)+\sin(\beta)\sin(\alpha))e^{i\alpha}\big(\|u_{+,j}\|^{-2}_{\mathcal{H}}\delta_{j,k}\big)_{1\leq j,k\leq n}M_1(z)\big) \\ & \times \big(e^{-i\beta}(\cos(\beta)\cos(\alpha)+\sin(\beta)\sin(\alpha))e^{i\alpha} \end{aligned} \tag{7.96}$$

$$+ e^{-i\beta}(\sin(\beta)\cos(\alpha) - \cos(\beta)\sin(\alpha))e^{i\alpha}\left(\|u_{+,j}\|_{\mathcal{H}}^{-2}\delta_{j,k}\right)_{1\le j,k\le n}M_1(z)\big)^{-1}.$$

A comparison of (7.92) and (7.96) then yields $(\|u_{+,j}\|_{\mathcal{H}}^2\delta_{j,k})_{1\le j,k\le n}M_\beta(z) = M_2(z)$, $\alpha = \alpha_1$, and $\beta = \alpha_2$, completing the proof. □

Clearly Remark 4.8 applies in the present matrix-valued context.

For different types of realization theorems in the context of conservative systems, see, for instance, [16]–[19], [142], and [143].

Finally we briefly turn to Hamiltonian systems on a half-line following Hinton and Shaw [76]–[80] (see also [75], [97], [98]). These systems describe matrix-valued Schrödinger and Dirac-type differential and difference operators (see, e.g., [52], [56], [59], [90], [99], and [145]). Let $A, B \in L^1([0,R])^{2n\times 2n}$ for all $R > 0$, $A(x) = A(x)^*$, $B(x) = B(x)^*$ for a.e. $x > 0$. Moreover, suppose that for some $1 \le r \le n$, $A(x) = \left(\begin{smallmatrix} W(x) & 0 \\ 0 & 0 \end{smallmatrix}\right)$, $W \in L^1([0,R])^{r\times r}$ for all $R > 0$, $W(x) > 0$ for a.e. $x > 0$. For $\underline{\psi}(z,\cdot) \in AC([0,R])^{2n}$ for all $R > 0$, $z \in \mathbb{C}$, consider the formally symmetric Hamiltonian system

$$J_{2n}\underline{\psi}'(z,x) = (zA(x) + B(x))\underline{\psi}(z,x), \quad x > 0 \tag{7.97}$$

and suppose Atkinson's definiteness condition

$$\int_a^b dx(\hat{\underline{\psi}}(z,x), A(x)\hat{\underline{\psi}}(z,x))_{\mathbb{C}^{2n}} > 0 \text{ for all } 0 \le a < b < \infty \tag{7.98}$$

whenever $\hat{\underline{\psi}}$ satisfies $0 \neq \hat{\underline{\psi}}(z,x) \in AC([0,R])^{2n}$ for all $R > 0$ and (7.97). Introduce for $0 \le c < d \le \infty$,

$$L_A^2((c,d)) = \{\underline{f} : (c,d) \to \mathbb{C}^{2n} \text{ measurable} \,|\, \int_c^d dx(\underline{f}(x), A(x)\underline{f}(x))_{\mathbb{C}^{2n}} < \infty\} \tag{7.99}$$

and for $x_0 > 0$,

$$N(z,0) = \{\underline{f} \in L_A^2((0,x_0)) \,|\, J_{2n}\underline{f}' = (zA + B)\underline{f} \text{ a.e. on } (0,x_0)\}, \tag{7.100}$$

$$N(z,\infty) = \{\underline{f} \in L_A^2((x_0,\infty)) \,|\, J_{2n}\underline{f}' = (zA + B)\underline{f} \text{ a.e. on } (x_0,\infty)\}. \tag{7.101}$$

Then (7.97) is defined to be in the limit point (respectively, limit circle) case at $e \in \{c,d\}$ if $\dim_{\mathbb{C}}(N(z_\pm,e)) = n$ (respectively, $\dim_{\mathbb{C}}(N(z_\pm,e)) = 2n$) for some (and hence for all) $z_+ \in \mathbb{C}_+$ and $z_- \in \mathbb{C}_-$. There are of course also intermediate cases between the limit point and limit circle case but we omit such considerations for simplicity. For more details in this connection see, for instance, [90] and [122].

Next, consider $\alpha_p, \beta_p \in M_n(\mathbb{C})$, $p = 1,2$, satisfying $\operatorname{rank}(\alpha) = \operatorname{rank}(\beta) = n$, where $\alpha = (\alpha_1, \alpha_2)$, $\beta = (\beta_1, \beta_2)$ are $2n \times n$ matrices over $\mathbb{C}$, and

$$\alpha_1\alpha_1^* + \alpha_2\alpha_2^* = I_n = \beta_1\beta_1^* + \beta_2\beta_2^*, \quad \alpha_1\alpha_2^* = \alpha_2\alpha_1^*, \quad \beta_1\beta_2^* = \beta_2\beta_1^*. \tag{7.102}$$

Let $\Psi_\alpha(z,x) \in M_{2n}$, $z \in \mathbb{C}$ be a fundamental system of solutions of (7.97) satisfying

$$\Psi_\alpha(z,0) = \begin{pmatrix} \alpha_1^* & -\alpha_2^* \\ \alpha_2^* & \alpha_1^* \end{pmatrix}, \quad z \in \mathbb{C} \tag{7.103}$$

and partition $\Psi_\alpha(z,x)$ into $n \times n$ blocks,

$$\Psi_\alpha(z,x) = \begin{pmatrix} \theta_{\alpha,1}(z,x) & \phi_{\alpha,1}(z,x) \\ \theta_{\alpha,2}(z,x) & \phi_{\alpha,2}(z,x) \end{pmatrix}. \tag{7.104}$$

Then $\Psi_\alpha(z,x)$ is entire in $z \in \mathbb{C}$ and one defines

$$M_{\alpha,\beta,R}(z) = -(\beta_1\phi_{\alpha,1}(z,R) + \beta_2\phi_{\alpha,2}(z,R))^{-1}(\beta_1\theta_{\alpha,1}(z,R) + \beta_2\theta_{\alpha,2}(z,R)). \tag{7.105}$$

$M_{\alpha,\beta,R}(z)$ is the Weyl-Titchmarsh matrix corresponding to the boundary value problem

$$J_{2n}\underline{\psi}'(z,x) = (zA(x) + B(x))\underline{\psi}(z,x), \quad 0 \le x \le R, \tag{7.106}$$
$$\alpha\underline{\psi}(z,0) = 0, \ \beta\underline{\psi}(z,R) = 0.$$

As shown in detail by Hinton and Shaw [76], [78], [79],

$$\lim_{R\uparrow\infty} M_{\alpha,\beta,R}(z) = M_\alpha(z), \quad z \in \mathbb{C}\backslash\mathbb{R} \tag{7.107}$$

exists and is independent of β if and only if (7.97) is in the limit point case at ∞. In the limit circle case at ∞, uniqueness and independence of β is lost and we denote by $\widehat{M}_\alpha(z)$ a parametrization of all possible limit points of $M_{\alpha,\beta,R}(z)$ as $R \uparrow \infty$. $M_\alpha(z)$ (respectively, $\widehat{M}_\alpha(z)$) are matrix-valued Herglotz functions with representations

$$M_\alpha(z) = C_\alpha + \int_{\mathbb{R}} d\Omega_\alpha(\lambda)((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}), \quad C_\alpha = C_\alpha^* \tag{7.108}$$

and one verifies

$$(\theta_{\alpha,p}(z,\cdot) + \phi_{\alpha,p}(z,\cdot)M_\alpha(z)) \in L^2_A((0,\infty)), \quad p = 1,2, \ z \in \mathbb{C}\backslash\mathbb{R}. \tag{7.109}$$

Moreover,

$$M_\alpha(z) = (-\alpha_2 + \alpha_1 M(z))(\alpha_1 + \alpha_2 M(z))^{-1}, \tag{7.110}$$

where $M(z) = M_{(I_n,0)}(z)$. Analogous relationships hold for $\widehat{M}_\alpha(z)$ in the limit circle case at ∞. A comparison of (7.110) and (6.40) suggests the introduction of

$$A(\alpha) = \begin{pmatrix} \alpha_1 & \alpha_2 \\ -\alpha_2 & \alpha_1 \end{pmatrix} \in \mathcal{A}_{2n}. \tag{7.111}$$

In particular, Theorem 6.6 applies (with $A_{1,1}(\alpha) = A_{2,2}(\alpha) = \alpha_1$, $A_{1,2}(\alpha) = -A_{2,1}(\alpha) = \alpha_2$).

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Appendix A. Examples of Scalar Herglotz Functions

For convenience of the reader we collect some standard examples of scalar Herglotz functions and their explicit representations (cf. [11], [21], Ch. V, [43], Ch. II, [48], Ch. 2).

In the following we denote Lebesgue measure on $\mathbb{R}$ by $d\lambda$ and a pure point measure supported at $x \in \mathbb{R}$ with mass one by $\mu_{\{x\}}$,

$$\operatorname{supp}(\mu_{\{x\}}) = \{x\}, \quad \mu_{\{x\}}(\{x\}) = 1. \tag{A.1}$$

We start with very simple examples and progressively discuss more sophisticated ones.

$$c + id = c + d\pi^{-1} \int_{\mathbb{R}} d\lambda\, ((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}), \quad c \in \mathbb{R},\ d \geq 0. \tag{A.2}$$

$$\ln(id) = \ln(d) + (i\pi/2) = \ln(d) + 2^{-1} \int_{\mathbb{R}} d\lambda\, ((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}), \quad d \geq 0. \tag{A.3}$$

$$c + dz, \quad c \in \mathbb{R},\ d \geq 0. \tag{A.4}$$

$$-z^{-1} = \int_{\mathbb{R}} d\mu_{\{0\}}(\lambda)\, (\lambda - z)^{-1}. \tag{A.5}$$

$$\ln(z) = \int_{-\infty}^{0} d\lambda\, ((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}), \tag{A.6}$$

$$\ln(-z^{-1}) = \int_{0}^{\infty} d\lambda\, ((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}), \tag{A.7}$$

where $\ln(\cdot)$ denotes the principal value of the logarithm (i.e., with cut along $(-\infty, 0]$ and $\ln(\lambda) > 0$ for $\lambda > 0$).

$$\begin{aligned} z^r &= \exp(r \ln(z)) \\ &= \cos(r\pi/2) + \pi^{-1}\sin(r\pi) \int_{-\infty}^{0} d\lambda\, |\lambda|^r ((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}), \quad 0 < r < 1, \end{aligned} \tag{A.8}$$

$$\begin{aligned} -z^{-r} &= -\exp(-r \ln(z)) \\ &= -\cos(r\pi/2) + \pi^{-1}\sin(r\pi) \int_{-\infty}^{0} d\lambda\, |\lambda|^{-r} ((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}), \quad 0 < r < 1. \end{aligned} \tag{A.9}$$

$$\begin{aligned} \tan(z) &= \sum_{n\in\mathbb{Z}} (((n+\tfrac{1}{2})\pi - z)^{-1} - (n+\tfrac{1}{2})\pi(1+(n+\tfrac{1}{2})^2\pi^2)^{-1}) \\ &= \int_{\mathbb{R}} d\omega(\lambda)\, ((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}), \end{aligned} \tag{A.10}$$

$$\omega = \sum_{n\in\mathbb{Z}} \mu_{\{(n+\frac{1}{2})\pi\}}, \tag{A.11}$$

$$\begin{aligned} -\cot(z) &= \sum_{n\in\mathbb{Z}} ((n\pi - z)^{-1} - n\pi(1+n^2\pi^2)^{-1}) \\ &= \int_{\mathbb{R}} d\omega(\lambda)\, ((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}), \end{aligned} \tag{A.12}$$

$$\omega = \sum_{n\in\mathbb{Z}} \mu_{\{n\pi\}}. \tag{A.13}$$

The psi or digamma function,

$$\psi(z) = \Gamma'(z)/\Gamma(z) = C + \sum_{n\in\mathbb{N}_0} ((-n - z)^{-1} + n(1+n^2)^{-1})$$

$$= \int_{\mathbb{R}} d\omega(\lambda)\,((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}), \tag{A.14}$$

$$\omega = \sum_{n\in\mathbb{N}_0} \mu_{\{-n\}}, \quad C = -\gamma + \sum_{n\in\mathbb{N}_0} ((n+1)^{-1} - n(1+n^2)^{-1}). \tag{A.15}$$

Here $\Gamma(z)$ denotes the gamma function, $\gamma = -\psi(1) = .572\ldots$ Euler's constant (cf. [1], Ch. 6), and $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$.

$$\frac{z-\lambda_2}{z-\lambda_1} = 1 + (\lambda_2 - \lambda_1)\int_{\mathbb{R}} d\mu_{\{\lambda_1\}}(\lambda)\,(\lambda - z)^{-1}, \quad \lambda_1 < \lambda_2, \tag{A.16}$$

$$\ln\left(\frac{z-\lambda_2}{z-\lambda_1}\right) = \int_{\lambda_1}^{\lambda_2} d\lambda\,(\lambda - z)^{-1}, \quad \lambda_1 < \lambda_2. \tag{A.17}$$

Next we turn to Weyl-Titchmarsh m-functions $m_{a(\alpha)}(z)$ associated with the operator H_α in $L^2([0,\infty);dx)$ defined by

$$\begin{aligned} &(H_\alpha g)(x) = -g''(x), \quad x > 0, \\ &\mathcal{D}(H_\alpha) = \{g \in L^2([0,\infty);dx) \,|\, g, g' \in AC([0,R]) \text{ for all } R > 0\ ; \\ &\qquad -g'' \in L^2([0,\infty);dx);\ \sin(\alpha)g'(0_+) + \cos(\alpha)g(0_+) = 0\}, \quad \alpha \in (0,\pi). \end{aligned} \tag{A.18}$$

These are Herglotz functions of the type

$$m_{a(\alpha)}(z) = \frac{-\sin(\alpha) + \cos(\alpha)iz^{1/2}}{\cos(\alpha) + \sin(\alpha)iz^{1/2}} = \cot(\alpha) + \int_{\mathbb{R}} d\omega_{a(\alpha)}(\lambda)\,(\lambda - z)^{-1}, \tag{A.19}$$

$$\omega_{a(\alpha)}(\lambda) = \begin{cases} 0,\ \lambda < 0,\ (\pi/2) \le \alpha < \pi \\ -2\frac{\cot(\alpha)}{\sin^2(\alpha)},\ -\infty < \lambda < -\cot^2(\alpha),\ 0 < \alpha < (\pi/2) \\ 0,\ -\cot^2(\alpha) < \lambda < 0,\ 0 < \alpha < (\pi/2) \\ \frac{2}{\pi}\lambda^{1/2},\ \lambda \ge 0,\ \alpha = (\pi/2) \\ \frac{2}{\pi\sin^2(\alpha)}\left(\lambda^{1/2} - \cot(\alpha)\arctan\left(\frac{\lambda^{1/2}}{\cot(\alpha)}\right)\right),\ \lambda \ge 0,\ \alpha \in (0,\pi)\backslash\{\pi/2\}, \end{cases} \tag{A.20}$$

where (cf. (2.12) and (3.10))

$$a(\alpha) = \begin{pmatrix} \cos(\alpha) & \sin(\alpha) \\ -\sin(\alpha) & \cos(\alpha) \end{pmatrix} \in \mathcal{A}_2. \tag{A.21}$$

Similarly,

$$m_{a(0)} = iz^{1/2} = -2^{-1/2} + \pi^{-1}\int_0^\infty d\lambda\,\lambda^{1/2}((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}) \tag{A.22}$$

corresponds to the remaining self-adjoint (Friedrichs) boundary condition $\alpha = 0$, that is, to $g(0_+) = 0$ in (A.18).

Finally we describe a class of Herglotz functions fundamental in Floquet theory of periodic Schrödinger operators on $\mathbb{R}$. Consider a sequence $\{\lambda_n\}_{n\in\mathbb{N}_0} \subset \mathbb{R}$,

$$0 = \lambda_0 < \lambda_1 \le \lambda_2 < \lambda_3 \le \lambda_4 < \cdots \tag{A.23}$$

such that asymptotically

$$\lambda_{2n},\, \lambda_{2n-1} \underset{n\to\infty}{=} (n\pi)^2 + O(1). \tag{A.24}$$

Define an entire function $\Delta(z)$ such that

$$\Delta(z) - 1 = \frac{(\lambda_0 - z^2)}{2} \prod_{n\in\mathbb{N}} \frac{(\lambda_{4n-1} - z^2)(\lambda_{4n} - z^2)}{(2n\pi)^4}, \tag{A.25}$$

$$\Delta(z) + 1 = 2 \prod_{n\in\mathbb{N}_0} \frac{(\lambda_{4n+1} - z^2)(\lambda_{4n+2} - z^2)}{((2n+1)\pi)^4} \tag{A.26}$$

and hence,

$$\Delta(z)^2 - 1 = (\lambda_0 - z^2) \prod_{n\in\mathbb{N}} \frac{(\lambda_{2n-1} - z^2)(\lambda_{2n} - z^2)}{(n\pi)^4}. \tag{A.27}$$

Moreover, define

$$\theta(z) = -\int_0^z d\zeta \, \frac{\Delta'(\zeta)}{(1-\Delta(\zeta)^2)^{1/2}}, \quad z \in \mathbb{C}_+, \tag{A.28}$$

where the square root branch in (A.28) is chosen to be positive on the interval $(0, \lambda_1^{1/2})$. Then

$$\cos(\theta(z)) = \Delta(z) \tag{A.29}$$

and, as shown in [113], Sect. 3.4, θ is a Herglotz function with a representation of the type

$$\theta(z) = c + z + \pi^{-1} \int_{\mathbb{R}} d\lambda \, \mathrm{Im}(\theta(\lambda)((\lambda - z)^{-1} - \lambda(1+\lambda^2)^{-1}) \tag{A.30}$$

for some $c \in \mathbb{R}$. In the case where the sequence $\{\lambda_n\}_{n\in\mathbb{N}_0}$ represents the periodic and antiperiodic eigenvalues associated with a Schrödinger operator $H = -\frac{d^2}{dx^2} + q$, with $q \in L^1_{\mathrm{loc}}(\mathbb{R})$ real-valued and of period one, $\Delta(z)$ represents the corresponding Floquet discriminant and $\theta(z)$ the Floquet (Bloch) momentum associated with H. In this case one verifies (see, e.g., [86], [93])

$$\theta(z) = \frac{i}{2} \int_0^1 dx \, G(z^2, x, x)^{-1}, \quad z \in \mathbb{C}_+, \tag{A.31}$$

with $G(\zeta, x, y) = (H - \zeta)^{-1}(x, y)$ the Green's function of H.

Analogous observations apply to one-dimensional Dirac-type operators.

Appendix B. Krein's Formula and Linear Fractional Transformations

The main purpose of this appendix is to provide a proof of (7.58) (cf. Theorem B.6) following its derivation in [58]. Our method of proof is based on Krein's formula, which describes the resolvent difference of two self-adjoint extensions A_1 and A_2 of a densely defined closed symmetric linear operator A with deficiency indices (n, n), $n \in \mathbb{N}$. (Reference [58] treats this topic in the general case where $n \in \mathbb{N} \cup \{\infty\}$. Here we specialize to the case $n < \infty$.) Since the latter formula is interesting in its own right we start with the basic setup following [3].

Let $\mathcal{H}$ be a complex separable Hilbert space, $\dot{A} : \mathcal{D}(\dot{A}) \to \mathcal{H}$, $\overline{\mathcal{D}(\dot{A})} = \mathcal{H}$ a densely defined closed symmetric linear operator in $\mathcal{H}$ with finite and equal deficiency indices $\mathrm{def}(\dot{A}) = (r, r)$, $r \in \mathbb{N}$. Let A_ℓ, $\ell = 1, 2$, be two distinct self-adjoint extensions of $\dot{A}$ and denote by A the maximal common part of A_1 and A_2, that is, A is the largest closed extension of $\dot{A}$ with $\mathcal{D}(A) = \mathcal{D}(A_1) \cap \mathcal{D}(A_2)$. Let $0 \le p \le r - 1$

be the maximal number of elements in $\mathcal{D}(A) = \mathcal{D}(A_1) \cap \mathcal{D}(A_2)$ which are linearly independent modulo $\mathcal{D}(\dot{A})$. Then A has deficiency indices $\mathrm{def}(A) = (n, n)$, $n = r - p$. Next, denote by $\ker(A^* - z)$, $z \in \mathbb{C}\backslash\mathbb{R}$ the deficiency subspaces of A and define

$$U_{1,z,z_0} = I + (z - z_0)(A_1 - z)^{-1} = (A_1 - z_0)(A_1 - z)^{-1}, \ z, z_0 \in \rho(A_1), \tag{B.1}$$

where I denotes the identity operator in $\mathcal{H}$ and $\rho(T)$ abbreviates the resolvent set of T. One verifies

$$U_{1,z_0,z_1} U_{1,z_1,z_2} = U_{1,z_0,z_2}, \ z_0, z_1, z_2 \in \rho(A_1) \tag{B.2}$$

and

$$U_{1,z,z_0} \ker(A^* - z_0) = \ker(A^* - z). \tag{B.3}$$

Let $\{u_j(i)\}_{1 \le j \le n}$ be an orthonormal basis for $\ker(A^* - i)$ and define

$$u_{1,j}(z) = U_{1,z,i}\, u_j(i), \ 1 \le j \le n, \ z \in \rho(A_1). \tag{B.4}$$

Then $\{u_{1,j}(z)\}_{1 \le j \le n}$ is a basis for $\ker(A^* - z)$, $z \in \rho(A_1)$ and since $U_{1,-i,i} = (A_1 - i)(A_1 + i)^{-1}$ is the unitary Cayley transform of A_1, $\{u_{1,j}(-i)\}_{1 \le j \le n}$ is in fact an orthonormal basis for $\ker(A^* + i)$.

The basic result on Krein's formula, as presented by Akhiezer and Glazman [3], Sect. 84, then reads as follows.

Theorem B.1. (Krein's formula, [3], Sect. 84)
There exists a $P_{1,2}(z) = (P_{1,2,j,k}(z))_{1 \le j,k \le n} \in M_n(\mathbb{C})$, $z \in \rho(A_2) \cap \rho(A_1)$, such that

$$\det(P_{1,2}(z)) \neq 0, \ z \in \rho(A_2) \cap \rho(A_1), \tag{B.5}$$

$$P_{1,2}(z)^{-1} = P_{1,2}(z_0)^{-1} - (z - z_0)(u_{1,j}(\bar{z}), u_{1,k}(z_0)), \ z, z_0 \in \rho(A_1), \tag{B.6}$$

$$\mathrm{Im}\,(P_{1,2}(i)^{-1}) = -I_n, \tag{B.7}$$

$$(A_2 - z)^{-1} = (A_1 - z)^{-1} + \sum_{j,k=1}^{n} P_{1,2,j,k}(z)(u_{1,k}(\bar{z}), \cdot\,)u_{1,j}(z), \quad z \in \rho(A_2) \cap \rho(A_1). \tag{B.8}$$

We note that $P_{1,2}(z)^{-1}$ extends by continuity from $z \in \rho(A_2) \cap \rho(A_1)$ to all of $\rho(A_1)$ since the right-hand side of (B.6) is continuous for $z \in \rho(A_1)$. The normalization condition (B.7) is not mentioned in [3] but it trivially follows from (B.6) and the fact

$$(u_j(i), u_k(i)) = \delta_{j,k}, \quad 1 \le j, k \le n \tag{B.9}$$

(where $\delta_{j,k}$ denotes Kronecker's symbol) and from

$$P_{1,2}^*(z) = P_{1,2}(\bar{z}), \quad z \in \rho(A_1) \cap \rho(A_2). \tag{B.10}$$

Taking $z = \overline{z_0}$ in (B.6) shows that $-P_{1,2}(z)^{-1}$ and hence $P_{1,2}(z)$ is a matrix-valued Herglotz function, that is,

$$\mathrm{Im}\,(P_{1,2}(z)) > 0, \ z \in \mathbb{C}_+. \tag{B.11}$$

Strict positive definiteness in (B.11) follows from the fact that $\{u_{1,k}(z)\}_{1 \le k \le n}$ are linearly independent for $z \in \mathbb{C}_+$ and hence $((u_{1,j}(z), u_{1,k}(z))_{1 \le j,k \le n} > 0$.

Krein's formula has been used in a great variety of problems in mathematical physics as can be seen from the extensive number of references provided, for instance, in [4]. (A complete bibliography on Krein's formula is impossible in this context.)

Next we describe the connection between $P_{1,2}(z)$ and von Neumann's parametrization of self-adjoint extensions of A. Due to (B.6), $P_{1,2}(z)^{-1}$ is determined for all $z \in \rho(A_1)$ in terms of $P_{1,2}(i)^{-1}$, $(A_1 - z)^{-1}$ and $\{u_j(i)\}_{1\le j\le n}$,

$$P_{1,2}(z)^{-1} = P_{1,2}(i)^{-1} - (z-i)I_n - (1+z^2)(u_j(i), (A_1 - z)^{-1}u_k(i))_{1\le j,k\le n}), \quad z \in \rho(A_1). \tag{B.12}$$

Hence it suffices to focus on

$$P_{1,2}(i)^{-1} = \operatorname{Re}(P_{1,2}(i)^{-1}) - iI_n. \tag{B.13}$$

Let

$$\mathcal{U}_\ell : \ker(A^* - i) \to \ker(A^* + i), \quad \ell = 1, 2, \tag{B.14}$$

be the linear isometric isomorphisms that parameterize A_ℓ according to von Neumann's formula

$$A_\ell(f + (I + \mathcal{U}_\ell)u_+) = Af + i(I - \mathcal{U}_\ell)u_+, \tag{B.15}$$
$$\mathcal{D}(A_\ell) = \{(g + (I + \mathcal{U}_\ell)u_+) \in \mathcal{D}(A^*) \,|\, g \in \mathcal{D}(A),\, u_+ \in \ker(A^* - i)\},\ \ell = 1, 2.$$

Denote by $U_\ell = (U_{\ell,j,k})_{1\le j,k\le n} \in M_n(\mathbb{C})$, $\ell = 1,2$ the unitary matrix representation of $\mathcal{U}_\ell$ with respect to the bases $\{u_j(i)\}_{1\le j\le n}$ and $\{u_{1,j}(-i)\}_{1\le j\le n}$ of $\ker(A^* - i)$ and $\ker(A^* + i)$ respectively, that is,

$$\mathcal{U}_\ell u_j(i) = \sum_{k=1}^n U_{\ell,k,j}u_{1,k}(-i),\ 1 \le j \le n,\ \ell = 1, 2. \tag{B.16}$$

Lemma B.2.
(i). $U_1 = -I_n$.
(ii). $(u_{1,j}(-i) + \sum_{k=1}^n \overline{U_{\ell,j,k}}u_k(i)) \in \mathcal{D}(A_\ell)$, $1 \le j \le n$, $\ell = 1,2$, *and*

$$(A_\ell - i)(u_{1,j}(-i) + \sum_{k=1}^n \overline{U_{\ell,j,k}}u_k(i)) = -2iu_{1,j}(-i),\ 1 \le j \le n,\ \ell = 1, 2. \tag{B.17}$$

Proof. (i). Since $u_{1,j}(-i) - u_j(i) = -2i(A_1 + i)^{-1}u_j(i) \in \mathcal{D}(A_1)$, $1 \le j \le n$ by (B.1) and (B.4), one infers

$$u_{1,j}(-i) - u_j(i) = c_j(I + \mathcal{U}_1)u_{+,j},\ 1 \le j \le n \tag{B.18}$$

for some $u_{+,j} \in \ker(A^* - i)$ and $c_j \in \mathbb{C}$. Since $\mathcal{D}(A^*)$ decomposes into the direct sum $\mathcal{D}(A^*) = \mathcal{D}(A) \dotplus \ker(A^* - i) \dotplus \ker(A^* + i)$, one infers

$$c_j u_{+,j} = -u_j(i), \quad c_j\mathcal{U}_1 u_{+,j} = -\mathcal{U}_1 u_j(i) = u_{1,j}(-i), \tag{B.19}$$

and hence $U_1 = -I_n$.
(ii). Using (B.16) one computes

$$\mathcal{U}_\ell \sum_{k=1}^n \overline{U_{\ell,j,k}}u_k(i) = \sum_{k=1}^n \sum_{m=1}^n \overline{U_{\ell,j,k}}U_{\ell,m,k}u_{1,m}(-i) = u_{1,j}(-i),\ 1 \le j \le n, \tag{B.20}$$

utilizing unitarity of U_ℓ, $\ell = 1, 2$. Hence,

$$u_{1,j}(-i) + \sum_{k=1}^n \overline{U_{\ell,j,k}}u_k(i) = (I + \mathcal{U}_\ell)(\sum_{k=1}^n \overline{U_{\ell,j,k}}u_k(i)) \in \mathcal{D}(A_\ell), \tag{B.21}$$

and thus (B.17) follows from

$$(A_\ell - i)(u_{1,j}(-i) + \sum_{k=1}^{n} \overline{U_{\ell,j,k}} u_k(i)) = (A^* - i)(u_{1,j}(-i) + \sum_{k=1}^{n} \overline{U_{\ell,j,k}} u_k(i)) \\ = -2i u_{1,j}(-i). \tag{B.22}$$

□

This yields the desired connection between $P_{1,2}(i)$ and U_ℓ, $\ell = 1, 2$.

Corollary B.3.

$$P_{1,2}(i) = \frac{i}{2}(I_n + U_2^{-1}) = \frac{i}{2}(U_2^{-1} - U_1^{-1}). \tag{B.23}$$

Proof. By (B.17), (B.8), and (B.9),

$$((A_2 - i)^{-1} - (A_1 - i)^{-1})u_{1,j}(-i) = \frac{i}{2}\sum_{k=1}^{n}(\delta_{j,k} + \overline{U_{2,j,k}})u_k(i) = \sum_{k=1}^{n} P_{1,2,k,j}(i)u_k(i). \tag{B.24}$$

Unitarity of U_2 and linear independence of the $u_k(i)$ then complete the proof of (B.23). □

Finally, we turn to our main goal, the Weyl-Titchmarsh M-matrices $M_1(z)$ and $M_2(z)$ associated with A_1 and A_2. Define (cf. [42], [58], [107])

$$M_\ell(z) = zI_n + (1 + z^2)\big((u_j(i), (A_\ell - z)^{-1}u_k(i))_{1\le j,k\le n}\big), \quad z \in \rho(A_\ell),\ \ell = 1, 2. \tag{B.25}$$

$M_\ell(z)$ as defined in (B.25) are known to be matrix-valued Herglotz functions. More precisely, one can prove

Lemma B.4. [58] *Assume A_1 to be a self-adjoint extension of A. Then the Weyl-Titchmarsh matrix $M_1(z)$ is analytic for $z \in \mathbb{C}\backslash\mathbb{R}$ and*

$$\mathrm{Im}(z)\mathrm{Im}(M_1(z)) \ge (\max(1, |z|^2) + |\mathrm{Re}(z)|)^{-1}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{B.26}$$

In particular, $M_1(z)$ is an $n \times n$ matrix-valued Herglotz function.

Proof. Using (B.25), an explicit computation yields

$$\mathrm{Im}(z)\mathrm{Im}(M_1(z)) \tag{B.27}$$
$$= \big((u_j(i), (I + A_1^2)^{1/2}((A_1 - \mathrm{Re}(z))^2 + (\mathrm{Im}(z))^2)^{-1}(I + A_1^2)^{1/2}u_k(i))\big)_{1\le j,k\le n}.$$

Next we note that for $z \in \mathbb{C}\backslash\mathbb{R}$,

$$\frac{1 + \lambda^2}{(\lambda - \mathrm{Re}(z))^2 + (\mathrm{Im}(z))^2} \ge \frac{1}{\max(1, |z|^2) + |\mathrm{Re}(z)|}, \quad \lambda \in \mathbb{R}. \tag{B.28}$$

Since by the Rayleigh-Ritz technique, projection onto a subspace contained in the domain of a self-adjoint operator bounded from below can only raise the lowerbound of the spectrum (cf. [126], Sect. XIII.1), (B.27) and (B.28) prove (B.26). □

Combining (B.12), (B.13), and (B.25) for $\ell = 1$ yields

$$P_{1,2}(z)^{-1} = \mathrm{Re}\,((P_{1,2}(i)^{-1}) - M_1(z). \tag{B.29}$$

One infers the following result relating $M_1(z)$ and $M_2(z)$.

Theorem B.5. [58]

$$M_2(z) = (P_{1,2}(i) + (I_n + iP_{1,2}(i))M_1(z))((I_n + iP_{1,2}(i)) - P_{1,2}(i)M_1(z))^{-1} \tag{B.30}$$

$$= e^{-i\alpha_2}(\cos(\alpha_2) + \sin(\alpha_2)M_1(z))(\sin(\alpha_2) - \cos(\alpha_2)M_1(z))^{-1}e^{i\alpha_2}, \tag{B.31}$$

where $\alpha_2 \in M_n(\mathbb{C})$ denotes a self-adjoint matrix related to U_2 by $U_2 = e^{2i\alpha_2}$.

Proof. Using

$$(u_j(i), u_k(i)) = \delta_{j,k}, \tag{B.32}$$

$$(u_j(i), u_{1,k}(z)) = \delta_{j,k} + (z-i)(u_j(i), (A_1 - z)^{-1}u_k(i)), \tag{B.33}$$

$$(u_{1,j}(\bar{z}), u_k(i)) = \delta_{j,k} + (z+i)(u_j(i), (A_1 - z)^{-1}u_k(i)), \tag{B.34}$$

and Krein's formula (B.8), one infers

$$\begin{aligned}
M_{2,j,k}(z) &= z\delta_{j,k} + (1+z^2)(u_j(i), (A_2 - z)^{-1}u_k(i)) \\
&= z\delta_{j,k} + (1+z^2)(u_j(i), (A_1 - z)^{-1}u_k(i)) \\
&\quad + \sum_{s,t=1}^{n}(u_j(i), u_{1,s}(z))P_{1,2,s,t}(z)(u_{1,t}(\bar{z}), u_k(i))(1+z^2) \\
&= M_{1,j,k}(z) + \sum_{s,t=1}^{n}((z+i)\delta_{j,s} + (1+z^2)(u_j(i), (A_1 - z)^{-1}u_s(i)) \\
&\quad \times (P_{1,2}(i)^{-1} - (z-i)I_n - (1+z^2)((u_p(i), (A_1 - z)^{-1}u_q(i))_{1\le p,q\le n}))^{-1}_{s,t} \\
&\quad \times ((z-i)\delta_{t,k} + (1+z^2)(u_t(i), (A_1 - z)^{-1}u_k(i))).
\end{aligned} \tag{B.35}$$

Hence,

$$M_2(z) = M_1(z) + (iI_n + M_1(z))(P_{1,2}(i)^{-1} + iI_n - M_1(z))^{-1}(-iI_n + M_1(z)), \tag{B.36}$$

which easily reduces to (B.30). Equation (B.31) then follows from (B.23) and the elementary trigonometric identity

$$\mathrm{Re}\ (P_{1,2}(i)^{-1}) = \tan(\alpha_2), \ \ U_2 = e^{2i\alpha_2}. \tag{B.37}$$

□

Equation (B.31) is connected with the pair $(U_2, U_1) = (e^{2i\alpha_2}, -I_n)$. If one is interested in a general pair of self-adjoint extensions (A_α, A_β) of A, associated with (U_α, U_β), one proceeds as follows:

Theorem B.6. [58] *Let $U_\alpha = e^{2i\alpha}, U_\beta = e^{2i\beta} \in M_n(\mathbb{C})$ be the matrix representations of the operators $\mathcal{U}_\alpha, \mathcal{U}_\beta$ associated with two self-adjoint extensions A_α, A_β of A with respect to the basis $\{u_j(i)\}_{1\le j\le n}$ of $\ker(A^* - i)$ and any (not necessarily orthogonal) basis $\{v_j\}_{1\le j\le n}$ of $\ker(A^* + i)$. Then*

$$\begin{aligned}
M_\beta(z) = (&-e^{-i\beta}(\sin(\beta)\cos(\alpha) - \cos(\beta)\sin(\alpha))e^{i\alpha} \\
&+ e^{-i\beta}(\cos(\beta)\cos(\alpha) + \sin(\beta)\sin(\alpha))e^{i\alpha}M_\alpha(z)) \\
&\times (e^{-i\beta}(\cos(\beta)\cos(\alpha) + \sin(\beta)\sin(\alpha))e^{i\alpha} \\
&+ e^{-i\beta}(\sin(\beta)\cos(\alpha) - \cos(\beta)\sin(\alpha))e^{i\alpha}M_\alpha(z))^{-1}.
\end{aligned} \tag{B.38}$$

Proof. We start by proving (B.38) with respect to the orthogonal bases $\{u_j(i)\}_{1\le j\le n}$ and $\{u_{1,j}(-i)\}_{1\le j\le n}$ applying Theorem B.5. Assuming that the pairs (A_α, A_1) and (A_β, A_1) are relatively prime, one infers from (B.31),

$$M_\alpha(z) = e^{-i\alpha}(\cos(\alpha)+\sin(\alpha)M_1(z))(\sin(\alpha)-\cos(\alpha)M_1(z))^{-1}e^{i\alpha}, \tag{B.39}$$

$$M_\beta(z) = e^{-i\beta}(\cos(\beta)+\sin(\beta)M_1(z))(\sin(\beta)-\cos(\beta)M_1(z))^{-1}e^{i\beta}, \tag{B.40}$$

Computing $M_1(z)$ (corresponding to A_1 and $U_1=-I_n$) from (B.39) yields

$$M_1(z) = -e^{i\alpha}(\cos(\alpha)-\sin(\alpha)M_\alpha(z))(\sin(\alpha)+\cos(\alpha)M_\alpha(z))^{-1}e^{-i\alpha}. \tag{B.41}$$

Insertion of (B.41) into (B.40) then proves (B.38). Inspection of the eight trigonometric terms in (B.38) shows that they are of the type $(c_1 I_n + c_2 U_\beta^{-1})(c_3 I_n + c_4 U_\alpha)$ with $c_m \in \{\pm 1/4, \pm i/4\}$, $1\le m\le 4$. That is, they are matrix representations of $F_{\alpha,\beta} := (-c_1\mathcal{U}_1^{-1} + c_2\mathcal{U}_\beta^{-1})(-c_3\mathcal{U}_1 + c_4\mathcal{U}_\alpha)$. But $F_{\alpha,\beta}$ map $\ker(A^*-i)$ into itself, and hence matrix representations of $F_{\alpha,\beta}$ are independent of the basis chosen in $\ker(A^*+i)$. ☐

The material of this appendix in the general case where $\operatorname{def}(A)=(n,n)$, $n\in\mathbb{N}\cup\{\infty\}$, is considered in detail in [58].

Since the boundary values $\lim_{\varepsilon\downarrow 0} M_\alpha(\lambda+i\varepsilon)$, $\lambda\in\mathbb{R}$, contain spectral information on the self-adjoint extension A_α of A, relationships of the type (B.38) entail important connections between the spectra of A_α and A_β. In particular, the well-known unitary equivalence of the absolutely continuous parts $A_{\alpha,ac}$ and $A_{\beta,ac}$ of A_α and A_β can be inferred from (B.38) as discussed in detail in Section 7.

We conclude with a simple illustration.

Example B.7. $\mathcal{H} = L^2((0,\infty);dx)$,

$$\begin{aligned}
&A = -\frac{d^2}{dx^2},\\
&\mathcal{D}(A) = \{g\in L^2((0,\infty);dx)\,|\,g,g'\in AC_{\text{loc}}((0,\infty)),\ g(0_+)=g'(0_+)=0\},\\
&A^* = -\frac{d^2}{dx^2},\\
&\mathcal{D}(A^*) = \{g\in L^2((0,\infty);dx)\,|\,g,g'\in AC_{\text{loc}}((0,\infty)),\ g''\in L^2((0,\infty);dx)\},\\
&A_1 = A_F = -\frac{d^2}{dx^2},\quad \mathcal{D}(A_1)=\{g\in\mathcal{D}(A^*)\mid g(0_+)=0\},\\
&A_2 = -\frac{d^2}{dx^2},\quad \mathcal{D}(A_2)=\{g\in\mathcal{D}(A^*)\mid g'(0_+)+2^{-1/2}(1-\tan(\alpha_2))g(0_+)=0\},\\
&\hspace{20em}\alpha_2\in[0,\pi)\backslash\{\pi/2\},
\end{aligned}$$

where A_F denotes the Friedrichs extension of A (corresponding to $\alpha_2=\pi/2$). One verifies,

$$\begin{aligned}
&\ker(A^*-z) = \{ce^{i\sqrt{z}x}, c\in\mathbb{C}\},\ \operatorname{Im}(\sqrt{z})>0,\ z\in\mathbb{C}\setminus[0,\infty),\\
&\operatorname{def}(A)=(1,1),\quad u_1(i,x)=2^{1/4}e^{i\sqrt{i}x},\quad u_{1,1}(-i,x)=2^{1/4}e^{i\sqrt{-i}x},\\
&(A_2-z)^{-1} = (A_1-z)^{-1} - (2^{-1/2}(1-\tan(\alpha_2))+i\sqrt{z})^{-1}(\overline{e^{i\sqrt{z}\cdot}},\,\cdot\,)e^{i\sqrt{z}\cdot},\\
&\hspace{20em} z\in\rho(A_2),\ \operatorname{Im}(\sqrt{z})>0,\\
&U_1=-1,\quad U_2=e^{2i\alpha_2},
\end{aligned}$$

$$P_{1,2}(z) = -(1-\tan(\alpha_2)+i\sqrt{2z})^{-1},\ z\in\rho(A_2),\quad P_{1,2}(i)^{-1} = \tan(\alpha_2)-i,$$
$$M_1(z) = i\sqrt{2z}+1,\quad M_2(z) = \frac{\cos(\alpha_2)+\sin(\alpha_2)(i\sqrt{2z}+1)}{\sin(\alpha_2)-\cos(\alpha_2)(i\sqrt{2z}+1)}.$$

The Krein extension $A_2 = A_K$ of A corresponds to $\tan(\alpha_2) = 1$ and hence coincides with the Neumann extension A_N of A (characterized by the boundary condition $g'(0_+) = 0$).

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