Operators
and
Matrices
Volume 18, Number 3 (2024), 535–557
doi:10.7153/oam-2024-18-31

THE PEAK MODEL FOR FINITE RANK SUPERSINGULAR PERTURBATIONS

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(*Communicated by B. Jacob*)

Abstract. In its original form the peak model for rank one supersingular perturbations of class $\mathfrak{H}_{-4}$ or higher of a nonnegative self-adjoint operator requires that the Gram matrix of the model should be diagonal. Here we remove the restriction on the Gram matrix. In particular we explain the origin of the Krein Q-function associated with the Gram matrix.

1. Introduction

The theory of higher order singular or else supersingular perturbations of a self-adjoint operator in a Hilbert space is, in principal, the theory of generalized, that is, exit space self-adjoint extensions, where perturbations are interpreted by means of generalized resolvents or, equivalently, generalized Nevanlinna families. For finite rank perturbations, the exit space $\mathscr{H}=\mathfrak{H}_m\dotplus\mathfrak{K}$ is made by extending a reference Hilbert space $\mathfrak{H}_m$ by a disjoint finite-dimensional linear space $\mathfrak{K}$. Depending on the precise definition of $\mathfrak{K}$, the cascade (A and B) and the peak models for supersingular perturbations are considered among researchers. Specifically, the cascade models for rank one supersingular perturbations of a nonnegative self-adjoint operator are developed in [21], see also references therein. In the B-model $\mathscr{H}$ is a Pontryagin space with a nontrivial index of indefiniteness. In the A-model, whether or not $\mathscr{H}$ is a Hilbert space depends on how one defines the scalar product in the scale of Hilbert spaces [21, Theorem 3.2]; *cf.* [30]. For classical, that is, singular perturbations the reader may consult the monographs [4, 36] and references there.

The peak model, first introduced in [34], is our main object of interest here. In the present model $\mathscr{H}$ is a Hilbert space, because the singular elements that span $\mathfrak{K}$ form the Gram matrix, $\mathscr{G}$, which is positive; this is the main motive in [34] for introducing an alternative to the cascade models. On the other hand, the peak model, as stated, has limitations in that the elements that generate $\mathfrak{K}$ must be orthogonal or, equivalently, $\mathscr{G}$ must be diagonal in order to be able to apply the standard theory of operator extensions.

Mathematics subject classification (2020): 47B25, 47A06, 34B05, 35P05.

Keywords and phrases: Supersingular perturbation, exit space extension, generalized resolvent, boundary triple, linear relation, γ-field, Weyl function.

The research was inspired by the topics presented at Insubria Summer School in Mathematical Physics, University of Insubria, Como (Italy), 18-22 September 2017.

Paper OaM-18-31

A quick example of a 6-dimensional Laplace operator with Dirac distribution already shows that the orthogonality condition does not necessarily hold.

Recall that, for a ν-dimensional $(\nu \geqslant 4)$ Laplace operator with Dirac distribution of class $\mathfrak{H}_{-m-2} \setminus \mathfrak{H}_{-m-1}$, $m = (\nu - 2)/2$ if ν is even and $m = (\nu - 3)/2$ if ν is odd. Two modifications are, for example, as follows. By lowering ν while taking instead the distributional derivative of Dirac distribution, the perturbation with $\nu = 3$ and $m = 1$ is considered in [34, Sec. 10]. A two-particle Rashba spin-orbit coupled operator with point-interaction considered in [31, Example 3.4], [29, Sec. 5] shows $m = 2$ for $\nu = 6$.

In the present study we remove the restriction on $\mathscr{G}$ by considering operator extensions to a subspace of $\mathscr{H}$ rather than to the whole $\mathscr{H}$ or, what is the same, by considering linear relations in $\mathscr{H}$ rather than operator extensions; the operator part of such a linear relation is precisely the operator extension to $\mathscr{H}_1$. The exit space $\mathscr{H}_1 := \mathfrak{H}_m \dotplus \mathfrak{K}_1$ is therefore constructed by taking a suitable subspace $\mathfrak{K}_1 \subseteq \mathfrak{K}$. In this way we still work within the framework of the peak model, because there is the smallest nontrivial subspace, $\mathfrak{K}_{\min}$, which is disjoint from $\mathfrak{H}_m$ and such that $\mathfrak{K}_{\min} \subseteq \mathfrak{K}_1 \subseteq \mathfrak{K}$. The existence of $\mathfrak{K}_{\min}$, but in the cascade A-model, was first observed in [30].

The characterization of the boundary value space for the operator extensions to $\mathscr{H}_1$ should be considered as our first main result out of the three. The second main result is that a generalized resolvent corresponding to the operator extension in $\mathscr{H}_1$ parametrized by a self-adjoint linear relation Θ is in bijective correspondence with a Nevanlinna family $z \mapsto (\mathscr{C}^{-1})^*(\mathring{Q}(z) - \Theta)\mathscr{C}^{-1}$. The transfer matrix $\mathscr{C}$ serves for a "scale parameter" depending on how one defines the scalar product in the scale of Hilbert spaces; this is because we avoid attaching ourselves to a specific (typically polynomial) definition of scale spaces. The matrix function $\mathring{Q}$ is a Nevanlinna function. For $\mathscr{G}$ diagonal, this $\mathring{Q}$ coincides with that in [34], where it is termed the Q-function associated with the Gram matrix $\mathscr{G}$. We explain the origin of $\mathring{Q}$ by demonstrating that it is the Weyl function corresponding to a boundary triple of a certain symmetric operator in $\mathfrak{K}_1$. In the terminology of [23] we present a realization for $\mathring{Q}$; it is minimal iff $\mathfrak{K}_1 = \mathfrak{K}_{\min}$. The latter is our third main result.

After introductory Sections 2, 3, operator extensions to $\mathscr{H}_1$ are studied in Section 4. Specifically, the characterization of the boundary value space of extensions, including a realization for $\mathring{Q}$, is presented in Theorem 1, and a generalized resolvent corresponding to a self-adjoint operator extension to $\mathscr{H}_1$ is presented in Theorem 2. In Section 5 we study some properties of $\mathring{Q}$ depending on $\mathfrak{K}_1$. There is also Appendix A, where we use the peak model as an example for an isometric boundary triple [20, Definition 1.9].

Throughout, we present our results using the language of linear relations in Hilbert spaces and the theory abstract boundary value spaces [7, 11–13, 16, 18–20]. Linear relations are referred to as relations and operators are identified with their graphs (single-valued relations).

2. Some background

Consider a closed symmetric relation T in a Hilbert space $\mathfrak{H}$, with equal and finite defect numbers (d,d). Then (*e.g.* [8, 16]) T has an (ordinary) boundary triple $\Pi_\Gamma = (\mathbb{C}^d, \Gamma_0, \Gamma_1)$, where the boundary operator $\Gamma := (\Gamma_0, \Gamma_1)$ from T^* (the adjoint in $\mathfrak{H}$ of T) to $\mathbb{C}^{2d}$ is surjective, and moreover the Green identity holds (*e.g.* [20, Definition 3.1], [19, Definition 7.11])

$$\langle f, g' \rangle_{\mathfrak{H}} - \langle f', g \rangle_{\mathfrak{H}} = \langle \Gamma_0 \widehat{f}, \Gamma_1 \widehat{g} \rangle_{\mathbb{C}^d} - \langle \Gamma_1 \widehat{f}, \Gamma_0 \widehat{g} \rangle_{\mathbb{C}^d}$$

for all $\widehat{f} = (f, f')$ and $\widehat{g} = (g, g')$ from T^*. The scalar product in $\mathfrak{H}$ is denoted by $\langle \cdot, \cdot \rangle_{\mathfrak{H}}$. Equivalently, by considering Γ with domain T^* as an operator from a Krein space $\mathfrak{H}^2$ with fundamental symmetry ($I_{\mathfrak{H}}$ is the identity in $\mathfrak{H}$)

$$\widehat{J}_{\mathfrak{H}} := \begin{pmatrix} 0 & -\mathrm{i} I_{\mathfrak{H}} \\ \mathrm{i} I_{\mathfrak{H}} & 0 \end{pmatrix} : \begin{matrix} \mathfrak{H} \\ \oplus \\ \mathfrak{H} \end{matrix} \to \begin{matrix} \mathfrak{H} \\ \oplus \\ \mathfrak{H} \end{matrix}$$

and an indefinite metric

$$[\widehat{f}, \widehat{g}] := -\mathrm{i} \langle f, g' \rangle_{\mathfrak{H}} + \mathrm{i} \langle f', g \rangle_{\mathfrak{H}}$$

to a Krein space $\mathbb{C}^{2d}$, with the fundamental symmetry $\widehat{J}_{\mathbb{C}^d}$ and an indefinite metric defined similarly, Π_Γ is said to be a boundary triple for T^* if Γ is unitary, *i.e.* if the inverse Γ^{-1} in the sense of relations coincides with the Krein space adjoint $\Gamma^+ := \widehat{J}_{\mathfrak{H}} \Gamma^* \widehat{J}_{\mathbb{C}^d}$; Γ^* is a Hilbert space adjoint. See [7] for Krein spaces.

Associated with Π_Γ is the γ-field γ_Γ and the matrix valued Weyl function M_Γ defined by

$$\gamma_\Gamma(z) := \pi_1 \widehat{\gamma}_\Gamma(z), \quad M_\Gamma(z) := \Gamma_1 \widehat{\gamma}_\Gamma(z), \quad z \in \mathbb{C} \setminus \mathbb{R},$$
$$\widehat{\gamma}_\Gamma := (\Gamma_0 |_{\widehat{\mathfrak{N}}_z(T^*)})^{-1}, \quad \pi_1 : \mathfrak{H}^2 \to \mathfrak{H}, \quad \widehat{f} \mapsto f.$$

The defect subspaces

$$\mathfrak{N}_z(T^*) := \ker(T^* - z), \quad \widehat{\mathfrak{N}}_z(T^*) := \{(f, zf) \,|\, f \in \mathfrak{N}_z(T^*)\}.$$

We use the notation $\operatorname{dom} T$, $\ker T$, $\operatorname{ran} T$ for the domain, kernel, range of T. As a rule we omit the identity operator. Because $T_0 := \ker \Gamma_0$ is a self-adjoint relation in $\mathfrak{H}$, by the von Neumann formula the functions γ_Γ and M_Γ extend to $\rho(T_0)$, the resolvent set of T_0. If T is densely defined, Γ on T^* is identified with Γ on $\operatorname{dom} T^*$, as well as $\widehat{\gamma}_\Gamma$ is identified with γ_Γ.

The Weyl function M_Γ corresponding to a boundary triple Π_Γ for T^* is both a Krein Q-function for a pair (T, T_0) [6, 14], *i.e.* it satisfies

$$M_\Gamma(z) - M_\Gamma(z_0)^* = (z - \overline{z_0}) \gamma_\Gamma(z_0)^* \gamma_\Gamma(z), \quad z, z_0 \in \rho(T_0) \tag{1}$$

and a Nevanlinna function [22], *i.e.* it is analytic on $\mathbb{C} \setminus \mathbb{R}$ and satisfies

$$M_\Gamma(z)^* = M_\Gamma(\overline{z}), \quad \operatorname{Im} M_\Gamma(z) / \operatorname{Im} z \geqslant 0.$$

Nevanlinna function is a special case of a Nevanlinna family, defined analogously but for relations. See [16] for various subclasses.

Let $\widetilde{T}$ be a self-adjoint extension of T in some possibly larger Hilbert space $\widetilde{\mathfrak{H}} \supseteq \mathfrak{H}$. Let $P_{\mathfrak{H}}$ be an orthogonal projection in $\widetilde{\mathfrak{H}}$ onto $\mathfrak{H}$. There is (*e.g.* [17, Theorems 6.1, 6.2]) a unique $d \times d$ relation valued Nevanlinna family τ such that

$$\begin{aligned} P_{\mathfrak{H}}(\widetilde{T}-z)^{-1}|_{\mathfrak{H}} =&(T_{-\tau(z)}-z)^{-1} \\ =&(T_0-z)^{-1}-\gamma_\Gamma(z)(\tau(z)+M_\Gamma(z))^{-1}\gamma_\Gamma(\overline{z})^* \end{aligned}$$

for $z \in \rho(\widetilde{T}) \cap \rho(T_0)$. The above generalized Krein–Naimark resolvent formula establishes a bijective correspondence between the sets of all generalized resolvents $P_{\mathfrak{H}}(\widetilde{T}-z)^{-1}|_{\mathfrak{H}}$ of T and all $d \times d$ relation valued Nevanlinna families τ; [17, 22, 35]. Particularly, $z \mapsto \tau(z)$ is a matrix function iff $\widetilde{T} \cap T_0 = T$, while $\tau(z) \equiv -\Theta$ is constant iff $\widetilde{T} \in \operatorname{Ext}(T)$, *i.e.* $T \subseteq \widetilde{T} \subseteq T^*$. The Štraus family $z \mapsto T_{-\tau(z)}$ in $\mathfrak{H}$ corresponding to $\widetilde{T}$ is given by $z \mapsto \ker(\Gamma_1 + \tau(z)\Gamma_0)$, see also [9, Theorem 2.7.3].

3. Preparatory statements

Throughout, L is a self-adjoint operator in a (complex and separable) Hilbert space $\mathfrak{H}_0$ with scalar product $\langle\cdot,\cdot\rangle_0$ and norm $\|\cdot\|_0 := \sqrt{\langle\cdot,\cdot\rangle_0}$. It is not assumed that L is semibounded.

DEFINITION 1. A sequence of Hilbert spaces

$$\cdots \subseteq \mathfrak{H}_2 \subseteq \mathfrak{H}_1 \subseteq \mathfrak{H}_0 \subseteq \mathfrak{H}_{-1} \subseteq \mathfrak{H}_{-2} \subseteq \cdots$$

is said to be the scale of Hilbert spaces associated with L, and each $\mathfrak{H}_n$ taken separately is termed the scale space, if the following conditions hold for $n \geqslant 0$:

(a) $\mathfrak{H}_n = (\operatorname{dom}|L|^{n/2}, \langle\cdot,\cdot\rangle_n)$ with scalar product

$$\langle f,g\rangle_n := \langle \Omega_n f, \Omega_n g\rangle_0\,, \quad f,g \in \mathfrak{H}_n\,,$$

the induced norm $\|f\|_n := \sqrt{\langle f,f\rangle_n}$, and a unitary operator Ω_n from $\mathfrak{H}_n$ onto $\mathfrak{H}_0$, $\Omega_0 := I$ (identity), such that:

(a$_1$) $\Omega_1(\mathfrak{H}_2) = \mathfrak{H}_1$ and $\Omega_n(\mathfrak{H}_{n+2}) = \mathfrak{H}_2$,

(a$_2$) $L\Omega_n = \Omega_n L$,

(a$_3$) Ω_n is self-adjoint in $\mathfrak{H}_0$,

(a$_4$) the Ω_n's are mutually commuting.

(b) The strong dual $\mathfrak{H}_{-n}$ of $\mathfrak{H}_n$ is a Hilbert space with the scalar product, $\langle\cdot,\cdot\rangle_{-n}$, defined via the duality pairing $\langle\cdot,\cdot\rangle : \mathfrak{H}_{-n} \times \mathfrak{H}_n \to \mathbb{C}$ as follows:

$$\langle \psi,\phi\rangle_{-n} := \langle \widetilde{\Omega}_n^{-1}\psi, \widetilde{\Omega}_n^{-1}\phi\rangle_0\,, \quad \psi,\phi \in \mathfrak{H}_{-n}$$

where a unitary operator $\widetilde{\Omega}_n$ from $\mathfrak{H}_0$ onto $\mathfrak{H}_{-n}$ is defined by

$$\langle \widetilde{\Omega}_n u, f\rangle := \langle u, \Omega_n f\rangle_0\,, \quad u \in \mathfrak{H}_0\,, \quad f \in \mathfrak{H}_n\,.$$

For $n \geqslant 0$, L_n is the domain restriction to $\mathfrak{H}_{n+2}$ of L. Notice that the range of L_n is contained in $\mathfrak{H}_n$. An operator L_n is self-adjoint in $\mathfrak{H}_n$ iff $\mathfrak{H}_n$ is dense in $\mathfrak{H}_0$. By ($a_{1,2}$) and the Riesz representation theorem

$$\langle \psi, f\rangle = \langle \widetilde{\Omega}_n^{-1}\psi, \Omega_n f\rangle_0$$

L_n is self-adjoint in $\mathfrak{H}_n$, so $\mathfrak{H}_{n+1} \subseteq \mathfrak{H}_n$ densely and continuously. Similarly $\mathfrak{H}_{-n}$ is dense in $\mathfrak{H}_{-n-1}$ by (b). Moreover, the self-adjointness of L_n in $\mathfrak{H}_n$ further yields

$$\Omega_n(\mathfrak{H}_{n+t}) = \mathfrak{H}_t$$

for all nonnegative integers t.

The definition of the triplet adjoint, as stated below, will suffice for our study.

DEFINITION 2. (*cf.* [21,34]) Consider the triple $\mathfrak{H}_n \subseteq \mathfrak{H}_0 \subseteq \mathfrak{H}_{-n}$ from the scale of Hilbert spaces associated with L, and let $L' \subseteq L$ be an operator in $\mathfrak{H}_n$. The triplet adjoint of L' with respect to this triple is a closed relation in $\mathfrak{H}_{-n}$ defined by

$$\{(\psi,\phi) \in \mathfrak{H}_{-n}^2 \,|\, (\forall f \in \operatorname{dom} L')\ \langle \phi, f\rangle = \langle \psi, Lf\rangle\}.$$

In particular, the triplet adjoint of L_n is denoted by L_{-n}.

By considering Ω_n as an operator in $\mathfrak{H}_0$, (a_3) allows us to view $\widetilde{\Omega}_n|_{\mathfrak{H}_n}$ as Ω_n. Thus, by (a_{1-4}) a bounded operator L_n from a Hilbert space $\mathfrak{H}_{n+2}$ to a Hilbert space $\mathfrak{H}_n$ has a continuation L_{-n}, which is a self-adjoint operator in $\mathfrak{H}_{-n}$ with dense domain $\mathfrak{H}_{2-n} = \widetilde{\Omega}_n(\mathfrak{H}_2)$.

REMARK 1. A polynomial description of $\Omega_n = \sqrt{P_n(L)}$ falls within our definition of the scale space; P_n is a positive polynomial in L or $|L|$, of degree $n \geqslant 0$. Thus:
$P_n(L) = (|L| + I)^n$ in [1–3, 5, 32].
$P_n(L) = L^n$, $0 \in \rho(L)$ in [15].
$P_n(L) = \prod_{j=1}^n (L - z_j)$, $L \geqslant 0$, and $z_1, \ldots, z_n < 0$ in [21, 34].
In these examples $\widetilde{\Omega}_n = \sqrt{P_n(L_{-n})}$.

In view of Definition 2 and the preceding remarks, everywhere else below we omit the index in $L_n \equiv L \equiv L_{-n}$ if no confusion can arise. With the same meaning $\widetilde{\Omega}_n \equiv \Omega_n$.

Symmetric operator Fix an integer $m \geqslant 1$ and consider the family $\{\varphi_s\}_{s=1}^d$ of linearly independent functionals from $\mathfrak{H}_{-m-2} \setminus \mathfrak{H}_{-m-1}$. In the theory of supersingular perturbations one looks for a generalized resolvent of the symmetric restriction, $L_{\min} \subseteq L$, to $f \in \mathfrak{H}_{m+2}$ such that $\langle \varphi, f\rangle = 0$; $\langle \varphi, \cdot\rangle$ stands for the vector valued functional with components $\langle \varphi_s, \cdot\rangle$. Then $L_{\min}$ is a closed densely defined symmetric operator in $\mathfrak{H}_m$, with defect numbers (d,d), $d < \infty$, and defect subspaces

$$\mathfrak{N}_z(L_{\min}^*) = G_z(\mathbb{C}^d), \quad G_z(c) := \sum_s c_s G_s(z), \quad z \in \rho(L),$$

$$G_s(z) = P(L)^{-1} g_s(z), \quad g_s(z) := (L-z)^{-1}\varphi_s, \quad P(L) := \Omega_m^2$$

and $c=(c_s)\in\mathbb{C}^d$. The summation indexes s, s', ... always run over $\{1,\dots,d\}$.

The triplet adjoint $L_{\max}$ of $L_{\min}$ with respect to $\mathfrak{H}_m\subseteq\mathfrak{H}_0\subseteq\mathfrak{H}_{-m}$ extends L to $\mathfrak{H}_{2-m}\dot{+}\mathfrak{N}_z(L_{\max})$ (direct sum, *cf.* [34, Definition 3.1]), where the eigenspace

$$\mathfrak{N}_z(L_{\max})=g_z(\mathbb{C}^d)\,,\quad g_z(c):=\sum_s c_s g_s(z)\,.$$

Up to this point one may also look at [21] with $d=1$.

Exit space Starting from now on, the cascade and the peak models break apart. In the peak model one considers the restriction, $A_{\max}$, of $L_{\max}$ to the model space $\mathscr{H}$, $\mathfrak{H}_m\subseteq\mathscr{H}\subseteq\mathfrak{H}_{-m}$, which is a Hilbert space defined by

$$\mathscr{H}:=(\mathfrak{H}_m\dot{+}\mathfrak{K},\langle\cdot,\cdot\rangle_{\mathscr{H}})$$

with an md-dimensional Hilbert subspace $\mathfrak{K}=(\mathfrak{K},\langle\cdot,\cdot\rangle_{-m})$ of $\mathfrak{H}_{-m}$ defined by ($\vee\equiv$ linear span)

$$\mathfrak{K}:=\vee\{g_i:=g_s(z_j)\}\,,\quad i=\alpha(s,j):=m(s-1)+j\,.$$

Clearly the numbers

$$\mathscr{Z}:=\{z_j\in\rho(L)\}$$

are assumed distinct. Unless specified otherwise, the summation indexes j, j', ... run over $\{1,\dots,m\}$.

REMARK 2. An index $i=\alpha(s,j)$ is uniquely determined by s and j, that is, the Kronecker symbol $\delta_{i,i'}=\delta_{s,s'}\delta_{j,j'}$ for $i'=\alpha(s',j')$.

The scalar product

$$\langle f+k,f'+k'\rangle_{\mathscr{H}}:=\langle f,f'\rangle_m+\langle k,k'\rangle_{-m}$$

for $f,f'\in\mathfrak{H}_m$ and $k,k'\in\mathfrak{K}$. A bijective correspondence $\mathfrak{K}\ni k\leftrightarrow d(k)\in\mathbb{C}^{md}$ is established via the Gram matrix $\mathscr{G}$ as follows:

$$k=\sum_i d_i(k)g_i\,,\quad d(k)=(d_i(k))=\mathscr{G}^{-1}(\langle g_i,k\rangle_{-m})\,,$$
$$\mathscr{G}=(\mathscr{G}_{ii'}:=\langle g_i,g_{i'}\rangle_{-m})\,.$$

Thus

$$\langle k,k'\rangle_{-m}=\langle d(k),\mathscr{G}d(k')\rangle_{\mathbb{C}^{md}}$$

and in this way $\mathscr{H}$ is isomorphic to a Hilbert sum $\mathfrak{H}_m\oplus(\mathbb{C}^{md},\langle\cdot,\mathscr{G}\cdot\rangle_{\mathbb{C}^{md}})$.

The set $\mathfrak{K}$ contains a subset, $\mathfrak{K}_{\min}$, which is least possible in order the exit space extensions should cover the case of defect numbers (d,d). To see this, consider a polynomial

$$\widetilde{P}(L):=\prod_j(L-z_j)\,.$$

It is a bijective operator from $\mathfrak{H}_m$ to $\mathfrak{H}_{-m}$ (with a possible continuation as described previously), which is seen by using the sum formula for the inverse (*cf.* [34, Eq. (6.4)], [33])

$$\widetilde{P}(L)^{-1} = \sum_j b_j (L - z_j)^{-1}, \quad b_j := \prod_{j \neq j'} (z_j - z_{j'})^{-1}. \tag{2}$$

(Clearly $b_1 := 1$ if $m = 1$.) Thus we have

LEMMA 1. $\mathfrak{K} \supseteq \mathfrak{K}_{\min}$ *where*

$$\mathfrak{K}_{\min} := \mathfrak{K} \cap \mathfrak{H}_{m-2} = \vee\{\mathfrak{f}_s := \widetilde{P}(L)^{-1}\varphi_s\}.$$

Proof. $\vee\{\mathfrak{f}_s\} \subseteq \mathfrak{K}_{\min}$ is due to (2). Consider an arbitrary $k \in \mathfrak{K}_{\min}$.
Since $\widetilde{P}(L)^{-1}(\mathfrak{H}_{-m-2}) = \mathfrak{H}_{m-2}$, $(\exists \psi \in \mathfrak{H}_{-m-2})$ $k = \widetilde{P}(L)^{-1}\psi$, and then by (2)

$$0 = \sum_j (L - z_j)^{-1}\phi_j, \quad \phi_j := b_j \psi - \sum_s d_i(k)\varphi_s.$$

Then

$$\begin{aligned} 0 &= \sum_j (L - z_1)(L - z_j)^{-1}\phi_j \\ &= \sum_{j \geqslant 1} \phi_j + \sum_{j \geqslant 2} (z_j - z_1)(L - z_2)^{-1}\phi_j \\ &\quad + \sum_{j \geqslant 3} (z_j - z_1)(z_j - z_2)(L - z_2)^{-1}(L - z_3)^{-1}\phi_j \\ &\quad + \cdots + (z_m - z_1)\cdots(z_m - z_{m-1})(L - z_2)^{-1}\cdots(L - z_m)^{-1}\phi_m. \end{aligned}$$

The elements $\sum_{j \geqslant r}$ belong to mutually disjoint sets for different $r \in \{1, \ldots, m\}$, namely, $\mathfrak{H}_{2r-m-4} \setminus \mathfrak{H}_{2r-m-3}$, which shows $(\forall r) \sum_{j \geqslant r} = 0$, and then $(\forall j)$ $\phi_j = 0$. As a result $(\forall j)$ $d_i(k)/b_j \equiv \chi_s$ and $\psi = \sum_s \chi_s \varphi_s$, *i.e.* $k \in \vee\{\mathfrak{f}_s\}$. $\square$

The Gram matrix of $\mathfrak{K}_{\min}$ is denoted by

$$\mathscr{G}_{\min} := (\langle \mathfrak{f}_s, \mathfrak{f}_{s'} \rangle_{-m})$$

and an element $k = k_{\min}(\chi) \in \mathfrak{K}_{\min}$ by

$$k_{\min}(\chi) := \sum_s \chi_s \mathfrak{f}_s, \quad \chi = (\chi_s) \in \mathbb{C}^d.$$

In this way $\mathfrak{K}_{\min} \leftrightarrow \mathbb{C}^d$ bijectively and moreover

$$d(k) = \hat{b}\chi \quad \text{for} \quad k = k_{\min}(\chi); \quad \hat{b} := \mathscr{G}^{-1}\mathscr{G}_b. \tag{3}$$

The rectangular injective $md \times d$ matrix

$$\mathscr{G}_b := (\langle g_i, \mathfrak{f}_{s'} \rangle_{-m}).$$

Notice moreover that the matrices $\mathscr{G}_{\min}$ and $\mathscr{G}_b$ (or $\hat{b}$) are related by the equality (with $\mathscr{G}_b^*$ the adjoint of $\mathscr{G}_b$)

$$\mathscr{G}_{\min} = \mathscr{G}_b^* \mathscr{G}^{-1} \mathscr{G}_b = \mathscr{G}_b^* \hat{b}\,.$$

The space $\mathfrak{K}_{\min}$ can be equivalently represented by using an initially given $P(L)$ instead of $\widetilde{P}(L)$ as follows. Let

$$p(L) := P(L)\widetilde{P}(L)^{-1}\,, \quad \mathfrak{e}_s := P(L)^{-1}\varphi_s$$

so that

$$p(L)\mathfrak{e}_s = \mathfrak{f}_s = \sum_{s'} \mathscr{C}_{s's}\mathfrak{e}_{s'}\,, \quad \mathscr{C} = (\mathscr{C}_{ss'}) := \mathscr{B}^{-1}\mathscr{A}\,,$$
$$\mathscr{A} := (\langle \mathfrak{e}_s, \mathfrak{f}_{s'} \rangle_{-m})\,, \quad \mathscr{B} := (\langle \mathfrak{e}_s, \mathfrak{e}_{s'} \rangle_{-m})\ (\text{Gram})\,.$$

From $\mathscr{G}_{\min} = \mathscr{C}^*\mathscr{B}\mathscr{C}$ one sees that $\mathscr{C}$ (and its adjoint $\mathscr{C}^*$) is nonsingular, and $\mathfrak{e}_s = \sum_{s'}(\mathscr{C}^{-1})_{s's}\mathfrak{f}_{s'}$. Moreover

LEMMA 2. $\mathfrak{K}_{\min} = \vee\{\mathfrak{e}_s\}$. $\square$

Triplet adjoint in exit space In the next lemma (*cf.* [34, Lemmas 5.1, 5.2], [21, Theorem 3.1]) we characterize the operator

$$A_{\max} := L_{\max} \cap \mathscr{H}^2$$

by considering $A_{\max}$ as an extension of the operator A_0 in $\mathscr{H}$ defined by the componentwise sum

$$A_0 := L_m \widehat{+}\, l\,, \quad l := \{(k,k') \in \mathfrak{K}^2 \,|\, d(k') = Z_d d(k)\}\,.$$

The matrix Z_d is the matrix direct sum of d diagonal $m \times m$ matrices

$$Z := \operatorname{diag}\{z_1, \dots, z_m\}\,.$$

The operator A_0 is closed in $\mathscr{H}$ with $\rho(A_0) = \rho(L) \cap \rho(l)$, $\rho(l) = \rho(Z_d) = \mathbb{C} \setminus \mathscr{Z}$.

LEMMA 3. *For $z \in \rho(A_0)$:*

1)

$$A_{\max} = A_0 \widehat{+} \widehat{\mathfrak{N}}_z(A_{\max})\,, \quad \mathfrak{N}_z(A_{\max}) = \mathfrak{N}_z(L_{\max})\,.$$

2)

$$A_{\max} = A_0 \widehat{+} \{(\widetilde{G}_z(c), z\widetilde{G}_z(c) + k_{\min}(c)) \,|\, c \in \mathbb{C}^d\}$$

where

$$\widetilde{G}_z(\cdot) := p(L)G_z(\cdot) = G_z(\mathscr{C}\cdot)\,.$$

Proof. 1) For the first equality, it suffices to verify $A_0 \subseteq L_{\max}$. But this follows from $f+k-g_z(c) \in \mathfrak{H}_{2-m}$ for $f \in \mathfrak{H}_{m+2}$, $k \in \mathfrak{K}$, $c = c(k)$, where

$$c(k) = (c_s(k)) \in \mathbb{C}^d, \quad c_s(k) := \sum_j d_{\alpha(s,j)}(k). \tag{4}$$

To see the second equality $\mathfrak{N}_z(A_{\max}) = \mathfrak{N}_z(L_{\max})$, first note that $\mathfrak{N}_z(A_{\max}) = \mathfrak{N}_z(L_{\max}) \cap \mathscr{H}$. Now $g_z(\mathbb{C}^d) \subseteq \mathscr{H}$ because

$$\widetilde{P}(z)^{-1}(L-z)^{-1} = \widetilde{P}(L)^{-1}(L-z)^{-1} + \sum_j \frac{b_j}{z-z_j}(L-z_j)^{-1} \tag{5}$$

by (2); *cf.* [34, Eq. (4.10)].

2) Straightforward from (5). □

By Lemma 3 the boundary form of $A_{\max}$ reads

$$\begin{aligned}
&\langle f_0 + \widetilde{G}_z(c), A_{\max}(f_0' + \widetilde{G}_z(c'))\rangle_{\mathscr{H}} - \langle A_{\max}(f_0 + \widetilde{G}_z(c)), f_0' + \widetilde{G}_z(c')\rangle_{\mathscr{H}} \\
&= \langle d(k), (\mathscr{G}_Z - \mathscr{G}_Z^*) d(k')\rangle_{\mathbb{C}^{md}} + \langle \widetilde{\Gamma}_0(f_0 + \widetilde{G}_z(c)), \widetilde{\Gamma}_1(f_0' + \widetilde{G}_z(c'))\rangle_{\mathbb{C}^d} \\
&\quad - \langle \widetilde{\Gamma}_1(f_0 + \widetilde{G}_z(c)), \widetilde{\Gamma}_0(f_0' + \widetilde{G}_z(c'))\rangle_{\mathbb{C}^d}
\end{aligned}$$

for $f_0 = f + k$, $f_0' = f' + k'$ from $\operatorname{dom} A_0$ and for $c, c' \in \mathbb{C}^d$. The matrix

$$\mathscr{G}_Z := \mathscr{G} Z_d$$

(with $\mathscr{G}_Z^*$ its adjoint), the boundary operator

$$\begin{aligned}
&\widetilde{\Gamma} = (\widetilde{\Gamma}_0, \widetilde{\Gamma}_1)\colon \operatorname{dom} A_{\max} \to \mathbb{C}^{2d}, \\
&\widetilde{\Gamma}_0(f + k + \widetilde{G}_z(c)) := c, \\
&\widetilde{\Gamma}_1(f + k + \widetilde{G}_z(c)) := \mathscr{C}^* \langle \varphi, f\rangle + \widetilde{R}(z)c - \mathscr{G}_b^* d(k)
\end{aligned} \tag{6}$$

and the matrix valued Nevanlinna function

$$\widetilde{R}(z) := \mathscr{C}^* R(z) \mathscr{C}, \quad R(z) = (R_{ss'}(z) := \langle \varphi_s, G_{s'}(z)\rangle).$$

REMARKS 1. 1. The function $\widetilde{R}$ extends to $z \in \rho(L)$.

2. Since $\mathfrak{H}_{m+2} \subseteq \mathfrak{H}_m$ densely and continuously, and $\langle \varphi_s, \cdot\rangle$ is bounded on $\mathfrak{H}_{m+2}$, $\langle \varphi_s, \cdot\rangle$ has a continuation to $\mathfrak{H}_m$, which we denote by the same symbol in $R(z)$. In [4, Definition 3.1.2] $R(\mathrm{i})$ is related to an admissible matrix for functionals of class $\mathfrak{H}_{-2} \setminus \mathfrak{H}_{-1}$, see also [28]. The reason behind all this is that our analysis in $\mathfrak{K}$ (or $\mathscr{H}$) can be transferred by scaling to the subspace of $\mathfrak{H}_0$ generated by $\widehat{g}_s(z_j) := (L - z_j)^{-1}\widehat{\varphi}_s$, with $\widehat{\varphi}_s := P(L)^{-1/2}\varphi_s \in \mathfrak{H}_{-2} \setminus \mathfrak{H}_{-1}$; see Appendix A for details. In this way $R_{ss'}(z) = \langle \widehat{\varphi}_s, \widehat{g}_{s'}(z)\rangle$, where $\langle \widehat{\varphi}_s, \cdot\rangle$ is a continuation to $\mathfrak{H}_0$.
3. With the operator $\Gamma = (\Gamma_0, \Gamma_1)\colon \operatorname{dom} L_{\min}^* \to \mathbb{C}^{2d}$ defined by

$$\begin{aligned}
&\Gamma_0(f + G_z(c)) := c, \quad f \in \mathfrak{H}_{m+2}, \quad c \in \mathbb{C}^d, \\
&\Gamma_1(f + G_z(c)) := \langle \varphi, f\rangle + R(z)c
\end{aligned}$$

the triple $\Pi_\Gamma = (\mathbb{C}^d, \Gamma_0, \Gamma_1)$ is a boundary triple for $L_{\min}^*$ with the γ-field $z \mapsto \gamma_\Gamma(z) = G_z(\cdot)$ and the Weyl function $M_\Gamma = R$.

At this point one makes an assumption in [34] that the matrix $\mathscr{G}_Z$ is Hermitian or, equivalently:

PROPOSITION 1. *The three statements are equivalent:*

(i) *The matrix* $\mathscr{G}_Z$ *is Hermitian.*

(ii) *The Gram matrix* $\mathscr{G}$ *is diagonal in* j, *and* $\mathscr{Z} \subseteq \mathbb{R} \cap \rho(L)$.

(iii) *The Nevanlinna function* R *satisfies* $R(z_j) \equiv \mathscr{R} = \mathscr{R}^*$ *for all* j.

The reason is: For an Hermitian $\mathscr{G}_Z$ the adjoint in $\mathscr{H}$ of $A_{\max}$, *i.e.* the operator

$$A_{\min} := A_{\max}^*$$

is closed densely defined symmetric in $\mathscr{H}$, and has defect numbers (d,d). Subsequently, one applies standard theory of extensions of symmetric operators, and then characterizes a generalized resolvent of $L_{\min}$ associated with a self-adjoint operator A_0 in $\mathscr{H}$.

Proof. In order to prove Proposition 1 the easiest way is to use the matrix notation

$$\mathscr{M} = (\mathscr{M}_{si'} := R_{ss'}(z_{j'}))$$

and to observe that

$$(\overline{z_j} - z_{j'})\mathscr{G}_{ii'} = (\mathscr{G}_Z^* - \mathscr{G}_Z)_{ii'} = (\mathscr{M}^*)_{is'} - \mathscr{M}_{si'}. \quad \square \tag{7}$$

For later reference we remark that $\mathscr{M}$ also appears in

$$\begin{aligned}&\langle d(k), (\mathscr{G}_Z - \mathscr{G}_Z^*)d(k')\rangle_{\mathbb{C}^{md}} \\ &= \langle c(k), \mathscr{M} d(k')\rangle_{\mathbb{C}^d} - \langle \mathscr{M} d(k), c(k')\rangle_{\mathbb{C}^d}\end{aligned} \tag{8}$$

with $c(k)$ as in (4). Thus $\mathscr{M} d(k) = \mathscr{R} c(k)$ if $\mathscr{G}_Z^* = \mathscr{G}_Z$.

In our approach we do not assume that $\mathscr{G}_Z$ is necessarily Hermitian. In this case define the operator $A'_{\max}$ in $\mathscr{H}$ by

$$A'_{\max} := A_0^* \widehat{+} \{(\widetilde{G}_z(c), z\widetilde{G}_z(c) + k_{\min}(c)) \,|\, c \in \mathbb{C}^d\} \tag{9}$$

and let $A_{\min}$ be as previously. By standard procedure one verifies that the adjoint A_0^* in $\mathscr{H}$ of A_0 is given by

$$A_0^* = L_m \widehat{+} l^*, \quad l^* = \{(k,k') \in \mathfrak{K}^2 \,|\, d(k') = \mathscr{G}^{-1}\mathscr{G}_Z^* d(k)\}$$

where l^* is the adjoint in $\mathfrak{K}$ of l. Moreover

LEMMA 4. *1) Consider* $\widetilde{\Gamma}$ *as an operator from a* $\widehat{J}_{\mathscr{H}}$*-space to a* $\widehat{J}_{\mathbb{C}^d}$*-space, with domain* $A_{\max}$, *and let* $\widetilde{\Gamma}^+$ *be its Krein space adjoint. Then the operator* $(\widetilde{\Gamma}^+)^{-1} = (\widetilde{\Gamma}_0, \widetilde{\Gamma}_1)$ *but now with domain* $A'_{\max}$.

2) In particular, $A_{\min}$ *is the domain restriction to* $\ker\widetilde{\Gamma}$ *of* $A'_{\max}$. $\square$

Instead of requiring $\mathscr{G}_Z$ to be Hermitian, in the next section we consider subspaces from the scale $\mathfrak{K}_{\min} \subseteq \mathfrak{K}$ such that (8) vanishes. Without making any additional assumptions, such subspaces always exist if $m \geqslant 2$; notice that $k \in \mathfrak{K}_{\min}$ satisfies $c(k) = 0$. If $m = 1$ then $\mathfrak{K}_{\min} = \mathfrak{K}$ and (8) vanishes iff $z_1 \in \mathbb{R} \cap \rho(L)$, *cf.* Proposition 1; hence L should be semibounded.

4. Generalized resolvent

Maximal exit subspace Fix $m \geqslant 2$ and define a subspace $\mathfrak{K}_{\max}$ of $\mathfrak{K}$ by

$$\mathfrak{K}_{\max} := \{k \in \mathfrak{K} \,|\, \operatorname{Im} \langle c(k), \mathscr{M} d(k) \rangle_{\mathbb{C}^d} = 0\}.$$

In order to characterize $\mathfrak{K}_{\max}$ it is convenient to interpret $d(\mathfrak{K}_{\max})$ as a neutral subspace of a W-space [7, 25] as follows. Define an Hermitian matrix

$$W := \mathrm{i}(\mathscr{G}_Z - \mathscr{G}_Z^*).$$

Then $(\mathbb{C}^{md}, [\cdot,\cdot])$ is a W-space with an indefinite inner product

$$[\xi, \xi'] := \langle \xi, W\xi' \rangle_{\mathbb{C}^{md}}, \quad \xi, \xi' \in \mathbb{C}^{md}.$$

By definition, a neutral subspace consists of those $\xi \in \mathbb{C}^{md}$ such that $[\xi,\xi] = 0$; it is maximal if it is not contained properly in a neutral subspace. Using $\mathfrak{K} \leftrightarrow \mathbb{C}^{md}$ and (8), by polarization therefore $d(\mathfrak{K}_{\max})$ is maximal neutral. By [25, Theorem 2.3.4], the dimension, d', of $\mathfrak{K}_{\max}$ satisfies $d' \leqslant \min\{\pi(W), \nu(W)\} + \dim\ker W$, where the number of positive (resp. negative) eigenvalues of W, counting multiplicities, is denoted by $\pi(W)$ (resp. $\nu(W)$).

PROPOSITION 2. *One has the direct sum decomposition*

$$d(\mathfrak{K}_{\max}) = d(\mathfrak{K} \cap \mathfrak{H}_{2-m}) \dotplus \ker W$$

where $\mathfrak{K} \cap \mathfrak{H}_{2-m}$, of dimension $(m-1)d$, is the set of those $k \in \mathfrak{K}$ such that $c(k) = 0$.
In particular, $\mathfrak{K}_{\max} = \mathfrak{K} \cap \mathfrak{H}_{2-m}$ if $d = 1$ and $W \neq 0$.

Proof. Step 1. For $k \in \mathfrak{K}$

$$Lk = lk + \sum_s c_s(k)\varphi_s.$$

If $k \in \mathfrak{K} \cap \mathfrak{H}_{1-m}$ then $Lk \in \mathfrak{H}_{-1-m}$. Since $lk \in \mathfrak{K}$ and $\varphi_s \in \mathfrak{H}_{-m-2} \setminus \mathfrak{H}_{-m-1}$ we have $c(k) = 0$, *i.e.*

$$\mathfrak{K} \cap \mathfrak{H}_{1-m} \subseteq \mathfrak{K}_* := \{k \in \mathfrak{K} \,|\, c(k) = 0\}.$$

Since $\mathfrak{K}_* \subseteq \mathfrak{K}_{\max} \subseteq \mathfrak{K}$, this shows

$$\mathfrak{K} \cap \mathfrak{H}_{1-m} = \mathfrak{K}_* \cap \mathfrak{H}_{1-m} = \mathfrak{K}_{\max} \cap \mathfrak{H}_{1-m}.$$

On the other hand

$$\mathfrak{K}_* = \vee\{(L - z_m)^{-1} g_i \,|\, j \leqslant m-1\}$$

i.e. $\mathfrak{K}_* \subseteq \mathfrak{H}_{2-m}$. Therefore

$$\mathfrak{K}_* = \mathfrak{K} \cap \mathfrak{H}_{2-m} = \mathfrak{K}_{\max} \cap \mathfrak{H}_{2-m}.$$

Step 2. To show the direct sum decomposition of $\mathfrak{K}_{\max}$, consider

$$\mathfrak{K}_0 := \mathfrak{K}_* \dotplus (\mathfrak{K}_{\max} \smallsetminus \mathfrak{K}_*)\,.$$

Clearly $\mathfrak{K}_0 \subseteq \mathfrak{K}_{\max}$. For the converse use that $\mathfrak{K}_{\max} \cap \mathfrak{K}_*^{\perp} \subseteq \mathfrak{K}_{\max} \smallsetminus \mathfrak{K}_*$. Thus $\mathfrak{K}_0 = \mathfrak{K}_{\max}$.

Since

$$\ker W \subseteq d(\mathfrak{K}_{\max}) = \{\xi \mid [\xi,\xi] = 0\}$$

and $(\exists(\xi_i) \in \ker W)$ $(\exists s)$ $\sum_i \xi_i \neq 0$, we have $\ker W \subseteq d(\mathfrak{K}_{\max} \smallsetminus \mathfrak{K}_*)$. For the converse, we apply the dimension argument. We have

$$\pi(W) + \nu(W) + d_0 = md\,, \quad d_0 := \dim\ker W$$

and

$$d' \leqslant d_* + d_0\,, \quad d_* := \min\{\pi(W), \nu(W)\}\,.$$

Since

$$(m-1)d + d_0 \leqslant d' \leqslant d_* + d_0$$

it therefore suffices to show $(m-1)d = d_*$.

Suppose $\pi(W) \leqslant \nu(W)$. Then

$$d_* = \pi(W) \leqslant md - (d_0 + \pi(W))\,.$$

Now $d_0 + \pi(W) \geqslant d' \geqslant d$ (the last $\geqslant$ uses $\mathfrak{K}_{\min} \subseteq \mathfrak{K}_{\max}$), so $d_* \leqslant md - d$. The case $\pi(W) \geqslant \nu(W)$ is treated analogously.

Step 3. If $d = 1$ then $d' \geqslant \dim\mathfrak{K}_* = m-1$. Since moreover $W \neq 0$, $d' \leqslant m-1$. This accomplishes the proof of the proposition. □

REMARKS 2. 1. $c(k) = 0$ for $k \in \mathfrak{K}_{\min}$ is seen directly from $d(\mathfrak{K}_{\min}) = \operatorname{ran}\hat{b}$ and $\sum_j b_j = 0$; recall (2), (3). Moreover, by (7)

$$\{0\} = \operatorname{ran}\hat{b} \cap \ker\mathscr{M} = \operatorname{ran}\hat{b} \cap \ker W\,.$$

If *e.g.* $m = 2$ then $\mathfrak{K}_* = \mathfrak{K}_{\min}$, *i.e.* $d(\mathfrak{K}_{\max}) = d(\mathfrak{K}_{\min}) \dotplus \ker W$.

2. In the course of proving Proposition 2 we have on the way established that

$$\mathfrak{K} \cap \mathfrak{H}_{1-m} = \mathfrak{K} \cap \mathfrak{H}_{2-m}\,.$$

Triplet adjoint in exit subspace Let $\mathfrak{K}_1 = (\mathfrak{K}_1, \langle\cdot,\cdot\rangle_{-m})$ be an arbitrary subspace from the scale $\mathfrak{K}_{\min} \subseteq \mathfrak{K}_{\max}$. The orthogonal complement in $\mathfrak{K}$ of $\mathfrak{K}_1$ is denoted by

$$\mathscr{H}_{\perp} := \mathfrak{K} \ominus \mathfrak{K}_1\,.$$

The corresponding Hilbert subspace of $\mathscr{H}$ is defined by

$$\mathscr{H}_1 := (\mathfrak{H}_m \dotplus \mathfrak{K}_1, \langle\cdot,\cdot\rangle_{\mathscr{H}})\,.$$

Notice that the orthogonal complement in $\mathscr{H}$ of $\mathscr{H}_1$ is $\mathscr{H}_\perp$.

Define a relation $B_{\max}$ in $\mathscr{H}$ by

$$B_{\max} := A_{\max}|_{\mathscr{H}_1} \widehat{+} (\{0\} \times \mathscr{H}_\perp).$$

By Lemma 3 and (9)

$$\mathrm{ran}((A_{\max} - A'_{\max})|_{\mathscr{H}_1}) \subseteq \mathscr{H}_\perp$$

and then the proof of the next lemma is accomplished by standard arguments.

LEMMA 5. *Let $B_{\min} := B^*_{\max}$ be the adjoint in $\mathscr{H}$ of $B_{\max}$. Then*

$$B_{\min} = A_{\min}|_{\mathscr{H}_1} \widehat{+} (\{0\} \times \mathscr{H}_\perp)$$

is a closed symmetric relation in $\mathscr{H}$ with defect numbers (d,d). The adjoint in $\mathscr{H}$ is given by

$$B^*_{\min} = B_{\max} = B_0 \widehat{+} \widehat{\mathfrak{N}}_z(B_{\max}), \quad z \in \rho(B_0).$$

The self-adjoint relation B_0 in $\mathscr{H}$ admits a canonical form

$$B_0 := \mathring{B}_0 \widehat{\oplus} (\{0\} \times \mathscr{H}_\perp), \quad \mathring{B}_0 := L_m \widehat{+} l_1$$

where (with $P_{\mathfrak{K}_1}$ an orthogonal projection in $\mathfrak{K}$ onto $\mathfrak{K}_1$)

$$l_1 := P_{\mathfrak{K}_1} l|_{\mathfrak{K}_1}$$

is the self-adjoint operator in $\mathfrak{K}_1$. The defect subspace

$$\mathfrak{N}_z(B_{\max}) = [(L-z)^{-1} - (l_1 - z)^{-1}](\mathfrak{K}_{\min}).$$

Moreover, if $\mathring{B}_{\min}$ denotes the operator part of $B_{\min}$, i.e.

$$\mathring{B}_{\min} = P_{\mathscr{H}_1} A_{\min}|_{\mathscr{H}_1}$$

($P_{\mathscr{H}_1}$ is an orthogonal projection in $\mathscr{H}$ onto $\mathscr{H}_1$), then $\mathring{B}_{\min}$ is a closed densely defined symmetric operator in $\mathscr{H}_1$, with equal defect numbers (d,d). The adjoint in $\mathscr{H}_1$, $\mathring{B}_{\max} := \mathring{B}^*_{\min}$, is the operator part of $B_{\max}$, i.e.

$$\mathring{B}_{\max} = \mathring{B}_0 \widehat{+} \widehat{\mathfrak{N}}_z(\mathring{B}_{\max}), \quad \mathfrak{N}_z(\mathring{B}_{\max}) = \mathfrak{N}_z(B_{\max}), \quad z \in \rho(B_0). \quad \square$$

The boundary value space of $B_{\max}$ in $\mathscr{H}$ is therefore completely determined by the boundary value space of $\mathring{B}_{\max}$ in $\mathscr{H}_1$. Recall $\widetilde{\Gamma}$ in (6).

THEOREM 1. *1) Consider $\widetilde{\Gamma}$ as an operator $A_{\max} \to \mathbb{C}^{2d}$. With an operator*

$$\mathring{\Gamma} := (\widetilde{\Gamma}|_{\mathscr{H}_1 \times \mathscr{H}}) \widehat{+} ((\{0\} \times \mathscr{H}_\perp) \times \{0\}) := (\mathring{\Gamma}_0, \mathring{\Gamma}_1)$$

from $B_{\max}$ *to* $\mathbb{C}^{2d}$*, the triple* $\Pi_{\mathring{\Gamma}}=(\mathbb{C}^d,\mathring{\Gamma}_0,\mathring{\Gamma}_1)$ *is a boundary triple for* $B_{\max}$ *with the* γ*-field* $\gamma_{\mathring{\Gamma}}$ *and the Weyl function* $M_{\mathring{\Gamma}}$ *given on* $\mathbb{C}^d$ *by*

$$\gamma_{\mathring{\Gamma}}(z)=[(L-z)^{-1}-(l_1-z)^{-1}]k_{\min}(\cdot)\,,$$
$$M_{\mathring{\Gamma}}(z)=\widetilde{R}(z)+\mathring{Q}(z)\,,\quad z\in\rho(\mathring{B}_0)$$

where the Nevanlinna function

$$\mathring{Q}(z):=(\langle\mathfrak{f}_s,(l_1-z)^{-1}\mathfrak{f}_{s'}\rangle_{-m})\,,\quad z\in\rho(l_1)\,.$$

2) *With an operator*

$$\mathring{\Gamma}:=\widetilde{\Gamma}|_{\mathscr{H}_1}:=(\mathring{\Gamma}_0,\mathring{\Gamma}_1)$$

from $\operatorname{dom}\mathring{B}_{\max}$ *to* $\mathbb{C}^{2d}$*, the triple* $\Pi_{\mathring{\Gamma}}=(\mathbb{C}^d,\mathring{\Gamma}_0,\mathring{\Gamma}_1)$ *is a boundary triple for* $\mathring{B}_{\max}$ *with the* γ*-field* $\gamma_{\mathring{\Gamma}}$ *and the Weyl function* $M_{\mathring{\Gamma}}$*.*

3) *Consider a closed symmetric operator*

$$\mathring{l}_1:=l_1|_{\mathfrak{K}_1\ominus\mathfrak{K}_{\min}}$$

in $\mathfrak{K}_1$*, with defect numbers* (d,d)*; the adjoint in* $\mathfrak{K}_1$ *is characterized by*

$$\mathring{l}_1^*=l_1\,\widehat{+}\,(\{0\}\times\mathfrak{K}_{\min})\,,$$
$$\mathfrak{N}_z(\mathring{l}_1^*)=(l_1-z)^{-1}(\mathfrak{K}_{\min})\,,\quad z\in\rho(l_1)\,.$$

Then the triple $\Pi_{\mathring{\mathring{\Gamma}}}=(\mathbb{C}^d,\mathring{\mathring{\Gamma}}_0,\mathring{\mathring{\Gamma}}_1)$*, where*

$$\mathring{\mathring{\Gamma}}=(\mathring{\mathring{\Gamma}}_0,\mathring{\mathring{\Gamma}}_1)\colon\,\mathring{l}_1^*\to\mathbb{C}^{2d}\,,$$
$$\mathring{\mathring{\Gamma}}_0(k,l_1k+k_{\min}(\chi)):=\chi\,,$$
$$\mathring{\mathring{\Gamma}}_1(k,l_1k+k_{\min}(\chi)):=-\mathscr{G}_b^*d(k)$$

is a boundary triple for $\mathring{l}_1^*$ *with the* γ*-field* $\gamma_{\mathring{\mathring{\Gamma}}}$ *and the Weyl function* $M_{\mathring{\mathring{\Gamma}}}$ *given on* $\mathbb{C}^d$ *by*

$$\gamma_{\mathring{\mathring{\Gamma}}}(z)=-(l_1-z)^{-1}k_{\min}(\cdot)\,,\quad M_{\mathring{\mathring{\Gamma}}}(z)=\mathring{Q}(z)\,,\quad z\in\rho(l_1)\,.$$

Proof. 1) $\mathring{\Gamma}$ can be given the form

$$\mathring{\Gamma}=(\widetilde{\Gamma}\cap\mathfrak{M})\,\widehat{+}\,\mathfrak{N}$$

where the closed relations $\mathfrak{M}$ and $\mathfrak{N}$ from $\mathscr{H}^2$ to $\mathbb{C}^{2d}$ are defined by

$$\mathfrak{M}:=(\mathscr{H}_1\times\mathscr{H})\times\mathbb{C}^{2d}\,,\quad\mathfrak{N}:=(\{0\}\times\mathscr{H}_\perp)\times\{0\}\,.$$

In order that $\Pi_{\mathring{\Gamma}}$ should be the boundary triple for $B_{\max}$ it is necessary and sufficient that the operator $\mathring{\Gamma}$ should be unitary from a $\widehat{J}_{\mathscr{H}}$-space to a $\widehat{J}_{\mathbb{C}^d}$-space. Since the Krein space adjoints $\mathfrak{N}^+=\mathfrak{M}^{-1}$ and $\mathfrak{M}^+=\mathfrak{N}^{-1}$, the Krein space adjoint of $\mathring{\Gamma}$ is given by

$$\mathring{\Gamma}^+=(\widetilde{\Gamma}\cap\mathfrak{M})^+\cap\mathfrak{N}^+=((\overline{(\widetilde{\Gamma}^+)^{-1}\,\widehat{+}\,\mathfrak{N}})\cap\mathfrak{M})^{-1}\,.$$

By Lemma 4

$$(\widetilde{\Gamma}^{+})^{-1}\,\widehat{+}\,\mathfrak{N}=\widetilde{\Gamma}\,\widehat{+}\,\mathfrak{N}\,.$$

Because the relation $\widetilde{\Gamma}\,\widehat{+}\,\mathfrak{N}$ is closed and $\mathfrak{N}\subseteq\mathfrak{M}$, one therefore gets $\mathring{\Gamma}^{+}=\mathring{\Gamma}^{-1}$ as required.

The computation of $\gamma_{\mathring{\Gamma}}$, $M_{\mathring{\Gamma}}$ is standard by applying Lemma 5. Note moreover that $\mathring{Q}(z)$, as stated, follows from

$$\mathring{Q}(z)=\mathscr{G}_b^{*}d((l_1-z)^{-1}k_{\min}(\cdot))\,.$$

2) With $\widetilde{\Gamma}\colon A_{\max}\to\mathbb{C}^{2d}$ as previously, one needs to verify that the operator

$$\mathring{\Gamma}:=((\widetilde{\Gamma}\cap\mathfrak{M})\,\widehat{+}\,\mathfrak{N})\,|_{\mathscr{H}_1^2}$$

is unitary from a $\widehat{J}_{\mathscr{H}_1}$-space to a $\widehat{J}_{\mathbb{C}^d}$-space; observe that the above $\mathring{\Gamma}$ coincides with $\widetilde{\Gamma}\,|_{\mathscr{H}_1}$ if considered as an operator $\operatorname{dom}\mathring{B}_{\max}\to\mathbb{C}^{2d}$. Thus, the inverse of the Krein space adjoint

$$\begin{aligned}(\mathring{\Gamma}^{+})^{-1}&=(\overline{\mathring{\Gamma}\,\widehat{+}\,(\mathscr{H}_{\perp}^2\times\{0\})})\,|_{\mathscr{H}_1^2}\\&=(\mathring{\Gamma}\,\widehat{+}\,(\mathscr{H}_{\perp}^2\times\{0\}))\,|_{\mathscr{H}_1^2}\\&=((\widetilde{\Gamma}\cap\mathfrak{M})\,\widehat{+}\,\mathfrak{N})\,|_{\mathscr{H}_1^2}=\mathring{\Gamma}\end{aligned}$$

as required.

3) Once $\mathring{l}_1$ has been established, the rest is straightforward. □

REMARK 3. With $\mathring{\Gamma}$ as in 1), $\mathring{\mathring{\Gamma}}\supsetneq\mathring{\Gamma}\,|_{\mathfrak{K}_1^2}$; in fact

$$\mathring{\mathring{\Gamma}}=\mathring{\Gamma}\,|_{\mathfrak{K}_1^2}\,\widehat{+}\,\{((0,k_{\min}(\chi)),(\chi,0))\,|\,\chi\in\mathbb{C}^d\}\,.$$

The subsequent results are presented only for $\mathring{B}_{\max}$.

Generalized resolvent A closed operator $\mathring{B}\in\operatorname{Ext}(\mathring{B}_{\min})$ is in bijective correspondence with a closed relation Θ in $\mathbb{C}^d$ via $\mathring{B}=\mathring{B}_{\Theta}:=\mathring{\Gamma}^{-1}(\Theta)$. We have

$$\mathring{B}_{\Theta}\subseteq\mathring{B}_{\max}\,,\quad\operatorname{dom}\mathring{B}_{\Theta}:=\{f\in\operatorname{dom}\mathring{B}_{\max}\,|\,(\mathring{\Gamma}_0f,\mathring{\Gamma}_1f)\in\Theta\}$$

and in particular $\mathring{B}_{\min}=\mathring{B}_{\Theta=\{0\}}$ and $\mathring{B}_0=\mathring{B}_{\Theta=\{0\}\times\mathbb{C}^d}$.

In the next theorem $U\colon f+k\mapsto(f,k)$ is a unitary operator from a Hilbert space $\mathscr{H}_1$ to an (external) Hilbert sum $\mathfrak{H}_m\oplus\mathfrak{K}_1$.

THEOREM 2. *1) Let Θ be a closed relation in $\mathbb{C}^d$. The resolvent of a closed operator $\mathring{B}_{\Theta}$ is given by*

$$U(\mathring{B}_{\Theta}-z)^{-1}U^{*}=\begin{pmatrix}\mathring{R}_{11}(z)&\mathring{R}_{12}(z)\\\mathring{R}_{21}(z)&\mathring{R}_{22}(z)\end{pmatrix}:\begin{matrix}\mathfrak{H}_m\\\oplus\\\mathfrak{K}_1\end{matrix}\to\begin{matrix}\mathfrak{H}_m\\\oplus\\\mathfrak{K}_1\end{matrix}$$

for $z\in\rho(\mathring{B}_\Theta)\cap\rho(\mathring{B}_0)$; *the entries*

$$\begin{aligned}
\mathring{R}_{11}(z) :=&(L-z)^{-1}+G_z\big(\mathscr{C}(\Theta-M_{\mathring{\Gamma}}(z))^{-1}\mathscr{C}^*\langle\varphi,(L-z)^{-1}\cdot\rangle\big)\,,\\
\mathring{R}_{12}(z) :=&-G_z\big(\mathscr{C}(\Theta-M_{\mathring{\Gamma}}(z))^{-1}\mathscr{G}_b^*d((l_1-z)^{-1}\cdot)\big)\,,\\
\mathring{R}_{21}(z) :=&-(l_1-z)^{-1}k_{\min}\big((\Theta-M_{\mathring{\Gamma}}(z))^{-1}\mathscr{C}^*\langle\varphi,(L-z)^{-1}\cdot\rangle\big)\,,\\
\mathring{R}_{22}(z) :=&(l_1-z)^{-1}+(l_1-z)^{-1}k_{\min}\big((\Theta-M_{\mathring{\Gamma}}(z))^{-1}\mathscr{G}_b^*d((l_1-z)^{-1}\cdot)\big)\,.
\end{aligned}$$

2) *Let* Θ *be a self-adjoint relation in* $\mathbb{C}^d$. *To a generalized resolvent* $P_{\mathfrak{H}_m}(\mathring{B}_\Theta-z)^{-1}|_{\mathfrak{H}_m}$ *there corresponds, via the generalized Krein–Naimark resolvent formula, a Nevanlinna family*

$$\tau\colon z\mapsto(\mathscr{C}^{-1})^*(\mathring{Q}(z)-\Theta)\mathscr{C}^{-1}\,.$$

Proof. 1) This part is due to Lemma 5, Theorem 1, and the Krein–Naimark resolvent formula.

2) We need to verify that the only solution $\tau(z)$ to

$$\mathring{R}_{11}(z)=(L-z)^{-1}-\gamma_\Gamma(z)(\tau(z)+M_\Gamma(z))\gamma_\Gamma(\bar{z})^*$$

is as stated; see Remark 1-3. The above equation reads

$$\begin{aligned}
&G_z(\mathscr{C}(\Theta-M_{\mathring{\Gamma}}(z))^{-1}\mathscr{C}^*\langle\varphi,(L-z)^{-1}\cdot\rangle)\\
&=-G_z((\tau(z)+M_\Gamma(z))^{-1}\langle\varphi,(L-z)^{-1}\cdot\rangle)
\end{aligned}$$

and then

$$\mathscr{C}(\Theta-M_{\mathring{\Gamma}}(z))^{-1}\mathscr{C}^*=-(\tau(z)+R(z))^{-1}$$

and

$$\mathscr{C}^{*\,-1}(\Theta-M_{\mathring{\Gamma}}(z))\mathscr{C}^{-1}=-(\tau(z)+R(z))$$

with both sides considered as relations. Subsequently, a relation $\tau(z)$ is the operator-wise sum of relations

$$\mathscr{C}^{*\,-1}M_{\mathring{\Gamma}}(z)\mathscr{C}^{-1}-R(z)=\mathscr{C}^{*\,-1}\mathring{Q}(z)\mathscr{C}^{-1}$$

and $-\mathscr{C}^{*\,-1}\Theta\mathscr{C}^{-1}$. □

REMARK 4. If $d=1$, $L\geqslant 0$, $\mathscr{Z}=\mathscr{Z}\cap(-\infty,0)$, $\mathscr{G}$ is diagonal, then an operator $\mathring{B}_\Theta=B_\Theta$ in $\mathscr{H}$, and then the resolvent in Theorem 2 is unitarily equivalent to that in [34, Theorem 6.1]. The scalar Q-function of the symmetric operator $\mathring{l}_1=l|_{\mathfrak{K}\ominus\mathfrak{K}_{\min}}$ in $\mathfrak{K}$ with defect numbers $(1,1)$ is

$$\mathring{Q}(z)=\langle b,\mathscr{G}(Z-z)^{-1}b\rangle_{\mathbb{C}^m}\,,\quad b:=(b_j)\in\mathbb{C}^m\,.$$

To compare with, the Q-function of the symmetric operator $\mathring{l}_1=\{0\}$ in $\mathfrak{K}_{\min}$ (*i.e.* $\mathfrak{K}_1=\mathfrak{K}_{\min}$) is given by

$$\mathring{Q}(z)=\langle b,\mathscr{G}b\rangle^2_{\mathbb{C}^m}\,/\,\langle b,\mathscr{G}(Z-z)b\rangle_{\mathbb{C}^m}\,.$$

Notice that $(\mathscr{G}Z-Z^*\mathscr{G})b\perp b$, and $\mathscr{G}Z\neq Z^*\mathscr{G}$ is allowed in this case.

5. Final remarks

Minimal realization The Nevanlinna function $\mathring{Q}$ can be given a standard form (*cf.* (1))

$$\mathring{Q}(z) = \mathring{Q}(\overline{z_0}) + (z-\overline{z_0})\gamma_{\mathring{\Gamma}}(z_0)^*(I+(z-z_0)(l_1-z)^{-1})\gamma_{\mathring{\Gamma}}(z_0)$$

for $z,\ z_0 \in \rho(l_1)$. One says in [23,27] the pair $(l_1, \gamma_{\mathring{\Gamma}})$ realizes $\mathring{Q}$, and a realization is minimal if ($\vee\ \equiv$ closed linear span)

$$\mathfrak{K}_1 = \vee\{(I+(z-z_0)(l_1-z)^{-1})\gamma_{\mathring{\Gamma}}(z_0)\chi \,|\, \chi \in \mathbb{C}^d\,;\, z\in\rho(l_1)\}\,.$$

Since the right-hand side $= \vee\{\mathfrak{N}_z(\mathring{l}_1^*)\,|\,z\in\rho(l_1)\}$, this means $\mathring{l}_1$ should be simple, *i.e.* $\mathring{l}_1$ should not admit orthogonal decompositions with a self-adjoint summand.

PROPOSITION 3. *$\mathring{l}_1$ is simple iff $\mathfrak{K}_1 = \mathfrak{K}_{\min}$.*

Proof. Sufficiency is clear, so we prove necessity. Consider $\mathfrak{K}_1$ as a set generated by elements $\{\mathfrak{h}_\mu\}_{\mu=1}^{d_1}$, with the corresponding Gram matrix

$$\mathscr{G}_1 := (\langle\mathfrak{h}_\mu, \mathfrak{h}_{\mu'}\rangle_{-m})$$

and $d_1 := \dim \mathfrak{K}_1$. An element k from $\mathfrak{K}_1$ is of the form

$$k = k(\eta) := \sum_\mu \eta_\mu \mathfrak{h}_\mu\,, \quad \eta = (\eta_\mu) = \mathscr{G}_1^{-1}\mathscr{W}^* d(k)$$

with $d(\mathfrak{K}_1) = \mathscr{G}^{-1}(\operatorname{ran}\mathscr{W})$. The transfer matrix

$$\mathscr{W} := (\langle g_i, \mathfrak{h}_\mu\rangle_{-m})\,.$$

Subsequently, l_1 maps $k(\eta)$ to $k(\mathring{Z}_{d_1}\eta)$, where the matrix

$$\mathring{Z}_{d_1} := \mathscr{G}_1^{-1}\mathscr{W}^* Z_d \mathscr{G}^{-1}\mathscr{W} \tag{10}$$

is similar to an Hermitian matrix: By recalling that $d(\mathfrak{K}_1)$ is a neutral subspace of a W-space it holds (with $\mathring{Z}_{d_1}^*$ the adjoint of $\mathring{Z}_{d_1}$)

$$\mathring{Z}_{d_1}^* \mathscr{G}_1 = \mathscr{G}_1 \mathring{Z}_{d_1}\,. \tag{11}$$

Let $\{\lambda_\mu\}$ be the eigenvalues of $\mathring{Z}_{d_1}$. By the spectral decomposition

$$\mathring{Z}_{d_1} = V_1^{-1}\operatorname{diag}\{\lambda_\mu\}V_1\,, \quad V_1 := U_1\mathscr{G}_1^{1/2}$$

with a $d_1\times d_1$ unitary matrix U_1, the eigenspace $\mathfrak{N}_\lambda(\mathring{l}_1)$, for some $\lambda\in\mathbb{R}$, consists of $k(\eta)\in\mathfrak{K}_1\ominus\mathfrak{K}_{\min}$ such that $(\forall\mu)\ (\lambda_\mu-\lambda)(V_1\eta)_\mu = 0$. Now, a simple $\mathring{l}_1$ has no eigenvalues, so that necessarily $\mathfrak{K}_1 = \mathfrak{K}_{\min}$. □

REMARK 5. With the notation as in Proposition 3 $\mathring{Q}$ can be given a yet another form

$$\mathring{Q}(z) = (\hat{b}^*\mathscr{W})(\mathring{Z}_{d_1}-z)^{-1}\mathscr{G}_1^{-1}(\hat{b}^*\mathscr{W})^*\,.$$

Invariance In order to emphasize that $\mathring{Q}$ is associated to $(\mathring{l}_1, l_1)$ in $\mathfrak{K}_1$, we use the notation

$$\mathring{Q} \equiv \mathring{Q}_{\mathfrak{K}_1}.$$

Because the diagonal entry [24, Lemma 2.3]

$$(\mathring{Q}_{\mathfrak{K}_1}(\lambda))_{ss} = \sup_{k \in \mathfrak{K}_1} \frac{|\langle k, \mathfrak{f}_s \rangle_{-m}|^2}{\langle k, (l-\lambda)k \rangle_{-m}}, \quad \lambda < \min \sigma(l_1)$$

(as usual the spectrum $\sigma(\cdot) := \mathbb{C} \setminus \rho(\cdot)$) and (*e.g.* [10]) a scalar valued Nevanlinna function is monotonically nondecreasing on any interval of $\mathbb{R}$ where it is analytic, one concludes that (*cf.* Remark 4)

$$(\mathring{Q}_{\mathfrak{K}_1'}(\lambda))_{ss} \leqslant (\mathring{Q}_{\mathfrak{K}_1}(\lambda))_{ss} \quad \text{if} \quad \mathfrak{K}_1' \subseteq \mathfrak{K}_1 \tag{12}$$

where $\mathfrak{K}_1'$ is some other subspace from the scale $\mathfrak{K}_{\min} \subseteq \mathfrak{K}_{\max}$. By the min-max principle $\min \sigma(l_1') \geqslant \min \sigma(l_1)$, $l_1' := P_{\mathfrak{K}_1'} l \,|_{\mathfrak{K}_1'}$. The preceding remarks imply the following, for $d = 1$: The points $\{\lambda \,|\, \mathring{Q}_{\mathfrak{K}_1}(\lambda) = \Theta - \widetilde{R}(\lambda)\}$ in $\rho(L) \cap (-\infty, \min \sigma(l_1))$ from the spectrum of a self-adjoint operator $\mathring{B}_\Theta$ in $\mathscr{H}_1$, $|\Theta| < \infty$, are nondecreasing whenever $\mathfrak{K}_1$ gets smaller.

These points need not increase, as $\mathfrak{K}_1$ gets smaller, if $\mathfrak{K}_1$ is invariant for l, *i.e.* if $l(\mathfrak{K}_1) \subseteq \mathfrak{K}_1$. In this case $l = l_1 \oplus (l \,|_{\mathscr{H}_\perp})$, and a generalized resolvent $P_{\mathfrak{K}_1}(l-z)^{-1} \,|_{\mathfrak{K}_1}$ coincides with $(l_1 - z)^{-1}$ (and is called orthogonal in [4, Chapter 2]); hence $\mathring{Q}_{\mathfrak{K}_1} = \mathring{Q}_{\mathfrak{K}}$. However

PROPOSITION 4. *$\mathfrak{K}_1$ is an invariant subspace for l iff $\mathfrak{K}_1 = \mathfrak{K}$.*

Proof. If $l(\mathfrak{K}_1) \subseteq \mathfrak{K}_1$ or, equivalently, $Z_d d(\mathfrak{K}_1) \subseteq d(\mathfrak{K}_1)$, then by Halmos [26, Theorem 3] there is an $md \times md$ matrix $C = (C_{ii'})$ that commutes with Z_d and satisfies $d(\mathfrak{K}_1) = \ker C$. The commutation criterion shows that C is diagonal in j (as previously, $i = \alpha(s,j)$, $i' = \alpha(s',j')$). On the other hand

$$\ker C \supseteq \operatorname{ran} \hat{b} = \vee \{ \sum_{j=1}^{m-1} b_j (e_{sm-m+j} - e_{sm}) \}$$

where $\{e_i\}_{i=1}^{md}$ is a standard basis of $\mathbb{C}^{md}$; hence $\sum_j b_j C e_i = 0$. But $Ce_i = (C_{1,i}, \ldots, C_{md,i})$ and $C_{1,i} = \delta_{j,1} C_{1,i}, \ldots, C_{md,i} = \delta_{j,m} C_{md,1}$, thus $(\forall i)$ $b_j C e_i = 0$, *i.e.* $C = 0$. □

Generalized resolvent of l_1 We present a (unique) Nevanlinna family τ_1 corresponding to $P_{\mathfrak{K}_{\min}}(l_1 - z)^{-1} \,|_{\mathfrak{K}_{\min}}$ in terms of $\mathring{Q}_{\mathfrak{K}_1}$. Below we use

$$\mathring{Z}_d = \mathscr{G}_{\min}^{-1} \mathscr{G}_b^* Z_d \hat{b}$$

as in (10) for $\mathfrak{K}_1 = \mathfrak{K}_{\min}$.

PROPOSITION 5. *To a generalized resolvent* $P_{\mathfrak{K}_{\min}}(l_1-z)^{-1}|_{\mathfrak{K}_{\min}}$ *there corresponds, via the generalized Krein–Naimark resolvent formula, a matrix valued Nevanlinna function*

$$\tau_1 : z \mapsto -\mathscr{G}_{\min}(\mathring{Q}_{\mathfrak{K}_1}(z)^{-1}\mathscr{G}_{\min}+z).$$

If $\mathfrak{K}_1=\mathfrak{K}_{\min}$ *then* $\tau_1(z)=-\mathscr{G}_{\min}\mathring{Z}_d$ *is an Hermitian matrix.*

Proof. Consider a simple symmetric operator $\{0\}$ in $\mathfrak{K}_{\min}$. The boundary triple $(\mathbb{C}^d,\Gamma_0^{\min},\Gamma_1^{\min})$ for $\mathfrak{K}_{\min}^2$ is given by $(\chi,\chi'\in\mathbb{C}^d)$

$$\Gamma_0^{\min}(k_{\min}(\chi),k_{\min}(\chi')) := \chi\,,$$
$$\Gamma_1^{\min}(k_{\min}(\chi),k_{\min}(\chi')) := \mathscr{G}_{\min}\chi'\,.$$

The γ-field and the Weyl function corresponding to the triple are given by $k_{\min}(\cdot)$ and $z\mathscr{G}_{\min}$, respectively. Subsequently, by using $\ker\Gamma_0^{\min}=\{0\}\times\mathfrak{K}_{\min}$ and by applying the generalized Krein–Naimark formula

$$\mathring{Q}_{\mathfrak{K}_1}(z) = -\mathscr{G}_{\min}(\tau_1(z)+z\mathscr{G}_{\min})^{-1}\mathscr{G}_{\min}$$

for $z\in\rho(l_1)$. Now $\mathring{Q}_{\mathfrak{K}_1}(z)$, as the Weyl family corresponding to $\Pi_{\mathring{\Gamma}}$, is nonsingular (or use that l_1 and $\{0\}\times\mathfrak{K}_{\min}$ are disjoint), so $\tau_1(z)$ is the matrix as stated.

If $\mathfrak{K}_1=\mathfrak{K}_{\min}$ then use that

$$\mathring{Q}_{\mathfrak{K}_{\min}}(z)=\mathscr{G}_{\min}(\mathring{Z}_d-z)^{-1}$$

for $z\in\rho(\mathring{Z}_d)$, *cf.* Remark 5, and recall from (11) that $\mathscr{G}_{\min}\mathring{Z}_d$ is Hermitian. □

REMARK 6. If $d=1$ then

$$\mathring{Q}_{\mathfrak{K}_1}(z)=\frac{z\|\mathfrak{f}\|_{-m}^2-\langle\mathfrak{f},L\mathfrak{f}\rangle_{-m}}{z\|\mathfrak{f}\|_{-m}^2+\tau_1(z)}\,\mathring{Q}_{\mathfrak{K}_{\min}}(z).$$

As already pointed out in Remark 4 $\langle b,\mathscr{G}Zb\rangle_{\mathbb{C}^m}$ is real valued; actually it equals $\langle\mathfrak{f},L\mathfrak{f}\rangle_{-m}$ (with $\mathfrak{f}\equiv\mathfrak{f}_s$ for $d=1$). Similarly $\langle b,\mathscr{G}b\rangle_{\mathbb{C}^m}=\|\mathfrak{f}\|_{-m}^2$. The scalar $\tau_1(z)=-\langle\mathfrak{f},L\mathfrak{f}\rangle_{-m}$ iff $\mathfrak{K}_1=\mathfrak{K}_{\min}$; otherwise, by (12) $\tau_1(\lambda)\leqslant-\langle\mathfrak{f},L\mathfrak{f}\rangle_{-m}$ for $\lambda<\min\sigma(l_1)$.

A. Appendix. The peak model in the reference space

We are given a linearly independent system $\{\widehat{\varphi}_s\in\mathfrak{H}_{-2}\smallsetminus\mathfrak{H}_{-1}\}$ and a closed densely defined symmetric restriction $\widehat{L}_0$ of L subject to the boundary condition $\langle\widehat{\varphi},u\rangle=0$, $u\in\mathfrak{H}_2$; $\langle\widehat{\varphi},\cdot\rangle$ is the vector valued functional with components $\langle\widehat{\varphi}_s,\cdot\rangle$. The adjoint $\widehat{L}_0^*$ in $\mathfrak{H}_0$ of $\widehat{L}_0$ extends L to $\mathfrak{H}_2\dotplus\mathfrak{N}_z(\widehat{L}_0^*)$, $z\in\rho(L)$, where the defect subspace

$$\mathfrak{N}_z(\widehat{L}_0^*)=\widehat{g}_z(\mathbb{C}^d)\,,\quad \widehat{g}_z(c):=\sum_s c_s\widehat{g}_s(z)\,,\quad \widehat{g}_s(z):=(L-z)^{-1}\widehat{\varphi}_s$$

and $c=(c_s)\in\mathbb{C}^d$.

Here we analyze the peak model transformed to $\mathfrak{H}_0$ by using a unitary operator $P(L)^{-1/2}$ from $\mathfrak{H}_{-n}$ onto $\mathfrak{H}_{m+n}$; $n \geqslant 0$. Thus, we view $\widehat{\varphi}_s$ as

$$\widehat{\varphi}_s := P(L)^{-1/2}\varphi_s\,, \quad \varphi_s \in \mathfrak{H}_{-m-2} \setminus \mathfrak{H}_{-m-1}$$

for some fixed integer $m \geqslant 1$. Then

$$\widehat{L}_0 = P(L)^{1/2} L_{\min} P(L)^{-1/2}\,, \quad \widehat{L}_0^* = P(L)^{1/2} L_{\min}^* P(L)^{-1/2}\,.$$

The triple $\Pi_{\widehat{\Gamma}} = (\mathbb{C}^d, \widehat{\Gamma}_0, \widehat{\Gamma}_1)$ with (recall Remark 1)

$$\widehat{\Gamma} = (\widehat{\Gamma}_0, \widehat{\Gamma}_1) := \Gamma P(L)^{-1/2}\,, \quad \operatorname{dom}\widehat{\Gamma} = \operatorname{dom}\widehat{L}_0^*$$

is a boundary triple for $\widehat{L}_0^*$ with the γ-field $\rho(L) \ni z \mapsto \gamma_{\widehat{\Gamma}}(z) = \widehat{g}_z(\cdot)$ and the Weyl function $M_{\widehat{\Gamma}} = R$. In this way R is the Q-function for both $(L_{\min}, L_m)$ and $(\widehat{L}_0, L)$.

What we really want to show is that the scaled boundary operator $\widetilde{\Gamma}$ in (6) defines an essentially unitary boundary triple $\Pi_{\widehat{\Gamma}'} = (\mathbb{C}^d, \widehat{\Gamma}'_0, \widehat{\Gamma}'_1)$ for $\widehat{L}_0^*$. This means the operator $\widehat{\Gamma}' := (\widehat{\Gamma}'_0, \widehat{\Gamma}'_1)$, with domain

$$\widehat{A}_{\max} := P(L)^{-1/2} A_{\max} P(L)^{1/2}$$

dense in $\widehat{L}_0^*$, is an isometry from a $\widehat{J}_{\mathfrak{H}_0}$-space to a $\widehat{J}_{\mathbb{C}^d}$-space, $\widehat{\Gamma}'^{-1} \subseteq \widehat{\Gamma}'^{+}$, and moreover the closure $\operatorname{clo}\widehat{\Gamma}' = \widehat{\Gamma}$. As usual, we consider $\widehat{\Gamma}'$ also as an operator $\operatorname{dom}\widehat{A}_{\max} \to \mathbb{C}^{2d}$. An essentially unitary boundary triple is a special case of an isometric boundary triple studied in [20]. The γ-field and the Weyl function are defined identically as in the case of an (ordinary) boundary triple.

To make our statement precise, define a subset $\widehat{\mathfrak{K}}$ of $\mathfrak{H}_0$ by

$$\widehat{\mathfrak{K}} := \vee\{\widehat{g}_i := \widehat{g}_s(z_j)\}\,, \quad i = \alpha(s,j)\,.$$

Note $\widehat{\mathfrak{K}} \cap \mathfrak{H}_{2m-1} = \{0\}$. Every $\widehat{k} \in \widehat{\mathfrak{K}}$ is in bijective correspondence with $d(\widehat{k}) = (d_i(\widehat{k}))$ via the Gram matrix $\mathscr{G} = (\langle \widehat{g}_i, \widehat{g}_{i'} \rangle_0)$; let (*cf.* (4))

$$c(\widehat{k}) = (c_s(\widehat{k})) \in \mathbb{C}^d\,, \quad c_s(\widehat{k}) := \sum_j d_i(\widehat{k})\,, \quad d(\widehat{k}) = \mathscr{G}^{-1}(\langle \widehat{g}_i, \widehat{k} \rangle_0)\,.$$

Then $c(\widehat{\mathfrak{K}}) = \mathbb{C}^d$ and moreover $c(\widehat{k}) = 0$ iff $\widehat{k} \in \widehat{\mathfrak{K}} \cap \mathfrak{H}_2$. Let

$$\mathfrak{L} := \mathfrak{H}_{2m+2} \dotplus \widetilde{P}(L)^{-1}(\mathfrak{N}_z(\widehat{L}_0^*))\,.$$

Then $\mathfrak{L}$ is dense in $\mathfrak{H}_0$: $\mathfrak{H}_{2m+2} \subseteq \mathfrak{L} \subseteq \mathfrak{H}_{2m} \subseteq \mathfrak{H}_2$.

THEOREM 3. *Define an operator* $\widehat{\Gamma}' := (\widehat{\Gamma}'_0, \widehat{\Gamma}'_1)$ *where*

$$\begin{aligned} &\widehat{\Gamma}'_0 \colon \mathfrak{L} \dotplus \widehat{\mathfrak{K}} \ni u + \widehat{k} \mapsto c(\widehat{k})\,, \\ &\widehat{\Gamma}'_1 \colon \mathfrak{L} \dotplus \widehat{\mathfrak{K}} \ni u + \widehat{k} \mapsto \langle \widehat{\varphi}, u \rangle + \mathscr{M} d(\widehat{k})\,. \end{aligned}$$

The triple $\Pi_{\widehat{\Gamma}'} = (\mathbb{C}^d, \widehat{\Gamma}'_0, \widehat{\Gamma}'_1)$ *is an isometric boundary triple for* $\widehat{L}_0^*$ *such that*

$$\operatorname{clo}\widehat{\Gamma}' = \widehat{\Gamma}, \quad \operatorname{ran}\widehat{\Gamma}'_0 = \mathbb{C}^d, \quad T_0 \subsetneq \overline{T_0} = L.$$

Here an essentially self-adjoint operator

$$T_0 := \widehat{L}_0^*|_{\ker\widehat{\Gamma}'_0} = L|_{\mathfrak{L}\dotplus(\widehat{\mathfrak{K}}\cap\mathfrak{H}_2)}.$$

The γ*-field and the Weyl function corresponding to* $\Pi_{\widehat{\Gamma}'}$ *are* $z \mapsto \widehat{g}_z(\cdot)$ *and* R.

Proof. It is rather straightforward that

$$\widehat{A}_{\max}(u+\widehat{k}) = Lu + \sum_i (Z_d d(\widehat{k}))_i \widehat{g}_i$$

and then the boundary form

$$\begin{aligned}&\langle u+\widehat{k}, \widehat{A}_{\max}(u'+\widehat{k}')\rangle_0 - \langle \widehat{A}_{\max}(u+\widehat{k}), u'+\widehat{k}'\rangle_0\\ &= \langle \widehat{\Gamma}'_0(u+\widehat{k}), \widehat{\Gamma}'_1(u'+\widehat{k}')\rangle_{\mathbb{C}^d} - \langle \widehat{\Gamma}'_1(u+\widehat{k}), \widehat{\Gamma}'_0(u'+\widehat{k}')\rangle_{\mathbb{C}^d}\end{aligned}$$

for $u, u' \in \mathfrak{L}$ and $\widehat{k}, \widehat{k}' \in \widehat{\mathfrak{K}}$. That $\widehat{A}_{\max} \subseteq \widehat{L}_0^*$ densely follows from

$$A_{\max} \subseteq L_{\max} = P(L)^{1/2}\widehat{L}_0^* P(L)^{-1/2}$$

so $\Pi_{\widehat{\Gamma}'}$ is an isometric boundary triple for $\widehat{L}_0^*$. Since $u+\widehat{k}$ is the sum of a $\mathfrak{H}_2$-function $u+\widehat{k}-\widehat{g}_z(c)$, $c = c(\widehat{k})$, and an eigenvector $\widehat{g}_z(c)$ of $\widehat{L}_0^*$, it follows that $\widehat{\Gamma}'_0 \subseteq \widehat{\Gamma}_0$ and $\widehat{\Gamma}'_1 \subseteq \widehat{\Gamma}_1$. Since moreover $\mathfrak{L} \dotplus \widehat{\mathfrak{K}}$ is a core for $\widehat{L}_0^*$, this shows $\operatorname{clo}\widehat{\Gamma}' = \widehat{\Gamma}$.

The last statement of the theorem uses $\mathfrak{N}_z(\widehat{A}_{\max}) = \mathfrak{N}_z(\widehat{L}_0^*)$. □

REMARKS 3. 1. $\mathscr{G}_Z$ need not be Hermitian.

2. Since T_0 is only essentially self-adjoint, $\Pi_{\widehat{\Gamma}'}$ is not a B-generalized boundary triple for $\widehat{L}_0^*$ [20, Definition 1.5]. (In [16, Lemma 5.5(ii)] A_0 must be self-adjoint.)

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(Received March 8, 2023)

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