



The linearization of boundary eigenvalue problems and reproducing kernel Hilbert spaces

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Abstract

The boundary eigenvalue problems for the adjoint of a symmetric relation S in a Hilbert space with finite, not necessarily equal, defect numbers, which are related to the selfadjoint Hilbert space extensions of S are characterized in terms of boundary coefficients and the reproducing kernel Hilbert spaces they induce. © 2001 Elsevier Science Inc. All rights reserved.

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1. Introduction

Let S be a densely defined symmetric operator in a Hilbert space \mathcal{H} with defect index (d_+, d_-) , $d = d_+ + d_- < \infty$ and let $b : \text{dom}(S^*) \rightarrow \mathbb{C}^d$ be a boundary mapping for S with Gram matrix Q ; for the definition, see Section 2. Consider the following boundary eigenvalue problem: for $h \in \mathcal{H}$, find $f \in \mathcal{H}$ such that

$$f \in \text{dom}(S^*), \quad (S^* - z)f = h, \quad \mathcal{U}(z)b(f) = 0, \quad (1.1)$$

where $\mathcal{U}(z)$ is a holomorphic matrix function on $\mathbb{C} \setminus \mathbb{R}$ of size $d_{\pm} \times d$ if $z \in \mathbb{C}^{\pm}$. The aim of this paper is to describe the linearization \tilde{A} of this problem. We call

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\tilde{A} a linearization of (1.1) if \tilde{A} is a selfadjoint extension of S in a Hilbert space $\tilde{\mathcal{H}}$ containing \mathcal{H} as a closed subspace and if for all $z \in \mathbb{C} \setminus \mathbb{R}$ and $h \in \mathcal{H}$, the unique solution of (1.1) is given by $f = \tilde{P}_{\mathcal{H}}(\tilde{A} - z)^{-1}h$, where $\tilde{P}_{\mathcal{H}}$ is the projection in $\tilde{\mathcal{H}}$ onto \mathcal{H} . Necessary and sufficient conditions on $\mathcal{U}(z)$ that (1.1) has such a linearization are given by (U1)–(U5) in Definition 3.1; see Theorem 5.4. These conditions are well known; see, for example, [5,11,13,19,20,26]. In [19], linear relations are avoided. The proofs in [11,20] are based on the theory of characteristic functions of unitary colligations. Here we give another proof. We use the reproducing kernel Hilbert space $\mathcal{H}(K_{\mathcal{U}})$ with the nonnegative reproducing kernel

$$K_{\mathcal{U}}(z, w) = i \frac{\mathcal{U}(z)Q^{-1}\mathcal{U}(w)^*}{z - \bar{w}}, \quad z \neq \bar{w}.$$

This space consists of holomorphic vector functions on $\mathbb{C} \setminus \mathbb{R}$. The operator $S_{\mathcal{U}}$ of multiplication by the independent variable in this space is a closed simple symmetric operator with defect index (ω_-, ω_+) , $d_+ - \omega_+ = d_- - \omega_- =: \tau \geq 0$; see Section 4. The linearization \tilde{A} of (1.1) is a canonical selfadjoint extension of the symmetric direct sum operator $S \oplus S_{\mathcal{U}}$ in $\tilde{\mathcal{H}} = \mathcal{H} \oplus \mathcal{H}(K_{\mathcal{U}})$ such that (in terms of graphs of operators)

$$\tilde{A} \cap \mathcal{H}^2 = S_0, \quad \tilde{A} \cap \mathcal{H}(K_{\mathcal{U}})^2 = S_{\mathcal{U}}, \tag{1.2}$$

where S_0 is a τ -dimensional symmetric extension of S in \mathcal{H} . The method yields a formula for \tilde{A} (see Theorem 5.4):

$$\tilde{A} = \left\{ \left\{ \begin{pmatrix} f \\ f_1 \end{pmatrix}, \begin{pmatrix} S^* f \\ g_1 \end{pmatrix} \right\} : f \in \text{dom}(S^*), \{f_1, g_1\} \in S_{\mathcal{U}}^*, \right. \\ \left. U_0 b(f) = 0, B_0 b(f) + \Gamma b_1(f_1, g_1) = 0 \right\},$$

where

- (a) the $\tau \times d$ matrix U_0 and $\omega \times d$ matrix B_0 have maximal rank and determine the operator S_0 and its adjoint S_0^* as follows

$$\begin{aligned} S_0 &= \{ \{f, S^* f\} : f \in \text{dom}(S^*), U_0 b(f) = 0, B_0 b(f) = 0 \}, \\ S_0^* &= \{ \{f, S^* f\} : f \in \text{dom}(S^*), U_0 b(f) = 0 \}; \end{aligned} \tag{1.3}$$

- (b) b_1 is an arbitrary boundary mapping for $S_{\mathcal{U}}$ in $\mathcal{H}(K_{\mathcal{U}})$ with Gram matrix Q_1 ;
- (c) Γ is an invertible $\omega \times \omega$ matrix such that $Q_1 + \Gamma(B_0 Q^{-1} B_0^*)^{-1} \Gamma^* = 0$.

The graph notation that we use here simplifies formulas like the ones in (1.2) and (1.3), but also can hardly be avoided. For example, $S_{\mathcal{U}}$ in $\mathcal{H}(K_{\mathcal{U}})$ need not be densely defined, and if it is not, its adjoint $S_{\mathcal{U}}^*$ is multivalued and the boundary mapping b_1 for $S_{\mathcal{U}}$ is not a mapping on $\text{dom}(S_{\mathcal{U}}^*)$, but on the graph of $S_{\mathcal{U}}^*$, that is, $b_1 : S_{\mathcal{U}}^* \rightarrow \mathbb{C}^{\omega}$, $\omega = \omega_+ + \omega_-$. This permits us also to drop the assumption that S is densely defined, which opens the possibility for more general boundary conditions

including integro-differential and interface conditions for the case that S arises from a differential expression. See, for example, [4,15,18,27].

The connection between $\mathcal{U}(z)$ and the formula for the linearization \tilde{A} is surprisingly simple. By multiplying the boundary eigenvalue condition $\mathcal{U}(z)b(f) = 0$ from the left by a suitable invertible (and even holomorphic) matrix function $\mathcal{A}(z)$, this condition can be row reduced to one of the form

$$\begin{pmatrix} U_0 \\ \mathcal{U}_0(z)B_0 \end{pmatrix} b(f) = 0,$$

where U_0 and B_0 are as in the formula for the linearization \tilde{A} and $\mathcal{U}_0(z)$ is an $\omega_{\pm} \times \omega$ matrix valued function on \mathbb{C}^{\pm} with the same properties as $\mathcal{U}(z)$ and one more, namely, that for all $z \in \mathbb{C} \setminus \mathbb{R}$, the $\omega \times \omega$ matrix

$$\begin{pmatrix} \mathcal{U}_0(z) \\ \mathcal{U}_0(\bar{z}) \end{pmatrix}$$

is invertible; see Theorem 3.2. The reproducing kernel Hilbert spaces associated with the kernels $K_{\mathcal{U}}(z, w)$ and $K_{\mathcal{U}_0}(z, w)$ are isomorphic and under the isomorphism the operators of multiplication by the independent variable coincide. An essential tool to obtain the description of the linearization of (1.1) is the characterization of $\mathcal{U}_0(z)$ in terms of a boundary mapping for $S_{\mathcal{U}}$ and a holomorphic basis of $\ker(S_{\mathcal{U}}^* - z)$; see Proposition 4.2.

If $\mathcal{U}(z)$ is a polynomial and satisfies (U1)–(U5) the theory of Bezoutians can be applied to yield an explicit formula for \tilde{A} . This is also possible when (U5) is replaced by the condition that the kernel $K_{\mathcal{U}}(z, w)$ has a finite number of negative squares (then the extending space $\tilde{\mathcal{H}}$ is a Pontryagin space containing the Hilbert space \mathcal{H} as a regular subspace). Our results in this case include and supplement those of Russakowskii in [21–23], who was the first to use Bezoutians in this context. They will be published in another paper. For an introduction to the linearization of Sturm–Liouville eigenvalue problems with boundary conditions which depend holomorphically on the eigenvalue parameter, we refer to the lecture series in [10], where further references can be found. The main results of this paper were presented by the first author at the International Workshop on Operator Theory and Applications held in Groningen, Netherlands, June 30–July 3, 1998.

2. Preliminaries

Recall that a *relation* from a set X to a set Y is a subset of the Cartesian product $X \times Y$, and a relation F from X to Y is called a *function* if $\{x, y\} \in F, \{x, z\} \in F$ implies $y = z$. A *linear relation* T in a Hilbert space $(\mathcal{H}, \langle \cdot, \cdot \rangle_{\mathcal{H}})$ is a linear subset of $\mathcal{H}^2 = \mathcal{H} \oplus \mathcal{H}$; T is called *closed* if T is a closed subset of \mathcal{H}^2 . The *inverse*

$$T^{-1} = \{\{f, g\}: \{g, f\} \in T\}$$

and the *adjoint*

$$T^* = \{\{u, v\} \in \mathcal{H}^2: \langle g, u \rangle_{\mathcal{H}} - \langle f, v \rangle_{\mathcal{H}} = 0 \forall \{f, g\} \in T\}$$

are also linear relations and T^* is always closed. A linear relation T is the graph of an operator if and only if its multivalued part $T(0) := \{y \in \mathcal{H}: \{0, y\} \in T\}$ is equal to $\{0\}$; we often identify an operator with its graph; see, for example, (1.3) or (2.3). The *domain* $\text{dom}(T)$, *range* $\text{ran}(T)$ and *kernel* $\text{ker}(T)$ of a linear relation T are defined by

$$\text{dom}(T) = \{x \in \mathcal{H}: \exists y \in \mathcal{H}, \{x, y\} \in T\},$$

$$\text{ran}(T) = \{y \in \mathcal{H}: \exists x \in \mathcal{H}, \{x, y\} \in T\},$$

$$\text{ker}(T) = \{x \in \mathcal{H}: \{x, 0\} \in T\}.$$

The *sum* $T + S$ and the *composition* TS of two linear relations T and S are defined by

$$T + S = \{\{f, g + h\}: \{f, g\} \in T, \{f, h\} \in S\},$$

$$ST = \{\{f, h\}: \exists g \in \mathcal{H}, \{f, g\} \in T, \{g, h\} \in S\}.$$

Since we identify operators with graphs,

$$\alpha I = \{\{x, \alpha x\}: x \in \mathcal{H}\}, \quad \alpha \in \mathbb{C},$$

and hence

$$T + \alpha I = \{\{f, g + \alpha f\}: \{f, g\} \in T\},$$

$$\alpha T = \{\{f, \alpha g\}: \{f, g\} \in T\}.$$

Then $T \cap \alpha I = \{\{f, g\} \in T: g = \alpha f\}$ is an operator with domain $\text{dom}(T \cap \alpha I) = \text{ker}(T - \alpha I)$. We often identify α with αI . Occasionally, we use the sum of two linear relations T and S as linear subsets of \mathcal{H}^2 :

$$T \dot{+} S = \{\{f + h, g + k\}: \{f, g\} \in T, \{h, k\} \in S\},$$

and this sum is called *direct* if $T \cap S = \{\{0, 0\}\}$ and *orthogonal* if $T \perp S$ and then we use the notation $T \oplus S$. For a detailed account of linear relations we refer to the recent book by Cross [6].

A linear relation T is called *symmetric* if $T \subset T^*$ and *selfadjoint* if $T = T^*$. A relation T is called *isometric* if $T^{-1} \subset T^*$ and *unitary* if $T^{-1} = T^*$; in the first case T is an ordinary isometric operator from $\text{dom}(T)$ to $\text{ran}(T)$ and in the second case T is a unitary operator on \mathcal{H} . The *Cayley transform* with respect to $\mu \in \mathbb{C} \setminus \mathbb{R}$

$$C_{\mu}(T) = \{\{g - \mu f, g - \bar{\mu} f\}: \{f, g\} \in T\}$$

defines a bijection on the class of linear relations on \mathcal{H} onto itself. Its inverse is given by

$$F_{\mu}(T) = \{\{u - v, \bar{\mu}u - \mu v\}: \{u, v\} \in T\}.$$

The formula $V = C_\mu(S)$ gives a one-to-one correspondence between all symmetric relations S in \mathcal{H} and all isometric operators V , in this case $\text{dom}(V) = \text{ran}(S - \mu)$ and $\text{ran}(V) = \text{ran}(S - \bar{\mu})$. The same formula gives a one-to-one correspondence between all selfadjoint relations A in \mathcal{H} and all unitary operators U , and the equality $A(0) = \ker(U - I)$ implies that in this correspondence A is multivalued if and only if 1 is an eigenvalue of U .

A symmetric relation S is called *simple* if

$$\mathcal{H} = \overline{\text{span}}\{ \ker(S^* - z) : z \in \mathbb{C} \setminus \mathbb{R} \}, \tag{2.1}$$

equivalently if

$$\bigcap_{z \in \mathbb{C} \setminus \mathbb{R}} \text{ran}(S - z) = \{0\}. \tag{2.2}$$

If S is simple, it is an operator. In general, S admits a unique decomposition into a simple operator and a selfadjoint part: there exists a decomposition of the space $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ and $S : S = S_1 \oplus S_2$, where S_1 is a simple symmetric operator in \mathcal{H}_1 and S_2 is a selfadjoint relation in \mathcal{H}_2 . A selfadjoint relation A has a ‘rectangular’ structure: A can be written as $A = A_1 \oplus A_\infty$, where $A_\infty := \{ \{0, x\} \in \mathcal{H}^2 : x \in A(0) \}$ is a selfadjoint relation in $\mathcal{H}_\infty = A(0)$ and A_1 is a selfadjoint operator in $\mathcal{H}_1 = \mathcal{H} \ominus \mathcal{H}_\infty$. Thus, the resolvent $(A - z)^{-1} = (A_1 - z)^{-1} \oplus 0$, $z \in \mathbb{C} \setminus \mathbb{R}$, is a bounded operator on \mathcal{H} whose kernel equals $A(0)$ and we have

$$(A - z)^{-1} = (A_1 - z)^{-1} P_{\mathcal{H}_1} : \mathcal{H} \rightarrow \mathcal{H}_1 \subset \mathcal{H}, \tag{2.3}$$

where $P_{\mathcal{H}_1}$ is the orthogonal projection in \mathcal{H} onto \mathcal{H}_1 .

The adjoint of a symmetric relation S can be decomposed as

$$S^* = S \dot{+} (S^* \cap zI) \dot{+} (S^* \cap \bar{z}I), \quad \text{direct sum in } \mathcal{H}^2,$$

where $z \in \mathbb{C} \setminus \mathbb{R}$. The dimension $\dim(S^* \cap zI)$ is constant on each of the open half planes \mathbb{C}^+ and \mathbb{C}^- and is denoted by d_+ , for $z \in \mathbb{C}^+$ and d_- , for $z \in \mathbb{C}^-$. The numbers d_+ and d_- are called the upper and lower defect numbers of S , the pair (d_+, d_-) is called the defect index. In the sequel, we assume $d = d_+ + d_- < \infty$.

A linear relation \tilde{T} in a Hilbert space $\tilde{\mathcal{H}}$ is called an *extension* of a linear relation S in a Hilbert space \mathcal{H} if \mathcal{H} is a closed subspace of $\tilde{\mathcal{H}}$ and $S \subset \tilde{T}$. The space $\tilde{\mathcal{H}} \ominus \mathcal{H}$ is called the *exit space*; if it is trivial \tilde{T} is called *canonical*. A symmetric relation always has selfadjoint extensions possibly with a nontrivial exit space (just as an isometric operator always has unitary extensions). S has canonical selfadjoint extensions if and only if $d_+ = d_-$.

A selfadjoint extension \tilde{T} of S is *minimal* if

$$\tilde{\mathcal{H}} = \overline{\text{span}}\{ \mathcal{H}, \text{ran}((\tilde{T} - z)^{-1}|_{\mathcal{H}}) : z \in \mathbb{C} \setminus \mathbb{R} \} \tag{2.4}$$

or, equivalently, the only subspace of $\tilde{\mathcal{H}} \ominus \mathcal{H}$ which is invariant under $(\tilde{T} - z)^{-1}$ for one, and hence for all, $z \in \mathbb{C} \setminus \mathbb{R}$, is the trivial subspace.

A *boundary mapping* for a closed symmetric relation S in \mathcal{H} with defect index (d_+, d_-) is a surjective linear operator $b : S^* \rightarrow \mathbb{C}^d$ with $\ker(b) = S$. If b is

a boundary mapping for S , then there is a unique $d \times d$ matrix Q such that for all $\{f, g\}, \{u, v\} \in S^*$,

$$\langle g, u \rangle_{\mathcal{H}} - \langle f, v \rangle_{\mathcal{H}} = ib(u, v)^*Qb(f, g). \tag{2.5}$$

Q is a selfadjoint and invertible matrix and has d_+ positive and d_- negative eigenvalues. The matrix Q is called the *Gram matrix* for b , for if $Q = (q_{jk})_{j,k=1}^d$, then $q_{jk} = \llbracket b^{-1}(e_k), b^{-1}(e_j) \rrbracket$, where $e_j \in \mathbb{C}^d$ is the j th unit vector and

$$\llbracket \{f, g\}, \{u, v\} \rrbracket := \frac{1}{i}(\langle g, u \rangle_{\mathcal{H}} - \langle f, v \rangle_{\mathcal{H}}). \tag{2.6}$$

Combining (2.5) and (2.6) we get

$$\llbracket \{f, g\}, \{u, v\} \rrbracket = b(u, v)^*Qb(f, g), \quad \{f, g\}, \{u, v\} \in S^*.$$

Note that if b is a boundary mapping for S with Gram matrix Q and if B is an invertible $d \times d$ matrix, then Bb is a boundary mapping for S with Gram matrix $B^{-*}QB^{-1}$. For each selfadjoint and invertible matrix Q with d_+ positive and d_- negative eigenvalues there exists a boundary mapping for S with Gram matrix Q .

The form $\llbracket \cdot, \cdot \rrbracket$ from (2.6) defines an indefinite inner product on \mathcal{H}^2 with respect to which the space $(\mathcal{H}^2, \llbracket \cdot, \cdot \rrbracket)$ is a Krein space. The inner product $\llbracket \cdot, \cdot \rrbracket$ appears also in the definition of the adjoint of a linear relation. The extension theory outlined here can be explained by the geometry of subspaces in Krein spaces; see Appendix A. For the Krein space terminology which we use throughout the paper we refer to the monographs of Azizov and Iokhvidov [1] and Bognar [2]. For similar symplectic algebra formulations we refer to the book of Everitt and Markus [16]. The extension theory in this paper is closely related to the extension theory in [17, Chapter 3]: there S is a densely defined symmetric operator in a Hilbert space \mathcal{H} with equal (finite or infinite) defect numbers d_{\pm} . A triple $(\mathcal{H}_0, \Gamma_1, \Gamma_2)$ consisting of a Hilbert space \mathcal{H}_0 and mappings $\Gamma_j : \text{dom}(S^*) \rightarrow \mathcal{H}_0$ is called a *boundary value space* of S if (i) for all $f, h \in \text{dom}(S^*)$,

$$\langle S^*f, h \rangle - \langle f, S^*h \rangle = \langle \Gamma_1 f, \Gamma_2 h \rangle_{\mathcal{H}_0} - \langle \Gamma_2 f, \Gamma_1 h \rangle_{\mathcal{H}_0}$$

and (ii) the mapping $(\Gamma_1, \Gamma_2)^T : \text{dom}(S^*) \rightarrow \mathcal{H}_0^2$ is surjective. The definition implies that $\text{dom}(S) = \ker(\Gamma_1, \Gamma_2)^T$. Hence, if $d_0 = d_+ = d_- < \infty$ and if we identify \mathcal{H}_0 with \mathbb{C}^{d_0} , then the mapping $b = (\Gamma_1, \Gamma_2)^T$ is a boundary mapping with Gram matrix

$$Q = i \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix},$$

where I denotes the identity matrix of appropriate size. Evidently, one can always transform a given boundary mapping b as defined above into one of the types considered in [17]. In [17], dissipative extensions are considered; for some recent results, see also [3]. The ‘boundary value space’ method is further developed in a series of interesting papers by Derkach and Malamud, see, for example, [8,9], where further references can be found. These papers are more focused on the description of the

generalized resolvents of S and Weyl functions with applications to moment and other problems, than on the description of the boundary coefficients as presented in this paper. Some of their results have been extended to the indefinite setting by Derkach in, for example, [7].

3. Boundary coefficients

For a symmetric linear relation S in a Hilbert space \mathcal{H} and boundary mapping b for S the formulation of the boundary eigenvalue problem, that is, the analog of problem (1.1) is admittedly somewhat artificial:

For $h \in \mathcal{H}$, find $\{f, g\} \in S^*$ such that $g - zf = h$ and $\mathcal{U}(z)b(f, g) = 0$. With $\mathcal{U}(z), z \in \mathbb{C} \setminus \mathbb{R}$, we associate the family of relations

$$T(z) = \{\{f, g\} \in S^*: \mathcal{U}(z)b(f, g) = 0\}, \quad z \in \mathbb{C} \setminus \mathbb{R}.$$

Evidently, $S \subset T(z) \subset S^*$ for all $z \in \mathbb{C} \setminus \mathbb{R}$. A linearization \tilde{A} of the boundary eigenvalue problem is a selfadjoint extension \tilde{A} of S such that

$$\tilde{P}_{\mathcal{H}}(\tilde{A} - z)^{-1}|_{\mathcal{H}} = (T(z) - z)^{-1}, \quad z \in \mathbb{C} \setminus \mathbb{R},$$

where $\tilde{P}_{\mathcal{H}}$ is the orthogonal projection in $\tilde{\mathcal{H}}$ onto \mathcal{H} . Because of this formula \tilde{A} is also called a linearization of $T(z)$. As we shall show, if $\mathcal{U}(z)$ satisfies (U1)–(U5) in Definition 3.1, then $T(z)$ admits a linearization and the converse also holds. In [11,14] $T(z)$ is called a Straus extension of S .

Definition 3.1 (*Boundary coefficient*). Let Q be an invertible selfadjoint $d \times d$ matrix with d_+ positive and d_- negative eigenvalues. A Q -boundary coefficient function \mathcal{U} is a matrix valued function defined on $\mathbb{C} \setminus \mathbb{R}$ with the following properties:

(U1) $\mathcal{U}(z)$ is a $d_+ \times d$ matrix if $z \in \mathbb{C}^+$ and $\mathcal{U}(z)$ is a $d_- \times d$ matrix if $z \in \mathbb{C}^-$.

(U2) $\mathcal{U}(z)$ is holomorphic on $\mathbb{C} \setminus \mathbb{R}$.

(U3) Each matrix $\mathcal{U}(z), z \in \mathbb{C} \setminus \mathbb{R}$, has maximal rank.

(U4) $\mathcal{U}(z)Q^{-1}\mathcal{U}(\bar{z})^* = 0, z \in \mathbb{C} \setminus \mathbb{R}$.

(U5) The kernel

$$K_{\mathcal{U}}(z, w) = i \frac{\mathcal{U}(z)Q^{-1}\mathcal{U}(w)^*}{z - \bar{w}}, \quad z \neq \bar{w}, \quad z, w \in \mathbb{C} \setminus \mathbb{R},$$

is nonnegative.

The kernel condition (U5) means that for any choice of the natural number n and $\lambda_1, \dots, \lambda_n \in \mathbb{C} \setminus \mathbb{R}$, the selfadjoint block matrix $(K_{\mathcal{U}}(\lambda_j, \lambda_k))_{j,k=1}^n$ is nonnegative. In particular,

$$\mathcal{U}(z)Q^{-1}\mathcal{U}(z)^* \geq 0 \quad \text{if } z \in \mathbb{C}^+ \quad \text{and} \quad \mathcal{U}(z)Q^{-1}\mathcal{U}(z)^* \leq 0 \quad \text{if } z \in \mathbb{C}^-. \quad (3.1)$$

The kernel condition is used to describe the exit space of the linearization of the family of extensions determined by $\mathcal{U}(z)$. In this section, we only make use of the special cases (3.1).

A Q -boundary coefficient $\mathcal{U}(z)$ is said to be *minimal* if

($\mathcal{U}3'$) the $d \times d$ matrix $\begin{pmatrix} \mathcal{U}(z) \\ \mathcal{U}(\bar{z}) \end{pmatrix}$ is invertible, $z \in \mathbb{C} \setminus \mathbb{R}$.

Note that ($\mathcal{U}3'$) implies ($\mathcal{U}3$).

A boundary coefficient $\mathcal{U}(z)$ is said to be *row reduced* to a boundary coefficient $\mathcal{V}(z)$ if

$$\mathcal{A}(z)\mathcal{U}(z) = \mathcal{V}(z)$$

for some invertible matrix function $\mathcal{A}(z)$ on $\mathbb{C} \setminus \mathbb{R}$ which is of size $d_{\pm} \times d_{\pm}$ for $z \in \mathbb{C}^{\pm}$. In the boundary eigenvalue problem in which the boundary coefficient $\mathcal{U}(z)$ appears, the variable z is the eigenvalue parameter. The following theorem says that any boundary coefficient can be row reduced to a boundary coefficient whose top rows are independent of the eigenvalue parameter and the remaining rows are essentially determined by a minimal boundary coefficient. The theorem shows that in this case $\mathcal{A}(z)$ can even be chosen holomorphic on $\mathbb{C} \setminus \mathbb{R}$.

Theorem 3.2. *Let Q be a selfadjoint invertible $d \times d$ matrix with d_+ positive and d_- negative eigenvalues. Let $\mathcal{U}(z)$ be a Q -boundary coefficient function. There exist a unique integer τ , $0 \leq \tau \leq \min\{d_+, d_-\}$, and a holomorphic function $\mathcal{A}(z)$ on $\mathbb{C} \setminus \mathbb{R}$ whose values are invertible matrices of size $d_{\pm} \times d_{\pm}$ for $z \in \mathbb{C}^{\pm}$ such that*

$$\mathcal{A}(z)\mathcal{U}(z) = \begin{pmatrix} I & 0 \\ 0 & \mathcal{U}_0(z) \end{pmatrix} \begin{pmatrix} U_0 \\ B_0 \end{pmatrix}, \tag{3.2}$$

where I is the $\tau \times \tau$ identity matrix, and with $\omega_{\pm} := d_{\pm} - \tau$, $\omega := d - 2\tau = \omega_+ + \omega_-$ the matrices U_0 , $\mathcal{U}_0(z)$, and B_0 have the following properties:

- (I) U_0 is a constant $\tau \times d$ matrix of maximal rank;
- (II) B_0 is a constant $\omega \times d$ matrix such that $B_0 Q^{-1} B_0^*$ is invertible and has ω_+ positive and ω_- negative eigenvalues;
- (III) the equality

$$\begin{pmatrix} U_0 \\ B_0 \end{pmatrix} Q^{-1} \begin{pmatrix} U_0 \\ B_0 \end{pmatrix}^* = \begin{pmatrix} 0 & 0 \\ 0 & Q_0^{-1} \end{pmatrix} \tag{3.3}$$

holds with $Q_0 := (B_0 Q^{-1} B_0^*)^{-1}$;

- (IV) $\mathcal{U}_0(z)$ is a minimal Q_0 -boundary coefficient of size $\omega_{\pm} \times \omega$.

The right-hand side of (3.2) is called a *minimal representation* of $\mathcal{U}(z)$.

In the proof of the theorem we use the following well-known lemma whose short proof we include for completeness.

Lemma 3.3. *Let \mathcal{H}_1 and \mathcal{H}_2 be Hilbert spaces and let $K : \Omega \rightarrow \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$ be a holomorphic (anti-holomorphic) contraction valued function defined on an open connected set $\Omega \subset \mathbb{C}$. There exist decompositions $\mathcal{H}_j = \mathcal{H}_j^0 \oplus \mathcal{H}_j^1$, $j = 1, 2$, such that $K(z)$ has the matrix representation*

$$K(z) = \begin{pmatrix} K_0(z) & 0 \\ 0 & V \end{pmatrix} \begin{pmatrix} \mathcal{H}_1^0 \\ \mathcal{H}_1^1 \end{pmatrix} \rightarrow \begin{pmatrix} \mathcal{H}_2^0 \\ \mathcal{H}_2^1 \end{pmatrix}, \tag{3.4}$$

in which $K_0 : \Omega \rightarrow \mathcal{L}(\mathcal{H}_1^0, \mathcal{H}_2^0)$ is a holomorphic (anti-holomorphic) strict contraction valued function, $V : \mathcal{H}_1^1 \rightarrow \mathcal{H}_2^1$ is unitary and the subspaces

$$\mathcal{H}_1^1 = \ker(I - K(z)^* K(z)), \quad \mathcal{H}_2^1 = \ker(I - K(z) K(z)^*)$$

are independent of z .

Proof. Choose a point $z_0 \in \Omega$ and set $\mathcal{H}_1^1 = \ker(I - K(z_0)^* K(z_0))$. For $x \in \mathcal{H}_1^1$, the function $f(z) = \langle K(z_0)^* K(z)x, x \rangle$ is a holomorphic function in $z \in \Omega$ and

$$|f(z)| \leq \|x\|^2 = \|K(z_0)x\|^2 = f(z_0).$$

By the maximum modulus principle $f(z) = f(z_0) \in \mathbb{R}$ for all $z \in \Omega$, and hence

$$\begin{aligned} 0 &\leq \|K(z)x - K(z_0)x\|^2 \\ &= \|K(z)x\|^2 - \|K(z_0)x\|^2 \\ &= \|K(z)x\|^2 - \|x\|^2 \\ &\leq 0, \end{aligned}$$

which implies that $K(z)|_{\mathcal{H}_1^1} = K(z_0)|_{\mathcal{H}_1^1}$ and $\mathcal{H}_1^1 = \ker(I - K(z)^* K(z))$ for all $z \in \Omega$. Hence, $V := K(z)|_{\mathcal{H}_1^1}$ is a unitary mapping from \mathcal{H}_1^1 onto $\mathcal{H}_2^1 := V \mathcal{H}_1^1$. The equalities

$$\begin{aligned} \langle K(z)\mathcal{H}_1^0, V \mathcal{H}_1^1 \rangle_2 &= \langle K(z)\mathcal{H}_1^0, K(z)\mathcal{H}_1^1 \rangle_2 \\ &= \langle \mathcal{H}_1^0, K(z)^* K(z)\mathcal{H}_1^1 \rangle_1 \\ &= \langle \mathcal{H}_1^0, \mathcal{H}_1^1 \rangle_1 \\ &= 0 \end{aligned}$$

imply that $K_0(z) := K(z)|_{\mathcal{H}_1^0}$ maps \mathcal{H}_1^0 into $\mathcal{H}_2^0 := \mathcal{H}_2 \ominus \mathcal{H}_2^1$. This proves the matrix representation (3.4) for $K(z)$. Moreover, $\ker(I - K_0(z)^* K_0(z)) = \mathcal{H}_1^1 \cap \mathcal{H}_1^0 = \{0\}$, and therefore $K_0(z)$ is a strict contraction. The last equality in Lemma 3.3 follows from considering the operator

$$K(z)^* = \begin{pmatrix} K_0(z)^* & 0 \\ 0 & V^{-1} \end{pmatrix} \begin{pmatrix} \mathcal{H}_2^0 \\ \mathcal{H}_2^1 \end{pmatrix} \rightarrow \begin{pmatrix} \mathcal{H}_1^0 \\ \mathcal{H}_1^1 \end{pmatrix}$$

in a similar way. In case K is anti-holomorphic, the statement follows by considering $\widehat{K} : \Omega \rightarrow \mathcal{L}(\mathcal{H}_2, \mathcal{H}_1)$ defined by $\widehat{K}(z) = K(z)^*$. \square

Proof of Theorem 3.2. In this proof, we consider \mathbb{C}^d equipped with the indefinite inner product

$$[x, y] = y^*Q^{-1}x, \quad x, y \in \mathbb{C}^d.$$

The space $(\mathbb{C}^d, [\cdot, \cdot])$ is a Krein space. Let $\mathbb{C}^d = \mathcal{Q}_+[\dot{+}]\mathcal{Q}_-$ be a fundamental decomposition of \mathbb{C}^d . For example, \mathcal{Q}_+ can be the subspace of \mathbb{C}^d generated by the eigenvectors of Q corresponding to its positive eigenvalues and \mathcal{Q}_- the subspace of \mathbb{C}^d generated by the eigenvectors of Q corresponding to its negative eigenvalues. Whatever the choice of the fundamental decomposition we have that $\dim(\mathcal{Q}_\pm) = d_\pm$. Denote by P_+ and P_- the orthogonal projections onto \mathcal{Q}_+ and \mathcal{Q}_- . We consider the subspaces

$$\mathcal{R}(z) := \text{ran}(\mathcal{U}(z)^*), \quad z \in \mathbb{C} \setminus \mathbb{R}.$$

For definiteness we assume that $\text{Im}(z) > 0$. The constructions for $\text{Im}(z) < 0$ are similar. For $x = \mathcal{U}(z)^*u, y = \mathcal{U}(z)^*v, u, v \in \mathbb{C}^{d_+}$, we have

$$[x, y] = (\mathcal{U}(z)^*v)^*Q^{-1}\mathcal{U}(z)^*u = v^*\mathcal{U}(z)Q^{-1}\mathcal{U}(z)^*u.$$

Since $\text{Im}(z) > 0$, Assumption (3.1) implies that $\mathcal{R}(z)$ is a nonnegative subspace of $(\mathbb{C}^d, [\cdot, \cdot])$. From $\dim(\mathcal{R}(z)) = d_+$, it follows that $\mathcal{R}(z)$ is a maximal nonnegative subspace of \mathbb{C}^d . Therefore, the operator $P_+\mathcal{U}(z)^*$ is surjective, and hence invertible. If $K(z)$ is the operator from the Hilbert space $(\mathcal{Q}_+, [\cdot, \cdot])$ to the Hilbert space $(\mathcal{Q}_-, -[\cdot, \cdot])$ defined by

$$K(z) = P_-\mathcal{U}(z)^*(P_+\mathcal{U}(z)^*)^{-1},$$

then $K(z)$ is a contraction and

$$\mathcal{R}(z) = \{(I_{\mathcal{Q}_+} + K(z))x_+ : x_+ \in \mathcal{Q}_+\}. \tag{3.5}$$

The operator $K(z)$ is called the *angular operator* of $\mathcal{R}(z)$; see [2]. Since $\mathcal{U}(z)$ is holomorphic, $K(z)$ is anti-holomorphic. In particular, we have that for $a \in \mathbb{C}^{d_+}$ there exists an $x_+ \in \mathcal{Q}_+$ such that

$$\mathcal{U}(z)^*a = (I_{\mathcal{Q}_+} + K(z))x_+.$$

Solving for $x_+ \in \mathcal{Q}_+$ we get $x_+ = P_+\mathcal{U}(z)^*a$. Therefore,

$$\mathcal{U}(z)^*a = (I_{\mathcal{Q}_+} + K(z))(P_+\mathcal{U}(z)^*)a \quad \text{for all } a \in \mathbb{C}^{d_+}. \tag{3.6}$$

It follows from Lemma 3.3 with $(\mathcal{H}_1, \langle \cdot, \cdot \rangle_1) = (\mathcal{Q}_+, [\cdot, \cdot])$ and $(\mathcal{H}_2, \langle \cdot, \cdot \rangle_2) = (\mathcal{Q}_-, -[\cdot, \cdot])$, that there exist decompositions $\mathcal{Q}_\pm = \mathcal{Q}_\pm^0[\dot{+}]\mathcal{Q}_\pm^1$ such that

$$K(z) = \begin{pmatrix} K_0(z) & 0 \\ 0 & V \end{pmatrix} \begin{pmatrix} \mathcal{Q}_+^0 \\ \mathcal{Q}_+^1 \end{pmatrix} \rightarrow \begin{pmatrix} \mathcal{Q}_-^0 \\ \mathcal{Q}_-^1 \end{pmatrix},$$

where $K_0(z) : \mathcal{Q}_+^0 \rightarrow \mathcal{Q}_-^0$ is a strict contraction, $K_0(z)$ is anti-holomorphic and $V : \mathcal{Q}_+^1 \rightarrow \mathcal{Q}_-^1$ is a unitary operator. Let $\tau = \dim(\mathcal{Q}_+^1) = \dim(\mathcal{Q}_-^1)$, $\omega_\pm = d_\pm - \tau$, and

$\omega = \omega_+ + \omega_- = d - 2\tau$. Since the spaces are finite-dimensional $K_0(z)$ is a uniform contraction, that is, $\|K_0(z)\| < 1$. The subspace $\mathcal{Q}_+^0[+] \mathcal{Q}_-^0$ is a Krein subspace of $(\mathbb{C}^d, [\cdot, \cdot])$ of dimension ω . The decomposition $\mathcal{Q}_+^0[+] \mathcal{Q}_-^0$ is a fundamental decomposition of this Krein space. We have $\omega_+ = \dim(\mathcal{Q}_+^0)$ and $\omega_- = \dim(\mathcal{Q}_-^0)$.

Now equality (3.5) becomes

$$\mathcal{R}(z) = \{x_0 + x_1 + K_0(z)x_0 + Vx_1: x_0 \in \mathcal{Q}_+^0, x_1 \in \mathcal{Q}_+^1\} = \mathcal{R}_0[+] \mathcal{R}_+(z),$$

where by (3.6),

$$\mathcal{R}_0 := \{x_1 + Vx_1: x_1 \in \mathcal{Q}_+^1\} = \mathcal{U}(z)^*(P_+ \mathcal{U}(z)^*)^{-1} \mathcal{Q}_+^1$$

is a neutral subspace and

$$\mathcal{R}_+(z) := \{x_0 + K_0(z)x_0: x_0 \in \mathcal{Q}_+^0\} = \mathcal{U}(z)^*(P_+ \mathcal{U}(z)^*)^{-1} \mathcal{Q}_+^0$$

is a maximal uniformly positive subspace of $(\mathcal{Q}_+^0[+] \mathcal{Q}_-^0, [\cdot, \cdot])$.

It follows from (U4) that the subspaces $\text{ran}(\mathcal{U}(z)^*)$ and $\text{ran}(\mathcal{U}(\bar{z})^*)$ are orthogonal with respect to $[\cdot, \cdot]$. The subspace $\mathcal{R}(\bar{z}) = \text{ran}(\mathcal{U}(\bar{z})^*)$ is a maximal nonpositive subspace of $(\mathbb{C}^d, [\cdot, \cdot])$. The angular operator for $\mathcal{R}(\bar{z})$ is given by

$$K(\bar{z}) = K(z)^* : (\mathcal{Q}_-, -[\cdot, \cdot]) \rightarrow (\mathcal{Q}_+, [\cdot, \cdot]),$$

that is, $\mathcal{R}(\bar{z}) = \{x_- + K(z)^*x_-: x_- \in \mathcal{Q}_-\}$. It follows that

$$\mathcal{R}(\bar{z}) = \mathcal{R}_0[+] \mathcal{R}_-(\bar{z}),$$

where $\mathcal{R}_-(z)$ is a maximal uniformly negative subspace of $(\mathcal{Q}_+^0[+] \mathcal{Q}_-^0, [\cdot, \cdot])$. Thus,

$$\mathcal{Q}_+^0[+] \mathcal{Q}_-^0 = \mathcal{R}_+(z)[+] \mathcal{R}_-(\bar{z}) \tag{3.7}$$

and the right-hand side of (3.7) is a fundamental decomposition of $(\mathcal{Q}_+^0[+] \mathcal{Q}_-^0, [\cdot, \cdot])$. Moreover,

$$\mathcal{R}_0[\perp] \mathcal{Q}_+^0[+] \mathcal{Q}_-^0.$$

Select a basis of the ω -dimensional space $\mathcal{Q}_+^0[+] \mathcal{Q}_-^0$. (Note that $\mathcal{Q}_+^0[+] \mathcal{Q}_-^0 \subset \mathbb{C}^d$.) Let the columns of the $d \times \omega$ matrix B_0^* be the vectors of this basis. The Gram matrix $B_0 Q^{-1} B_0^*$ of the columns of B_0^* with respect to the indefinite inner product $[\cdot, \cdot]$ is invertible and has ω_+ positive and ω_- negative eigenvalues. Hence, B_0 has property (II). The Gram matrix $B_0 B_0^*$ of the columns of B_0^* with respect to the Euclidean inner product is invertible and the matrix $B_0^*(B_0 B_0^*)^{-1} B_0$ is the orthogonal projection with respect to the Euclidean inner product of \mathbb{C}^d onto $\mathcal{Q}_+^0[+] \mathcal{Q}_-^0$.

Let a_1, \dots, a_τ be a basis of the subspace \mathcal{Q}_+^1 . Then $(I_{\mathcal{Q}_+^1} + V)a_j, j = 1, 2, \dots, \tau$, is a basis of \mathcal{R}_0 . Let the columns of the $d \times \tau$ matrix U_0^* be the $d \times 1$ vectors $(I_{\mathcal{Q}_+^1} + V)a_j, j = 1, 2, \dots, \tau$. Then U_0 has property (I).

Property (III) now follows from the fact that \mathcal{R}_0 is a neutral subspace of $(\mathbb{C}^d, [\cdot, \cdot])$ and orthogonal to $\mathcal{Q}_+^0[+] \mathcal{Q}_-^0$ in $[\cdot, \cdot]$.

We now construct $\mathcal{U}_0(z)$. Let b_1, \dots, b_{ω_+} be a basis of the space \mathcal{Q}_+^0 . Then $(I_{\mathcal{Q}_+^0} + K_0(z))b_j, j = 1, 2, \dots, \omega_+$, is a basis of $\mathcal{R}_+(z)$. Let the columns of the $d \times \omega_+$

matrix $\mathcal{W}_1(z)^*$ be the $d \times 1$ vectors $(I_{\mathcal{Q}_+^0} + K_0(z))b_j$, $j = 1, 2, \dots, \omega_+$. Since the function $K_0(z)$ is anti-holomorphic, the function $\mathcal{W}_1(z)^*$ is anti-holomorphic. Put

$$\mathcal{U}_0(z)^* = (B_0 B_0^*)^{-1} B_0 \mathcal{W}_1(z)^*.$$

Clearly, $\mathcal{U}_0(z)^*$ is an $\omega \times \omega_+$ matrix and the function $\mathcal{U}_0(z)^*$ is anti-holomorphic. Since the columns of the matrix $\mathcal{W}_1(z)^*$ belong to $\mathcal{Q}_+^0[+] \mathcal{Q}_-^0$ we have

$$B_0^* \mathcal{U}_0(z)^* = B_0^* (B_0 B_0^*)^{-1} B_0 \mathcal{W}_1(z)^* = \mathcal{W}_1(z)^*.$$

Thus, the columns of the matrix $(U_0^* \ B_0^* \mathcal{U}_0(z)^*)$ form an anti-holomorphic basis for $\mathcal{R}(z) = \text{ran}(\mathcal{U}(z)^*)$. Another anti-holomorphic basis of this space is formed by the columns of $\mathcal{U}(z)^*$. Denote by $\mathcal{A}(z)^*$ the ‘change of coordinates matrix’ between these two basis of $\mathcal{R}(z)$, that is, the matrix with the property

$$\mathcal{U}(z)^* \mathcal{A}(z)^* = (U_0^* \ B_0^* \mathcal{U}_0(z)^*).$$

By (3.6), we have $\mathcal{A}(z)^* = (P_+ \mathcal{U}(z)^*)^{-1}$. Clearly, $\mathcal{A}(z)$ is a $d_+ \times d_+$ invertible matrix and the function $\mathcal{A}(z)$ is holomorphic on \mathbb{C}^+ . An analogous construction leads to the $d \times \omega_-$ matrix $\mathcal{W}(\bar{z})^*$ and to the $\omega \times \omega_-$ matrix $\mathcal{U}_0(\bar{z})^* := B_0 \mathcal{W}(\bar{z})^*$ and finally to the $d_- \times d_-$ matrix $\mathcal{A}(\bar{z})^*$ such that

$$\mathcal{U}(\bar{z})^* \mathcal{A}(\bar{z})^* = (U_0^* \ B_0^* \mathcal{U}_0(\bar{z})^*).$$

Thus, $\mathcal{U}(z)$ has the minimal representation (3.2).

It remains to show property (IV). Properties (U1) and (U2) follow from the construction of $\mathcal{U}_0(z)$. The $d \times \omega$ matrix $(B_0^* \mathcal{U}_0(z)^* \ B_0^* \mathcal{U}_0(\bar{z})^*)$ consists of the basis vectors of $\mathcal{R}_+(z)$ and of $\mathcal{R}_-(\bar{z})$. Since these two subspaces form a fundamental decomposition of $\mathcal{Q}_+^0[+] \mathcal{Q}_-^0$ the columns of $(B_0^* \mathcal{U}_0(z)^* \ B_0^* \mathcal{U}_0(\bar{z})^*)$ are linearly independent. Thus, the matrix $B_0^* (\mathcal{U}_0(z)^* \ \mathcal{U}_0(\bar{z})^*)$ has rank ω and therefore $\omega \times \omega$ matrix

$$\begin{pmatrix} \mathcal{U}_0(z) \\ \mathcal{U}_0(\bar{z}) \end{pmatrix} \text{ is invertible, } z \in \mathbb{C} \setminus \mathbb{R},$$

that is, (U3') holds.

From (3.2) and (3.3) we obtain the equalities

$$\begin{aligned} \begin{pmatrix} 0 & 0 \\ 0 & \mathcal{U}_0(z) Q_0^{-1} \mathcal{U}_0(w)^* \end{pmatrix} &= \begin{pmatrix} U_0 Q^{-1} U_0^* & U_0 Q^{-1} B_0^* \mathcal{U}_0(w)^* \\ \mathcal{U}_0(z) B_0 Q^{-1} U_0^* & \mathcal{U}_0(z) B_0 Q^{-1} B_0^* \mathcal{U}_0(w)^* \end{pmatrix} \\ &= \begin{pmatrix} U_0 \\ \mathcal{U}_0(z) B_0 \end{pmatrix} Q^{-1} \begin{pmatrix} U_0 \\ \mathcal{U}_0(w) B_0 \end{pmatrix}^* \\ &= \mathcal{A}(z) \mathcal{U}(z) Q^{-1} \mathcal{U}(w)^* \mathcal{A}(w)^*. \end{aligned} \tag{3.8}$$

Properties (U4) and (U5) of $\mathcal{U}_0(z)$ follow from (3.8) and from the corresponding properties (U4) and (U5) of $\mathcal{U}(z)$. Thus, $\mathcal{U}_0(z)$ is a minimal Q_0 -boundary coefficient. \square

Lemma 3.4. *Let S be a closed symmetric linear relation with defect (d_+, d_-) , $d = d_+ + d_- < \infty$, let τ be an integer with $0 < \tau < d$, and let b be a boundary mapping for S with Gram matrix Q . Equivalent are:*

(a) *For a closed linear relation T we have $S \subset T \subset S^*$, and $\dim(T/S) = \tau$.*

(b) *There exists a $(d - \tau) \times d$ matrix A of maximal rank such that*

$$T = \{ \{f, g\} \in S^* : Ab(f, g) = 0 \}.$$

(c) *There exists a $\tau \times d$ matrix B of maximal rank such that*

$$T^* = \{ \{f, g\} \in S^* : Bb(f, g) = 0 \}.$$

If (a)–(c) hold, then $BQ^{-1}A^ = 0$ and the matrices A and B are determined uniquely up to multiplication from the left by invertible matrices.*

(d) *If (a)–(c) hold and if C is a $\tau \times d$ matrix of maximal rank such that $CQ^{-1}A^* = 0$ and*

$$V = \{ \{f, g\} \in S^* : Cb(f, g) = 0 \},$$

then $T^ = V$.*

Proof. We use the same setting as in the proof of Theorem 3.2. We consider \mathbb{C}^d to be equipped with the indefinite inner product $[x, y] = y^*Q^{-1}x$, $x, y \in \mathbb{C}^d$. The space $(\mathbb{C}^d, [\cdot, \cdot])$ is a Krein space with signature (d_+, d_-) . The mapping $Qb : S^*/S \rightarrow \mathbb{C}^d$ is an isomorphism between the Krein spaces $(S^*/S, [[\cdot, \cdot]])$ and $(\mathbb{C}^d, [\cdot, \cdot])$. For a matrix $M \times M^*$ we denote the adjoint of M with respect to the Euclidean inner product. For a $d \times r$ matrix M^* whose columns are vectors in \mathbb{C}^d we have

$$\begin{aligned} x \in \ker(MQ^{-1}) &\Leftrightarrow y^*MQ^{-1}x = 0 \quad (\forall y \in \mathbb{C}^d) \\ &\Leftrightarrow x^*Q^{-1}M^*y = 0 \quad (\forall y \in \mathbb{C}^d) \\ &\Leftrightarrow x \in (\text{ran}(M^*))^{[\perp]}, \end{aligned}$$

where $[\perp]$ denotes the orthogonal complement in $(\mathbb{C}^d, [\cdot, \cdot])$. Thus,

$$\ker(MQ^{-1}) = (\text{ran}(M^*))^{[\perp]}. \tag{3.9}$$

If $T = \{ \{f, g\} \in S^* : Mb(f, g) = 0 \}$, and M has maximal rank, then $Qb(T) = \ker(MQ^{-1})$. Since $Qb(T^*)$ is the orthogonal complement of $\ker(MQ^{-1})$ in $(\mathbb{C}^d, [\cdot, \cdot])$ equality (3.9) implies $Qb(T^*) = \text{ran}(M^*)$. Thus,

$$Qb(T) = \ker(MQ^{-1}) \quad \text{if and only if } Qb(T^*) = \text{ran}(M^*). \tag{3.10}$$

If (a) holds, then $\dim(Qb(T)) = \tau$ and $\dim(Qb(T^*)) = \dim(Qb(T)^{[\perp]}) = d - \tau$. Set A^* to be a $d \times (d - \tau)$ matrix whose columns are basis vectors of $Qb(T^*)$. Then

(3.10) with $M = A$ implies that (b) holds. The implication (b) \Rightarrow (a) follows from the fact that $S = \ker(b)$. The equivalence (a) \Leftrightarrow (c) follows from the fact that (a) is equivalent to

$$S \subset T^* \subset S^* \quad \text{and} \quad \dim(T^*/S) = d - \tau,$$

which follows from (3.10).

Now assume that (a)–(c) hold. It follows from (3.10) that $Qb(T^*) = \text{ran}(A^*) = \ker(\text{BQ}^{-1})$. Consequently, $\text{BQ}^{-1}A^* = 0$. The uniqueness statement about A and B follows from (3.10).

Statement (d) follows from the fact that $\ker(B) = \text{ran}(\text{Q}^{-1}A^*) = \ker(C)$. \square

Lemma 3.5. *Let S be a closed symmetric linear relation with defect (d_+, d_-) , $d = d_+ + d_- < \infty$, and let b be a boundary mapping for S with Gram matrix Q . Assume that (a)–(c) in Lemma 3.4 hold. Then T is symmetric if and only if $\text{BQ}^{-1}B^* = 0$. In this case, $\tau \leq \min\{d_+, d_-\}$ and the defect index of T is (ω_+, ω_-) , $\omega_{\pm} = d_{\pm} - \tau$. The $(d - \tau) \times d$ matrix A can be chosen to be of the form*

$$A = \begin{pmatrix} B \\ B_0 \end{pmatrix},$$

where B_0 is an $\omega \times d$ matrix of maximal rank, $\omega = d - 2\tau$, such that $\text{BQ}^{-1}B_0^* = 0$ and $B_0\text{Q}^{-1}B_0^*$ is invertible. Then $b_0 = B_0b|_{T^*}$ is a boundary mapping for T with Gram matrix $Q_0 = (B_0\text{Q}^{-1}B_0^*)^{-1}$.

Proof. We use the notation and facts from the proof of Lemma 3.4. The relation T is symmetric if and only if $Qb(T) \subset Qb(T^*)$, and consequently, $Qb(T) = \text{ran}(B^*) \subset \ker(\text{BQ}^{-1}) = Qb(T^*)$. The last inclusion is equivalent to $\text{BQ}^{-1}B^* = 0$. Hence, T is symmetric if and only if $\text{BQ}^{-1}B^* = 0$.

Assume that T is symmetric. Then

$$\text{ran}(B^*) \subset Qb(T^*) = \text{ran}(A^*) \tag{3.11}$$

and the columns of the matrix A^* can be chosen to be any basis vectors for $Qb(T^*)$. In particular, we can choose A^* to be of the form $(B^* \ B_0^*)$, where the columns of $d \times \omega$ matrix B_0^* are chosen to complete the basis of $Qb(T^*)$. It follows from Lemma 3.4 that

$$0 = \text{BQ}^{-1}A^* = \text{BQ}^{-1} \begin{pmatrix} B \\ B_0 \end{pmatrix}^* = (\text{BQ}^{-1}B^* \ \text{BQ}^{-1}B_0^*).$$

In particular, $\text{BQ}^{-1}B_0^* = 0$ or, equivalently, $(\text{ran}B^*)[\perp](\text{ran}B_0^*)$. Thus, $Qb(T^*) = (\text{ran}B^*)[\dot{+}](\text{ran}B_0^*)$. Since $Qb(T^*)[\perp\perp] = \text{ran}(B^*)$, we conclude that the inner product $[\cdot, \cdot]$ is nondegenerate on $\text{ran}(B_0^*)$. This implies that $B_0\text{Q}^{-1}B_0^*$ is invertible and we put $Q_0 := (B_0\text{Q}^{-1}B_0^*)^{-1}$. Further, $(\text{ran}(B_0^*), [\cdot, \cdot])$ is a Krein space of dimension $\omega = d - 2\tau$ and therefore $(\text{ran}(B_0^*)[\perp\perp], [\cdot, \cdot])$ is a Krein space of dimension 2τ . Since it contains the neutral τ -dimensional subspace $\text{ran}(B^*)$, the signature of

$(\text{ran}(B_0^*)^{[\perp]}, [\cdot, \cdot])$ is (τ, τ) . The equality $\mathbb{C}^d = \text{ran}(B_0^*)^{[\perp]}[\cdot]$ $\text{ran}(B_0^*)$, implies that the signature of $(\text{ran}(B_0^*), [\cdot, \cdot])$ is (ω_+, ω_-) , $\omega_{\pm} = d_{\pm} - \tau$. This also implies that the signature of the matrix Q_0 is (ω_+, ω_-) .

Put $b_0 := B_0b|_{T^*}$. Since $Qb(T^*) \supset \text{ran}(B_0^*)$ and since the $\omega \times \omega$ matrix $B_0Q^{-1}B_0^*$ is invertible we conclude that $b_0 : T^* \rightarrow \mathbb{C}^{\omega}$ is surjective. Considering b_0 as a mapping from the $\omega + \tau$ -dimensional space T^*/S onto \mathbb{C}^{ω} we see that its kernel must be τ -dimensional. Since $Qb(T) = \text{ran}(B^*)$ and $B_0Q^{-1}B^* = 0$, we have $T/S \subset \ker(b_0)$. Now $\dim(T/S) = \tau$ implies that $T = \ker(b_0)$. Thus, b_0 is a boundary mapping for T . Since $Qb(T^*) = \text{ran}(A^*) = \text{ran}(\begin{pmatrix} B^* & B_0^* \end{pmatrix})$, for $\{f, g\}, \{u, v\} \in T^*$ there exist $x, y \in \mathbb{C}^{\tau+\omega}$ such that $Qb(f, g) = \begin{pmatrix} B^* & B_0^* \end{pmatrix}x$ and $Qb(u, v) = \begin{pmatrix} U_0^* & B_0^* \end{pmatrix}y$ and we have

$$\begin{aligned} \llbracket \{f, g\}, \{u, v\} \rrbracket &= (b(u, v))^*Qb(f, g) \\ &= y^* \begin{pmatrix} B \\ B_0 \end{pmatrix} Q^{-1}QQ^{-1} \begin{pmatrix} B \\ B_0 \end{pmatrix}^* x \\ &= y^* \begin{pmatrix} 0 & 0 \\ 0 & Q_0^{-1} \end{pmatrix} x. \end{aligned} \tag{3.12}$$

We also calculate

$$\begin{aligned} (B_0b(u, v))^*Q_0(B_0b(f, g)) &= y^* \begin{pmatrix} B \\ B_0 \end{pmatrix} Q^{-1}B_0^*Q_0B_0Q^{-1} \begin{pmatrix} B \\ B_0 \end{pmatrix}^* x \\ &= y^* \begin{pmatrix} BQ^{-1}B_0^* \\ Q_0^{-1} \end{pmatrix} Q_0 \begin{pmatrix} BQ^{-1}B_0^* \\ Q_0^{-1} \end{pmatrix}^* x \\ &= y^* \begin{pmatrix} 0 \\ Q_0^{-1} \end{pmatrix} Q_0 \begin{pmatrix} 0 \\ Q_0^{-1} \end{pmatrix}^* x \\ &= y^* \begin{pmatrix} 0 \\ 1 \end{pmatrix} (0 \quad Q_0^{-1})x \\ &= y^* \begin{pmatrix} 0 & 0 \\ 0 & Q_0^{-1} \end{pmatrix} x. \end{aligned} \tag{3.13}$$

Combining (3.12) and (3.13) we get

$$\llbracket \{f, g\}, \{u, v\} \rrbracket = (B_0b(u, v))^*Q_0(B_0b(f, g)) \quad \text{for all } \{f, g\}, \{u, v\} \in T^*,$$

and therefore the Gram matrix of the boundary mapping $b_0 = B_0b|_{T^*}$ is Q_0 . Since the signature of the matrix Q_0 is (ω_+, ω_-) , the defect index of T is (ω_+, ω_-) . \square

Corollary 3.6. *Let S be a closed symmetric linear relation with defect (d_+, d_-) , $d = d_+ + d_- < \infty$, and let b be a boundary mapping for S with Gram matrix Q . Let $\mathcal{U}(z)$ be a Q -boundary coefficient and assume $\mathcal{U}(z)$ has the minimal representation (3.2). Then:*

- (a) The relation $S_0 := \{ \{f, g\} \in S^* : U_0 b(f, g) = 0, B_0 b(f, g) = 0 \}$ is a closed linear symmetric extension of S with defect index (ω_+, ω_-) and $\dim(S_0/S) = \tau$.
- (b) The mapping $b_0 := B_0 b|_{S_0^*}$ is a boundary mapping for S_0 with Gram matrix $Q_0 = (B_0 Q^{-1} B_0^*)^{-1}$.
- (c) For all $z \in \mathbb{C} \setminus \mathbb{R}$, we have $\{ \{f, g\} \in S^* : \mathcal{U}(z) b(f, g) = 0 \} = \{ \{f, g\} \in S_0^* : \mathcal{U}_0(z) b_0(f, g) = 0 \}$.

4. Representation of minimal boundary coefficient and reproducing kernel Hilbert spaces

We begin with a lemma about the existence of a holomorphic basis of eigenfunctions of the adjoint of a symmetric relation.

Lemma 4.1. *Let S be a closed symmetric linear relation in a Hilbert space \mathcal{H} with defect index (d_+, d_-) . There exists a holomorphic row vector function $\Phi : \mathbb{C}^\pm \rightarrow \mathcal{H}^{d^\pm}$ such that the components of $\Phi(z)$ constitute a basis for $\ker(S^* - z)$, $z \in \mathbb{C} \setminus \mathbb{R}$.*

Proof. Let \tilde{A} be any selfadjoint extension of S in $\tilde{\mathcal{H}}$. Let $\tilde{P}_{\mathcal{H}}$ denote the orthogonal projection in $\tilde{\mathcal{H}}$ onto \mathcal{H} . For $\mu \in \mathbb{C}^+$ let

$$\begin{aligned} \Phi(\mu) &= (\phi_1(\mu), \dots, \phi_{d_+}(\mu)), \\ \Phi(\bar{\mu}) &= (\phi_1(\bar{\mu}), \dots, \phi_{d_-}(\bar{\mu})) \end{aligned}$$

be row vectors whose entries form a basis for $\ker(S^* - \mu)$ and $\ker(S^* - \bar{\mu})$. Define for $z \in \mathbb{C}^+$,

$$\begin{aligned} \tilde{\Phi}(z) &= (I + (z - \mu)\tilde{P}_{\mathcal{H}}(\tilde{A} - z)^{-1})\Phi(\mu) \\ &= ((I + (z - \mu)\tilde{P}_{\mathcal{H}}(\tilde{A} - z)^{-1})\phi_1(\mu), \\ &\quad \dots, (I + (z - \mu)\tilde{P}_{\mathcal{H}}(\tilde{A} - z)^{-1})\phi_{d_+}(\mu)) \end{aligned}$$

and for $z \in \mathbb{C}^-$,

$$\tilde{\Phi}(z) = (I + (z - \bar{\mu})\tilde{P}_{\mathcal{H}}(\tilde{A} - z)^{-1})\Phi(\bar{\mu}).$$

We show that $\tilde{\Phi}(z)$ has the desired properties. We restrict the proof to $z \in \mathbb{C}^+$; the case $z \in \mathbb{C}^-$ can be treated similarly. For arbitrary $\{u, v\} \in S$ we have that

$$\begin{aligned} &\langle (I + (z - \mu)\tilde{P}_{\mathcal{H}}(\tilde{A} - z)^{-1})\phi_j(\mu), v - \bar{z}u \rangle \\ &= \langle \phi_j(\mu), v - \bar{z}u \rangle + (z - \mu)\langle \phi_j(\mu), (\tilde{A} - \bar{z})^{-1}(v - \bar{z}u) \rangle \\ &= \langle \phi_j(\mu), v - \bar{z}u \rangle + (z - \mu)\langle \phi_j(\mu), u \rangle \end{aligned}$$

$$\begin{aligned}
 &= \langle \phi_j(\mu), v - \bar{\mu}u \rangle \\
 &= 0
 \end{aligned}$$

as $v - \bar{\mu}u \in \text{ran}(S - \bar{\mu}) = (\ker(S^* - \mu))^\perp$. It follows that the components of the vector

$$(I + (z - \mu)\tilde{P}_{\mathcal{H}}(\tilde{A} - z)^{-1})\Phi(\mu)$$

are orthogonal to $\text{ran}(S - \bar{z}) = (\ker(S^* - z))^\perp$. This proves that the components of $\Phi(z)$ belong to $\ker(S^* - z)$. To show that they are linearly independent it suffices to show that if $\phi \in \ker(S^* - \mu)$ and

$$(I + (z - \mu)\tilde{P}_{\mathcal{H}}(\tilde{A} - z)^{-1})\phi = 0, \tag{4.1}$$

then $\phi = 0$. If (4.1) holds, then there is a $\tilde{h} \in \tilde{\mathcal{H}} \ominus \mathcal{H}$ such that $(z - \mu)(\tilde{A} - z)^{-1}\phi = \tilde{h} - \phi$ or, equivalently, $\{(z - \mu)\phi, \tilde{h} - \phi\} \in (\tilde{A} - z)^{-1}$ or $\{\tilde{h} - \phi, z\tilde{h} - \mu\phi\} \in \tilde{A}$. From $\tilde{A} = A^*$ we get

$$\begin{aligned}
 0 &= \llbracket \{\tilde{h} - \phi, z\tilde{h} - \mu\phi\}, \{\tilde{h} - \phi, z\tilde{h} - \mu\phi\} \rrbracket \\
 &= 2 \text{Im}(z)\|\tilde{h}\|^2 + 2 \text{Im}(\mu)\|\phi\|^2.
 \end{aligned}$$

As $\text{Im}(z), \text{Im}(\mu) > 0$ we see $\phi = 0$. \square

If, as in Lemma 4.1, the components of $\Phi(z)$ form a basis, we shall simply say that $\Phi(z)$ is a basis; if additionally the components are holomorphic we call $\Phi(z)$ a holomorphic basis. In the sequel, we also use the following notation. If $z \in \mathbb{C}^\pm$ and $\Phi(z) = (\phi_1(z), \dots, \phi_{d_\pm}(z))$ is a basis for $\ker(S^* - z)$, then $\widehat{\Phi}(z)$ stands for the basis for $S^* \cap zI$ given by

$$\widehat{\Phi}(z) = (\{\phi_1(z), z\phi_1(z)\}, \dots, \{\phi_{d_\pm}(z), z\phi_{d_\pm}(z)\})$$

and, if b is a boundary mapping for S , $b(\widehat{\Phi}(z))$ is the $d \times d_\pm$ matrix

$$b(\widehat{\Phi}(z)) = (b(\phi_1(z), z\phi_1(z)), \dots, b(\phi_{d_\pm}(z), z\phi_{d_\pm}(z))).$$

If $(\mathcal{H}, \langle \cdot, \cdot \rangle)$ is an inner product space and if $v = (v_1, \dots, v_m)$ and $w = (w_1, \dots, w_n)$ are vectors with entries in \mathcal{H} , then $\langle v, w \rangle$ stands for the $n \times m$ matrix

$$\langle v, w \rangle = \begin{pmatrix} \langle v_1, w_1 \rangle & \langle v_2, w_1 \rangle & \cdots & \langle v_m, w_1 \rangle \\ \langle v_1, w_2 \rangle & \langle v_2, w_2 \rangle & \cdots & \langle v_m, w_2 \rangle \\ \vdots & \vdots & \vdots & \vdots \\ \langle v_1, w_n \rangle & \langle v_2, w_n \rangle & \cdots & \langle v_m, w_n \rangle \end{pmatrix}.$$

In the following proposition, we construct minimal boundary coefficients from a boundary mapping for a symmetric relation S and a holomorphic basis of $\ker(S^* - z)$.

Proposition 4.2. *Let S be a closed symmetric linear relation in a Hilbert space \mathcal{H} with defect index (d_+, d_-) , $d = d_+ + d_- < \infty$.*

- (a) *Let $\Phi(z)$ be a holomorphic basis for $\ker(S^* - z)$, $z \in \mathbb{C} \setminus \mathbb{R}$, and let b be a boundary mapping for S with Gram matrix Q . Then the matrix valued function $\mathcal{U}(z) := (Qb(\widehat{\Phi}(\bar{z})))^*$, $z \in \mathbb{C} \setminus \mathbb{R}$, is a minimal $(-Q)$ -boundary coefficient.*
- (b) *Let $\Phi_1(z)$ be another holomorphic basis for $\ker(S^* - z)$, $z \in \mathbb{C} \setminus \mathbb{R}$, and let b_1 be another boundary mapping for S with Gram matrix Q_1 and $\mathcal{U}_1(z) := (Q_1 b_1(\widehat{\Phi}_1(\bar{z})))^*$, $z \in \mathbb{C} \setminus \mathbb{R}$. Then*

$$\mathcal{U}(z) = \mathcal{A}(z)\mathcal{U}_1(z)A$$

for some invertible matrix function $\mathcal{A}(z)$ of size $d_{\mp} \times d_{\mp}$ if $z \in \mathbb{C}^{\pm}$ and a constant invertible $d \times d$ matrix A such that $AQ^{-1}A^ = Q_1^{-1}$.*

Proof. (a) For $z \in \mathbb{C}^{\pm}$ the row vector $\widehat{\Phi}(\bar{z})$ has d_{\mp} components which are vectors from $S^* \cap \bar{z}I$. The mapping Qb maps each component from $\widehat{\Phi}(\bar{z})$ to a $d \times 1$ vector in \mathbb{C}^d . Thus, $Qb(\widehat{\Phi}(\bar{z}))$ is a $d \times d_{\mp}$ matrix and $\mathcal{U}(z)$ is a $d_{\mp} \times d$ matrix. This proves (U1). Since $\widehat{\Phi}(z)$ is holomorphic, $\widehat{\Phi}(\bar{z})$ is anti-holomorphic, and consequently $Qb(\widehat{\Phi}(\bar{z}))$ is also anti-holomorphic. Therefore, $\mathcal{U}(z)$ is holomorphic and (U2) is proved. Since the vectors in $\widehat{\Phi}(z)$ and $\widehat{\Phi}(\bar{z})$ are linearly independent and since Qb is a bijection on $(S^* \cap zI) \dot{+} (S^* \cap \bar{z}I)$ it follows that the matrix $(Qb(\widehat{\Phi}(\bar{z})) \quad Qb(\widehat{\Phi}(z))) = (\mathcal{U}(z)^* \quad \mathcal{U}(\bar{z})^*)$ is invertible. Thus, the property (U3') holds. We calculate $\mathcal{U}(z)(-Q^{-1})\mathcal{U}(w)^*$:

$$\begin{aligned} \mathcal{U}(z)(-Q^{-1})\mathcal{U}(w)^* &= b(\widehat{\Phi}(\bar{z}))^*Q(-Q^{-1})Qb(\widehat{\Phi}(\bar{w})) \\ &= b(\widehat{\Phi}(\bar{z}))^*(-Q)b(\widehat{\Phi}(\bar{w})) \\ &= -[[\widehat{\Phi}(\bar{w}), \widehat{\Phi}(\bar{z})]] \\ &= \frac{1}{i}(z - \bar{w})\langle \Phi(\bar{w}), \Phi(\bar{z}) \rangle. \end{aligned}$$

Thus, \mathcal{U} has the property (U4) and

$$K_{\mathcal{U}}(z, w) = \langle \Phi(\bar{w}), \Phi(\bar{z}) \rangle, \quad z \neq \bar{w}, \quad z, w \in \mathbb{C} \setminus \mathbb{R}. \tag{4.2}$$

It follows that the block matrix $(K_{\mathcal{U}}(\lambda_j, \lambda_k))_{j,k=1}^n$ is Gram matrix of vectors in $\Phi(\bar{\lambda}_1), \dots, \Phi(\bar{\lambda}_n)$. Therefore, the function $\mathcal{U}(z)$ has the property (U5).

- (b) Let b and b_1 be two boundary mappings for S with Gram matrices Q and Q_1 and let $\Phi(z)$ and $\Phi_1(z)$ be holomorphic basis for $\ker(S^* - z)$. Then there exist invertible matrices A and $\mathcal{A}(z)$ such that $Qb = A^*Q_1b_1$, $AQ^{-1}A^* = Q_1^{-1}$ and $\Phi(z) = \Phi_1(z)\mathcal{A}(\bar{z})^*$. The linearity of b_1 implies that $Qb(\widehat{\Phi}(z)) = A^*Q_1b_1(\widehat{\Phi}_1(z)\mathcal{A}(\bar{z})^*) = A^*Q_1b_1(\widehat{\Phi}_1(z))\mathcal{A}(\bar{z})^*$ and therefore (b) is proved. \square

To show that Proposition 4.2 has a converse we make use of the theory of reproducing kernel Hilbert spaces. Let Q be a $d \times d$ invertible selfadjoint matrix with d_+

positive and d_- negative eigenvalues. Let $\mathcal{U}(z)$ be a \mathbb{Q} -boundary coefficient. With the kernel $K_{\mathcal{U}}(z, w)$ in (M5) we associate a reproducing kernel Hilbert space $\mathcal{H}(K_{\mathcal{U}})$. It is the completion of the linear space of the holomorphic functions

$$z \mapsto \sum_{j=1}^n K_{\mathcal{U}}(z, w_j)x_j, \quad z \in \mathbb{C} \setminus \mathbb{R}, \quad w_j \in \mathbb{C}^{\pm}, \quad x_j \in \mathbb{C}^{d_{\pm}},$$

$$j = 1, \dots, n, \quad n \in \mathbb{N},$$

with respect to the inner product

$$\left\langle \sum_{j=1}^n K_{\mathcal{U}}(\cdot, w_j)x_j, \sum_{k=1}^m K_{\mathcal{U}}(\cdot, u_k)y_k \right\rangle = \sum_{j=1}^n \sum_{k=1}^m y_k^* K_{\mathcal{U}}(u_k, w_j)x_j.$$

This completion consists of column vector functions $f(z)$ which are holomorphic on $\mathbb{C} \setminus \mathbb{R}$, and are of size $d_{\pm} \times 1$ on \mathbb{C}^{\pm} . The inner product of $f(z)$ in $\mathcal{H}(K_{\mathcal{U}})$ with a function $z \mapsto K_{\mathcal{U}}(z, w)x$ reproduces the value of $f(z)$ at $z = w$ in the direction x :

$$x^* f(w) = \langle f(\cdot), K_{\mathcal{U}}(\cdot, w)x \rangle.$$

By the continuity of the kernel $K_{\mathcal{U}}(z, w)$ for any finite subset $F \subset \mathbb{C} \setminus \mathbb{R}$ the linear manifold

$$\mathcal{H}_F^{\circ}(K_{\mathcal{U}}) := \text{span}\{z \mapsto K_{\mathcal{U}}(z, w)x \mid (z \in \mathbb{C} \setminus \mathbb{R}): w \in \mathbb{C}^{\pm} \setminus F, x \in \mathbb{C}^{d_{\pm}}\} \tag{4.3}$$

is dense in $\mathcal{H}(K_{\mathcal{U}})$.

Lemma 4.3. *Let \mathbb{Q} and \mathbb{Q}_1 be $d \times d$ invertible selfadjoint matrices with d_+ positive and d_- negative eigenvalues. Let \mathcal{U} be a \mathbb{Q} -boundary coefficient, let \mathcal{U}_1 be a \mathbb{Q}_1 -boundary coefficient and assume that*

$$\mathcal{U}(z) = \mathcal{A}(z)\mathcal{U}_1(z)A$$

for some invertible matrix function $\mathcal{A}(z)$ of size $d_{\mp} \times d_{\mp}$ if $z \in \mathbb{C}^{\pm}$ and a constant invertible $d \times d$ matrix A such that $A\mathbb{Q}^{-1}A^* = \mathbb{Q}_1^{-1}$. Then the operator of multiplication $\mathcal{A}(\cdot) : f(z) \mapsto \mathcal{A}(z)f(z)$ is an isomorphism from $\mathcal{H}(K_{\mathcal{U}})$ onto $\mathcal{H}(K_{\mathcal{U}_1})$ and under this isomorphism the operators $S_{\mathcal{U}}$ and $S_{\mathcal{U}_1}$ of multiplication by the independent variable z coincide.

In particular, if \mathcal{U} has a minimal representation (3.2), then the reproducing kernel spaces $\mathcal{H}(K_{\mathcal{U}})$ and $\mathcal{H}(K_{\mathcal{U}_0})$ are isomorphic and under the isomorphism the operators of multiplication by the independent variable z coincide.

Proof. The kernels associated with the boundary coefficients \mathcal{U} and \mathcal{U}_1 are

$$K_{\mathcal{U}}(z, w) = i \frac{\mathcal{U}(z)\mathbb{Q}^{-1}\mathcal{U}(w)^*}{z - \bar{w}}, \quad K_{\mathcal{U}_1}(z, w) = i \frac{\mathcal{U}_1(z)\mathbb{Q}_1^{-1}\mathcal{U}_1(w)^*}{z - \bar{w}}$$

and so from $\mathcal{U}(z) = \mathcal{A}(z)\mathcal{U}_1(z)A$ and $AQ^{-1}A^* = Q_1^{-1}$ we obtain

$$K_{\mathcal{U}}(z, w) = i \frac{\mathcal{A}(z)\mathcal{U}_1(z)AQ^{-1}A^*\mathcal{U}_1(w)^*\mathcal{A}(w)^*}{z - \bar{w}} = \mathcal{A}(z)K_{\mathcal{U}_1}(z, w)\mathcal{A}(w)^*.$$

Hence, for all $w \in \mathbb{C}^\pm$ and $x \in \mathbb{C}^{d_\pm}$, $z \in \mathbb{C}^\pm$ and $y \in \mathbb{C}^{d_\pm}$,

$$\langle K_{\mathcal{U}}(\cdot, w)x, K_{\mathcal{U}}(\cdot, z)y \rangle_{\mathcal{H}_{\mathcal{U}}} = \langle K_{\mathcal{U}_1}(\cdot, w)\mathcal{A}(w)^*x, K_{\mathcal{U}_1}(\cdot, z)\mathcal{A}(z)^*y \rangle_{\mathcal{H}_{\mathcal{U}_1}},$$

which implies that the linear operator which maps $K_{\mathcal{U}}(\cdot, w)x$ to $K_{\mathcal{U}_1}(\cdot, w)\mathcal{A}(w)^*x$ extends by continuity to an isometry from $\mathcal{H}(K_{\mathcal{U}})$ to $\mathcal{H}(K_{\mathcal{U}_1})$. We denote its adjoint by W . Then for $w \in \mathbb{C}^\pm$ and $x \in \mathbb{C}^{d_\pm}$,

$$\begin{aligned} x^*(Wh)(w) &= \langle (Wh)(\cdot), K_{\mathcal{U}}(\cdot, w)x \rangle_{\mathcal{H}_{\mathcal{U}}} \\ &= \langle h(\cdot), K_{\mathcal{U}_1}(\cdot, w)\mathcal{A}(w)^*x \rangle_{\mathcal{H}_{\mathcal{U}_1}} \\ &= x^*\mathcal{A}(w)h(w) \end{aligned}$$

and so W is the operator of multiplication by $\mathcal{A}(\cdot)$ and is a partial isometry from $\mathcal{H}(K_{\mathcal{U}_1})$ onto $\mathcal{H}(K_{\mathcal{U}})$. As $\mathcal{A}(z)$ is invertible, W is in fact a unitary operator. Evidently, the operators of multiplication by z in $\mathcal{H}(K_{\mathcal{U}})$ and $\mathcal{H}(K_{\mathcal{U}_1})$ are isomorphic under W . \square

Thus, to study the operator $S_{\mathcal{U}}$ of multiplication by z in $\mathcal{H}(K_{\mathcal{U}})$ we may assume without loss of generality that $\mathcal{U}(z)$ is a minimal Q -boundary coefficient. The following theorem gives a representation of a minimal boundary coefficient $\mathcal{U}(z)$ in terms of the operator $S_{\mathcal{U}}$ of multiplication by z in the reproducing kernel Hilbert space $\mathcal{H}(K_{\mathcal{U}})$.

Theorem 4.4. *Let Q be a $d \times d$ invertible selfadjoint matrix with d_+ positive and d_- negative eigenvalues. Let $\mathcal{U}(z)$ be a minimal Q -boundary coefficient.*

- (a) *The operator $S_{\mathcal{U}}$ of multiplication by z in the reproducing kernel Hilbert space $\mathcal{H}(K_{\mathcal{U}})$ is a closed simple symmetric operator with defect index (d_-, d_+) . Its adjoint is given by*

$$S_{\mathcal{U}}^* = \overline{\text{span}}\{ \{ K_{\mathcal{U}}(\cdot, w)x, \bar{w}K_{\mathcal{U}}(\cdot, w)x \} : w \in \mathbb{C}^\pm, x \in \mathbb{C}^{d_\pm} \}. \tag{4.4}$$

- (b) *There exist a boundary mapping b_1 for $S_{\mathcal{U}}$ with Gram matrix $-Q$ and a holomorphic basis $\widehat{\Phi}_1(z)$ for $\ker(S_{\mathcal{U}}^* - z)$, $z \in \mathbb{C} \setminus \mathbb{R}$, such that*

$$\mathcal{U}(z) = (Qb_1(\widehat{\Phi}_1(\bar{z})))^*.$$

- (c) *Let b_2 be an arbitrary boundary mapping for $S_{\mathcal{U}}$ with Gram matrix Q_2 and let $\widehat{\Phi}_2(z)$ be an arbitrary holomorphic basis for $\ker(S_{\mathcal{U}}^* - z)$, $z \in \mathbb{C} \setminus \mathbb{R}$. Then*

$$\mathcal{U}(z) = \mathcal{A}(z)(Q_2b_2(\widehat{\Phi}_2(\bar{z})))^*A$$

for some invertible matrix function $\mathcal{A}(z)$ of size $d_{\mp} \times d_{\mp}$ if $z \in \mathbb{C}^\pm$ and a constant invertible $d \times d$ matrix A such that $AQ^{-1}A^ = -Q_2^{-1}$.*

Proof. To prove (a) consider the linear manifold

$$T_{\max}^{\circ} = \left\{ \left\{ \sum_{j=1}^n K_{\mathcal{U}}(\cdot, w_j)x_j, \sum_{j=1}^n \bar{w}_j K_{\mathcal{U}}(\cdot, w_j)x_j \right\}; \right. \\ \left. n \in \mathbb{N}, w_j \in \mathbb{C}^{\pm}, x_j \in \mathbb{C}^{d_{\pm}} \right\}$$

in the space $\mathcal{H}(K_{\mathcal{U}})^2$. The closure of this manifold in $\mathcal{H}(K_{\mathcal{U}})^2$ is the linear relation T_{\max} . Consider the boundary form $[[\cdot, \cdot]]$ on T_{\max}° :

$$\begin{aligned} & \left[\left[\left\{ \sum_{j=1}^n K_{\mathcal{U}}(\cdot, w_j)x_j, \sum_{j=1}^n \bar{w}_j K_{\mathcal{U}}(\cdot, w_j)x_j \right\}, \right. \right. \\ & \left. \left. \left\{ \sum_{k=1}^m K_{\mathcal{U}}(\cdot, u_k)y_k, \sum_{k=1}^m \bar{u}_k K_{\mathcal{U}}(\cdot, u_k)y_k \right\} \right] \right] \\ & := \frac{1}{i} \left(\left\langle \sum_{j=1}^n \bar{w}_j K_{\mathcal{U}}(\cdot, w_j)x_j, \sum_{k=1}^m K_{\mathcal{U}}(\cdot, u_k)y_k \right\rangle \right. \\ & \quad \left. - \left\langle \sum_{j=1}^n K_{\mathcal{U}}(\cdot, w_j)x_j, \sum_{k=1}^m \bar{u}_k K_{\mathcal{U}}(\cdot, u_k)y_k \right\rangle \right) \\ & = \frac{1}{i} \sum_{j=1}^n \sum_{k=1}^m (\bar{w}_j y_k^* K_{\mathcal{U}}(u_k, w_j)x_j - u_k y_k^* K_{\mathcal{U}}(u_k, w_j)x_j) \\ & = \frac{1}{i} \sum_{j=1}^n \sum_{k=1}^m (\bar{w}_j - u_k) y_k^* K_{\mathcal{U}}(u_k, w_j)x_j \\ & = \frac{1}{i} \sum_{j=1}^n \sum_{k=1}^m (\bar{w}_j - u_k) y_k^* i \frac{\mathcal{U}(u_k)Q^{-1}\mathcal{U}(w_j)^*}{u_k - \bar{w}_j} x_j \\ & = - \sum_{j=1}^n \sum_{k=1}^m y_k^* \mathcal{U}(u_k)Q^{-1}\mathcal{U}(w_j)^* x_j \\ & = - \left(\sum_{k=1}^m \mathcal{U}(u_k)^* y_k \right)^* Q^{-1} \left(\sum_{j=1}^n \mathcal{U}(w_j)^* x_j \right). \end{aligned} \tag{4.5}$$

Since the form $[[\cdot, \cdot]]$ is continuous on $\mathcal{H}(K_{\mathcal{U}})^2$ the subspace $(T_{\max}^{\circ}, [[\cdot, \cdot]])$ is a dense subspace of the pseudo-Krein space $(T_{\max}, [[\cdot, \cdot]])$. The isotropic part of T_{\max} is the closure T_{\min} of the following linear manifold:

$$T_{\min}^{\circ} := \left\{ \left\{ \sum_{j=1}^n K_{\mathcal{U}}(\cdot, w_j)x_j, \sum_{j=1}^n \bar{w}_j K_{\mathcal{U}}(\cdot, w_j)x_j \right\}; \right. \\ \left. \sum_{j=1}^n \mathcal{U}(w_j)^* x_j = 0, n \in \mathbb{N}, w_j \in \mathbb{C}^{\pm}, x_j \in \mathbb{C}^{d_{\pm}} \right\}.$$

Since we assume that $\mathcal{U}(z)$ is a minimal boundary coefficient it follows that the mapping $b^{\circ} : T_{\max}^{\circ} \rightarrow \mathbb{C}^d$ defined by

$$b^{\circ} \left(\left\{ \sum_{j=1}^n K_{\mathcal{U}}(\cdot, w_j)x_j, \sum_{j=1}^n \bar{w}_j K_{\mathcal{U}}(\cdot, w_j)x_j \right\} \right) := \sum_{j=1}^n \mathcal{U}(w_j)^* x_j$$

is onto. This mapping is continuous with respect to the topology of $\mathcal{H}(K_{\mathcal{U}})^2$. Clearly, $\ker(b^{\circ}) = T_{\min}^{\circ}$. Therefore, $\dim(T_{\max}^{\circ}/T_{\min}^{\circ}) = d$. Denote by b the extension of b° to T_{\max} by continuity. Then $\ker(b) = T_{\min}$. The mapping b is a boundary mapping for T_{\max} . It follows from (4.5) that Gram matrix of b is $-Q^{-1}$.

Let $\mu \in \mathbb{C}^+$. Put

$$\begin{aligned} \mathcal{M}_{\mu} &= \text{span}\{ \{K_{\mathcal{U}}(\cdot, \bar{\mu})x, \mu K_{\mathcal{U}}(\cdot, \bar{\mu})x\} : x \in \mathbb{C}^{d_-} \} \subset T_{\max}^{\circ} \cap \mu I, \\ \mathcal{M}_{\bar{\mu}} &= \text{span}\{ \{K_{\mathcal{U}}(\cdot, \mu)x, \bar{\mu} K_{\mathcal{U}}(\cdot, \mu)x\} : x \in \mathbb{C}^{d_+} \} \subset T_{\max}^{\circ} \cap \bar{\mu} I. \end{aligned} \tag{4.6}$$

Since $\mathcal{U}(z)$ is a minimal boundary coefficient we conclude that

$$\dim(\mathcal{M}_{\mu}) = d_- \quad \text{and} \quad \dim(\mathcal{M}_{\bar{\mu}}) = d_+,$$

and

$$\mathcal{M}_{\mu} \cap \mathcal{M}_{\bar{\mu}} = \{0\} \quad \text{and} \quad (\mathcal{M}_{\mu} \llbracket \dot{+} \rrbracket \mathcal{M}_{\bar{\mu}}) \cap T_{\min}^{\circ} = \{0\}.$$

Since

$$d = d_- + d_+ = \dim(\mathcal{M}_{\mu} \llbracket \dot{+} \rrbracket \mathcal{M}_{\bar{\mu}}) \leq \dim(T_{\max}^{\circ}/T_{\min}^{\circ}) = d,$$

we conclude that the following decomposition of T_{\max}° holds:

$$T_{\max}^{\circ} = T_{\min}^{\circ} \llbracket \dot{+} \rrbracket \mathcal{M}_{\mu} \llbracket \dot{+} \rrbracket \mathcal{M}_{\bar{\mu}}, \quad \text{direct sums in } \mathcal{H}^2.$$

Continuity of the inner product $\llbracket \cdot, \cdot \rrbracket$ in the space $\mathcal{H}(K_{\mathcal{U}})^2$ implies that the same decomposition will be true for the closures:

$$T_{\max} = T_{\min} \llbracket \dot{+} \rrbracket \mathcal{M}_{\mu} \llbracket \dot{+} \rrbracket \mathcal{M}_{\bar{\mu}}, \quad \text{direct sums in } \mathcal{H}^2. \tag{4.7}$$

Evidently, T_{\min} is the isotropic part of T_{\max} . We now want to apply Proposition A.2 from Appendix A. We need to be specific about the fundamental symmetry of the Krein space $(\mathcal{H}(K_{\mathcal{U}})^2, \llbracket \cdot, \cdot \rrbracket)$ that induces the decomposition (4.7). That fundamental symmetry is

$$J_{\mu} = \frac{1}{i \operatorname{Im}(\mu)} \begin{pmatrix} -\operatorname{Re}(\mu) & 1 \\ -|\mu|^2 & \operatorname{Re}(\mu) \end{pmatrix}. \tag{4.8}$$

We now have to prove that

$$J_\mu T_{\max} + T_{\max} = \mathcal{H}(K_{\mathcal{U}})^2. \tag{4.9}$$

Using the notation introduced in (4.3), it is sufficient to prove that

$$J_\mu(T_{\max}^\circ) + T_{\max}^\circ = \mathcal{H}^\circ_{\{\mu, \bar{\mu}\}}(K_{\mathcal{U}})^2, \tag{4.10}$$

since the closure of the left-/right-hand side of (4.10) is the left-/right-hand side of (4.9). Let $w, v \in (\mathbb{C} \setminus \mathbb{R}) \setminus \{\mu, \bar{\mu}\}$ and let a and c be vectors of appropriate size. Put

$$a' = \frac{1}{2(\mu - \bar{w})(\bar{\mu} - \bar{w})}a \quad \text{and} \quad c' = -\frac{1}{2(\mu - \bar{v})(\bar{\mu} - \bar{v})}c.$$

A straightforward calculation shows that

$$\begin{aligned} & (\mu - \bar{\mu})J_\mu \left(\bar{w} \begin{pmatrix} K_{\mathcal{U}}(\cdot, w)a' \\ \bar{w}K_{\mathcal{U}}(\cdot, w)a' \end{pmatrix} + \begin{pmatrix} K_{\mathcal{U}}(\cdot, v)c' \\ \bar{v}K_{\mathcal{U}}(\cdot, v)c' \end{pmatrix} \right) \\ & + \left((2\mu\bar{\mu} - \bar{w}(\mu + \bar{\mu})) \begin{pmatrix} K_{\mathcal{U}}(\cdot, w)a' \\ \bar{w}K_{\mathcal{U}}(\cdot, w)a' \end{pmatrix} \right. \\ & \quad \left. + ((\mu + \bar{\mu}) - 2\bar{w}) \begin{pmatrix} K_{\mathcal{U}}(\cdot, v)c' \\ \bar{v}K_{\mathcal{U}}(\cdot, v)c' \end{pmatrix} \right) \\ & = \begin{pmatrix} K_{\mathcal{U}}(\cdot, w)a \\ K_{\mathcal{U}}(\cdot, v)c \end{pmatrix}. \end{aligned}$$

Taking linear combinations over all $w, v \in (\mathbb{C} \setminus \mathbb{R}) \setminus \{\mu, \bar{\mu}\}$ leads to (4.10).

Thus, we have proved that $T_{\max}^* = T_{\min}$. We now give another characterization of T_{\min} . By the definition of the adjoint, $\{f, g\} \in \mathcal{H}(K_{\mathcal{U}})^2$ belongs to T_{\max}^* if and only if for each $\{K_{\mathcal{U}}(\cdot, w)a, \bar{w}K_{\mathcal{U}}(\cdot, w)a\} \in T_{\max}$ we have

$$\begin{aligned} 0 &= \llbracket \{f, g\}, \{K_{\mathcal{U}}(\cdot, w)a, \bar{w}K_{\mathcal{U}}(\cdot, w)a\} \rrbracket \\ &= \frac{1}{i}(\langle g, K_{\mathcal{U}}(\cdot, w)a \rangle - \langle f, \bar{w}K_{\mathcal{U}}(\cdot, w)a \rangle) \\ &= \frac{1}{i}(a^*g(w) - a^*wf(w)). \end{aligned} \tag{4.11}$$

Since (4.11) holds for all $w \in \mathbb{C}^\pm$ and for all $a \in \mathbb{C}^{d_\pm}$ we conclude that $\{f, g\} \in \mathcal{H}(K_{\mathcal{U}})^2$ belongs to T_{\max}^* if and only if $g(z) = zf(z)$, $z \in \mathbb{C}^\pm$. Therefore, the operator of multiplication by z in $\mathcal{H}(K_{\mathcal{U}})$ equals T_{\min} ,

$$S_{\mathcal{U}} = T_{\min}.$$

Thus, $S_{\mathcal{U}}$ is a closed and symmetric operator with defect index (d_-, d_+) . Since $S_{\mathcal{U}}^* = T_{\min}^* = T_{\max}$, (4.4) holds and consequently $S_{\mathcal{U}}$ is simple. This completes the proof of part (a).

The proof of (b) follows. Put $b_1 = Q^{-1}b$, where b is the boundary mapping for $S_{\mathcal{U}}$ with Gram matrix $-Q^{-1}$ introduced in the proof of part (a). Then b_1 is a

boundary mapping for $S_{\mathcal{U}}$ with Gram matrix $-\mathbf{Q}$. Note that for the j th basis vector e_j of $\mathbb{C}^{d_{\mp}}$, $j = 1, \dots, d_{\mp}$, the vectors $K_{\mathcal{U}}(\cdot, \bar{z})e_j$, $j = 1, \dots, d_{\mp}$, form a basis of $\ker(S_{\mathcal{U}}^* - z)$, $z \in \mathbb{C}^{\pm}$. Let $\widehat{\Phi}_1(z)$, $z \in \mathbb{C}^{\pm}$, be the vector whose components are the vectors $K_{\mathcal{U}}(\cdot, \bar{z})e_j$, $j = 1, \dots, d_{\mp}$. Since $\mathcal{U}(z)$ is holomorphic on \mathbb{C}^{\pm} , $\widehat{\Phi}_1(z)$ is holomorphic there too. Using the above definitions we get

$$\begin{aligned} b_1(\widehat{\Phi}_1(z)) &= \mathbf{Q}^{-1}b(\widehat{\Phi}_1(z)) \\ &= \mathbf{Q}^{-1}(\mathcal{U}(\bar{z})^*e_1 \ \cdots \ \mathcal{U}(\bar{z})^*e_{d_{\mp}}) \\ &= \mathbf{Q}^{-1}\mathcal{U}(\bar{z})^*. \end{aligned}$$

This readily implies (b).

Part (c) follows from Proposition 4.2(b). The theorem is proved. \square

Corollary 4.5. *Let S be a closed simple symmetric operator in a Hilbert space $(\mathcal{H}, \langle \cdot, \cdot \rangle_{\mathcal{H}})$ with defect index (d_+, d_-) , $d = d_+ + d_- < \infty$. Then there exist a $d \times d$ invertible matrix \mathbf{Q} with d_+ positive and d_- negative eigenvalues and a minimal $(-\mathbf{Q})$ -boundary coefficient $\mathcal{U}(z)$ such that S is isomorphic to the operator $S_{\mathcal{U}}$ of multiplication by the independent variable in the reproducing kernel Hilbert space $\mathcal{H}(K_{\mathcal{U}})$ and*

$$S^* = \overline{\text{span}}\{\{\phi, z\phi\}: \phi \in \ker(S^* - z), z \in \mathbb{C} \setminus \mathbb{R}\}.$$

Proof. Assume that S is a closed simple symmetric operator in a Hilbert space $(\mathcal{H}, \langle \cdot, \cdot \rangle_{\mathcal{H}})$ with defect index (d_+, d_-) , $d = d_+ + d_- < \infty$. Let $\mathcal{U}(z) = (\mathbf{Q}b(\widehat{\Phi}(\bar{z})))^*$, where b is a boundary mapping for S with Gram matrix \mathbf{Q} and $\widehat{\Phi}(z)$ is a holomorphic basis for $\ker(S^* - z)$. By Proposition 4.2 $\mathcal{U}(z)$ is a minimal $(-\mathbf{Q})$ -boundary coefficient. It follows that the kernel

$$K_{\mathcal{U}}(z, w) = -i \frac{\mathcal{U}(z)\mathbf{Q}^{-1}\mathcal{U}(w)^*}{z - \bar{w}}$$

is nonnegative. We show that S in \mathcal{H} is isomorphic to the operator $S_{\mathcal{U}}$ of multiplication by the independent variable in the reproducing kernel space $(\mathcal{H}(K_{\mathcal{U}}), \langle \cdot, \cdot \rangle_{\mathcal{H}(K_{\mathcal{U}})})$. By Theorem 4.4 the defect index of $S_{\mathcal{U}}$ is equal to that of S . Denote by $U : \mathcal{H} \rightarrow \mathcal{H}(K_{\mathcal{U}})$ the linear operator

$$U(\Phi(\bar{w})x) = K_{\mathcal{U}}(\cdot, w)x, \quad w \in \mathbb{C}^{\pm}, \quad x \in \mathbb{C}^{d_{\pm}}.$$

From (4.2)

$$\langle \Phi(\bar{w})x, \Phi(\bar{z})y \rangle_{\mathcal{H}} = y^*K_{\mathcal{U}}(z, w)x = \langle K_{\mathcal{U}}(\cdot, w)x, K_{\mathcal{U}}(\cdot, z)y \rangle_{\mathcal{H}(K_{\mathcal{U}})}.$$

Hence, U is isometric. As S is simple, $\text{dom}(S^*)$ is dense in \mathcal{H} and as the kernel functions $K_{\mathcal{U}}(\cdot, w)x$ are total in $\mathcal{H}(K_{\mathcal{U}})$ the range of U is dense in $\mathcal{H}(K_{\mathcal{U}})$. Therefore, the closure of U is a unitary operator which we also denote by U . Using Theorem 4.4 we conclude:

$$S \subset U^{-1}S_{\mathcal{H}}U \subset U^{-1}S_{\mathcal{H}}^*U$$

$$= \overline{\text{span}}\{\{\Phi(\overline{w})x, \overline{w}\Phi(\overline{w})x\}: w \in \mathbb{C}^{\pm}, x \in \mathbb{C}^{d_{\pm}}\} \subset S^*.$$

Since $\dim(S^*/S) = \dim(S_{\mathcal{H}}^*/S_{\mathcal{H}}) = d$, we have $S = U^{-1}S_{\mathcal{H}}U$ and the formula for S^* holds. \square

5. Linearization of the boundary eigenvalue problem

Theorem 5.1. For $j = 0, 1$, let S_j be a closed symmetric relation in a Hilbert space $(\mathcal{H}_j, \langle \cdot, \cdot \rangle_j)$ with defect index (ω_j^+, ω_j^-) , $\omega_j = \omega_j^+ + \omega_j^- < \infty$, and let $b_j : S_j^* \rightarrow \mathbb{C}^{\omega_j}$ be a boundary mapping for S_j with Gram matrix Q_j .

- (a) $S_0 \oplus S_1$ has a canonical selfadjoint extension \tilde{A} in the Hilbert space $\tilde{\mathcal{H}} = \mathcal{H}_0 \oplus \mathcal{H}_1$ such that $\tilde{A} \cap \mathcal{H}_j^2 = S_j$, $j = 0, 1$, if and only if

$$\omega_0^+ = \omega_1^- \quad \text{and} \quad \omega_0^- = \omega_1^+. \tag{5.1}$$

- (b) Assume that (5.1) holds and set $\omega = \omega_0 = \omega_1$. The formula

$$\tilde{A} = \left\{ \left\{ \begin{pmatrix} f_0 \\ f_1 \end{pmatrix}, \begin{pmatrix} g_0 \\ g_1 \end{pmatrix} \right\} : \{f_0, g_0\} \in S_0^*, \{f_1, g_1\} \in S_1^*, \right. \\ \left. b_0(f_0, g_0) + \Gamma b_1(f_1, g_1) = 0 \right\} \tag{5.2}$$

gives a one-to-one correspondence between all canonical selfadjoint extensions \tilde{A} of $S_0 \oplus S_1$ in $\mathcal{H}_0 \oplus \mathcal{H}_1$ with $\tilde{A} \cap \mathcal{H}_j^2 = S_j$, $j = 0, 1$, and all $\omega \times \omega$ invertible matrices Γ with $Q_1 + \Gamma^*Q_0\Gamma = 0$.

Proof. Let $\mu \in \mathbb{C}^+$. Then the Cayley transform

$$V = C_{\mu}(S) = \{\{g - \mu f, g - \overline{\mu}f\}: \{f, g\} \in S\}$$

gives a one-to-one correspondence between all selfadjoint relations S in a Hilbert space and all unitary operators V and also a one-to-one correspondence between all symmetric relations S and all isometric operators V ,

$$V : \text{dom}(V) = \text{ran}(S - \mu) \rightarrow \text{ran}(V) = \text{ran}(S - \overline{\mu}).$$

The inverse is given by

$$S = F_{\mu}(V) = \{\{u - v, \overline{\mu}u - \mu v\}: \{u, v\} \in V\}.$$

Clearly, $C_{\mu}(\mathcal{H}_j^2) = F_{\mu}(\mathcal{H}_j^2) = \mathcal{H}_j^2$, $j = 0, 1$.

Recall that a symmetric relation has a canonical selfadjoint extension if and only if its defect numbers are equal. In the case of $S_0 \oplus S_1$, a canonical selfadjoint extension \tilde{A} of $S_0 \oplus S_1$ exists if and only if

$$\omega_0^+ + \omega_1^+ = \omega_0^- + \omega_1^- \tag{5.3}$$

If (5.3) holds and $V_j = C_\mu(S_j)$, $j = 0, 1$, the formula

$$\begin{aligned} \tilde{U} &= C_\mu(\tilde{A}) \\ &= \begin{pmatrix} V_0 & 0 & 0 & 0 \\ 0 & V_{00} & V_{01} & 0 \\ 0 & V_{10} & V_{11} & 0 \\ 0 & 0 & 0 & V_1 \end{pmatrix} : \begin{pmatrix} \text{ran}(S_0 - \mu) \\ \ker(S_0^* - \bar{\mu}) \\ \ker(S_1^* - \bar{\mu}) \\ \text{ran}(S_1 - \mu) \end{pmatrix} \rightarrow \begin{pmatrix} \text{ran}(S_0 - \bar{\mu}) \\ \ker(S_0^* - \mu) \\ \ker(S_1^* - \mu) \\ \text{ran}(S_1 - \bar{\mu}) \end{pmatrix} \end{aligned} \tag{5.4}$$

gives a one-to-one correspondence between all canonical selfadjoint extensions \tilde{A} of $S_0 \oplus S_1$ and all unitary operators

$$U = \begin{pmatrix} V_{00} & V_{01} \\ V_{10} & V_{11} \end{pmatrix} : \begin{pmatrix} \ker(S_0^* - \bar{\mu}) \\ \ker(S_1^* - \bar{\mu}) \end{pmatrix} \rightarrow \begin{pmatrix} \ker(S_0^* - \mu) \\ \ker(S_1^* - \mu) \end{pmatrix} \tag{5.5}$$

Since the Cayley transform of an intersection of linear relations is the intersection of the corresponding Cayley transforms we have that $\tilde{A} \cap \mathcal{H}_j^2 = S_j$ if and only if $\tilde{U} \cap \mathcal{H}_j^2 = V_j$, $j = 0, 1$. Since, for example,

$$\begin{aligned} \tilde{U} \cap \mathcal{H}_0^2 &= \left\{ \left\{ \begin{pmatrix} f_0 \\ \varphi_0 \end{pmatrix}, \begin{pmatrix} V_0 f_0 \\ V_{00} \varphi_0 \end{pmatrix} \right\} : \right. \\ &\quad \left. f_0 \in \text{dom}(V_0), \varphi_0 \in \ker(S_0^* - \bar{\mu}), V_{10} \varphi_0 = 0 \right\}, \end{aligned}$$

we conclude that $\tilde{A} \cap \mathcal{H}_0^2 = S_0$ if and only if $\ker(V_{10}) = \{0\}$. Analogously, $\tilde{A} \cap \mathcal{H}_1^2 = S_1$ if and only if $\ker(V_{01}) = \{0\}$.

We now prove (a). If \tilde{A} with the desired properties exists, the injectivity of V_{10} and V_{01} imply

$$\omega_0^- \leq \omega_1^+, \quad \omega_1^- \leq \omega_0^+.$$

By (5.3) equalities prevail. Conversely, if (5.1) holds, bijections V_{10} and V_{01} exist and with $V_{00} = 0$ and $V_{11} = 0$ they give rise to a unitary mapping \tilde{U} of the form (5.4). The inverse Cayley transform $\tilde{A} = F_\mu(\tilde{U})$ now has the desired properties.

We proceed with the proof of (b). Assume that \tilde{A} is a canonical selfadjoint extension of $S_0 \oplus S_1$ in $\tilde{\mathcal{H}} = \mathcal{H}_0 \oplus \mathcal{H}_1$ such that $\tilde{A} \cap \mathcal{H}_j^2 = S_j$, $j = 0, 1$. Applying the inverse Cayley transformation to both sides of the second equality in (5.4) we obtain

$$\tilde{A} = S_0 \oplus S_1 \dot{+} N, \quad \text{direct sum in } \tilde{\mathcal{H}}^2, \tag{5.6}$$

where, in terms of the operator U given in (5.5),

$$N = \left\{ \left\{ (I - U) \begin{pmatrix} \varphi_0 \\ \varphi_1 \end{pmatrix}, (\bar{\mu} - \mu U) \begin{pmatrix} \varphi_0 \\ \varphi_1 \end{pmatrix} \right\} : \right. \\ \left. \varphi_0 \in \ker(S_0^* - \bar{\mu}), \varphi_1 \in \ker(S_1^* - \bar{\mu}) \right\}.$$

The elements in N are of the form

$$\left\{ \begin{pmatrix} f_0 \\ f_1 \end{pmatrix}, \begin{pmatrix} g_0 \\ g_1 \end{pmatrix} \right\}$$

with

$$\begin{aligned} f_0 &= \varphi_0 - V_{00}\varphi_0 - V_{01}\varphi_1, \\ g_0 &= \bar{\mu}\varphi_0 - \mu V_{00}\varphi_0 - \mu V_{01}\varphi_1, \\ f_1 &= \varphi_1 - V_{10}\varphi_0 - V_{11}\varphi_1, \\ g_1 &= \bar{\mu}\varphi_1 - \mu V_{10}\varphi_0 - \mu V_{11}\varphi_1, \end{aligned} \tag{5.7}$$

where $\varphi_0 \in \ker(S_0^* - \bar{\mu}), \varphi_1 \in \ker(S_1^* - \bar{\mu})$. The mapping

$$\begin{pmatrix} \varphi_0 \\ \varphi_1 \end{pmatrix} \mapsto \{f_0, g_0\}$$

is a bijection from $\ker(S_0^* - \bar{\mu}) \oplus \ker(S_1^* - \bar{\mu})$ onto $(S_0 \cap \mu I) \dot{+} (S_0 \cap \bar{\mu} I)$, direct sum in \mathcal{H}_0^2 . The injectivity follows from the facts that the last sum is direct and that V_{01} is invertible. The surjectivity follows from the fact that $\{\varphi_0, \bar{\mu}\varphi_0\}$ is the projection of $\{f_0, g_0\} \in (S_0 \cap \mu I) \dot{+} (S_0 \cap \bar{\mu} I)$ onto $S_0 \cap \mu I$ and $\varphi_1 = V_{01}^{-1}(f_0 - \varphi_0 + V_{00}\varphi_0)$. Similarly, the mapping

$$\begin{pmatrix} \varphi_0 \\ \varphi_1 \end{pmatrix} \mapsto \{f_1, g_1\}$$

is a bijection from $\ker(S_0^* - \bar{\mu}) \oplus \ker(S_1^* - \bar{\mu})$ onto $(S_1 \cap \mu I) \dot{+} (S_1 \cap \bar{\mu} I)$, direct sum in \mathcal{H}_1^2 . Hence, the four equalities in (5.7) define a bijection

$$\Upsilon : \{f_0, g_0\} \mapsto \{f_1, g_1\}$$

from $(S_0 \cap \mu I) \dot{+} (S_0 \cap \bar{\mu} I)$ onto $(S_1 \cap \mu I) \dot{+} (S_1 \cap \bar{\mu} I)$, and N is the graph of this bijection:

$$N = \left\{ \left\{ \begin{pmatrix} f_0 \\ f_1 \end{pmatrix}, \begin{pmatrix} g_0 \\ g_1 \end{pmatrix} \right\} : \right. \\ \left. \{f_0, g_0\} \in (S_0 \cap \mu I) \dot{+} (S_0 \cap \bar{\mu} I), \{f_1, g_1\} = \Upsilon(f_0, g_0) \right\}. \tag{5.8}$$

Since N is a restriction of a selfadjoint relation we have $N \subset N^*$ and therefore any two elements

$$\left\{ \begin{pmatrix} f_0 \\ f_1 \end{pmatrix}, \begin{pmatrix} g_0 \\ g_1 \end{pmatrix} \right\}, \left\{ \begin{pmatrix} f'_0 \\ f'_1 \end{pmatrix}, \begin{pmatrix} g'_0 \\ g'_1 \end{pmatrix} \right\} \in N$$

satisfy the identity

$$\langle g_0, f'_0 \rangle_0 - \langle f_0, g'_0 \rangle_0 = -(\langle g_1, f'_1 \rangle_1 - \langle f_1, g'_1 \rangle_1).$$

Hence, if for $j = 0, 1$, we provide $(S_j \cap \mu I) \dot{+} (S_j \cap \bar{\mu} I)$ with the indefinite inner product

$$\| \{f_j, g_j\}, \{f'_j, g'_j\} \|_j := \frac{1}{i} (\langle g_j, f'_j \rangle_j - \langle f_j, g'_j \rangle_j),$$

the mapping

$$\Upsilon : ((S_0 \cap \mu I) \dot{+} (S_0 \cap \bar{\mu} I), \| \cdot, \cdot \|_0) \rightarrow ((S_0 \cap \mu I) \dot{+} (S_0 \cap \bar{\mu} I), \| \cdot, \cdot \|_1) \tag{5.9}$$

satisfies

$$\| \Upsilon(f_0, g_0), \Upsilon(f'_0, g'_0) \|_1 = -\| \{f_0, g_0\}, \{f'_0, g'_0\} \|_0$$

for all $\{f_0, g_0\}, \{f'_0, g'_0\} \in (S_0 \cap \mu I) \dot{+} (S_0 \cap \bar{\mu} I)$, that is, $\Upsilon^* \Upsilon = -I$. As \tilde{A} is self-adjoint in \mathcal{H} , by (5.6)

$$\tilde{A}^* = \tilde{A} = (S_0^* \oplus S_1^*) \cap N^*. \tag{5.10}$$

In this formula N^* is the adjoint of N in $\tilde{\mathcal{H}}$ and S_j^* stands for the adjoint of S_j in $\mathcal{H}_j, j = 0, 1$.

Let

$$\{\alpha_{01}, \beta_{01}\}, \dots, \{\alpha_{0\omega}, \beta_{0\omega}\}$$

be a basis for $(S_0 \cap \mu I) \dot{+} (S_0 \cap \bar{\mu} I)$ and set

$$\Upsilon(\alpha_{0r}, \beta_{0r}) = \{\alpha_{1r}, \beta_{1r}\}, \quad r = 1, 2, \dots, \omega. \tag{5.11}$$

Then

$$\{\alpha_{11}, \beta_{11}\}, \dots, \{\alpha_{1\omega}, \beta_{1\omega}\}$$

is a basis for $(S_1 \cap \mu I) \dot{+} (S_1 \cap \bar{\mu} I)$. For $j = 0, 1$, let Γ_j be the $\omega \times \omega$ matrix of which the r th column vector is the column vector $b_j(\alpha_{jr}, \beta_{jr})$. Evidently, Γ_j is invertible and

$$\begin{aligned} (\Gamma_j^* Q_j \Gamma_j)_{rs} &= b_j(\alpha_{jr}, \beta_{jr})^* Q_j b_j(\alpha_{js}, \beta_{js}) \\ &= \| \{\alpha_{js}, \beta_{js}\}, \{\alpha_{jr}, \beta_{jr}\} \|_j, \quad r = 1, \dots, \omega. \end{aligned}$$

These equalities and (5.11) imply that $\Upsilon^* \Upsilon = -I$ is equivalent to

$$\Gamma_0^* Q_0 \Gamma_0 = -\Gamma_1^* Q_1 \Gamma_1.$$

Finally, (5.10) implies

$$\begin{aligned} \tilde{A} &= \left\{ \left\{ \begin{pmatrix} f_0 \\ f_1 \end{pmatrix}, \begin{pmatrix} g_0 \\ g_1 \end{pmatrix} \right\} : \{f_0, g_0\} \in S_0^*, \{f_1, g_1\} \in S_1^*, \right. \\ &\quad \left. \llbracket \{f_0, g_0\}, \{\alpha_{0r}, \beta_{0r}\} \rrbracket_0 + \llbracket \{f_1, g_1\}, \Upsilon(\alpha_{0r}, \beta_{0r}) \rrbracket_1 = 0, r = 1, \dots, \omega \right\} \\ &= \left\{ \left\{ \begin{pmatrix} f_0 \\ f_1 \end{pmatrix}, \begin{pmatrix} g_0 \\ g_1 \end{pmatrix} \right\} : \{f_0, g_0\} \in S_0^*, \{f_1, g_1\} \in S_1^*, \right. \\ &\quad \left. \Gamma_0^* Q_0 b_0(f_0, g_0) + \Gamma_1^* Q_1 b_1(f_1, g_1) = 0 \right\}. \end{aligned}$$

Thus, if we set $\Gamma = Q_0^{-1} \Gamma_0^* \Gamma_1^* Q_1$, then

$$Q_1 + \Gamma^* Q_0 \Gamma = 0 \tag{5.12}$$

and

$$\begin{aligned} \tilde{A} &= \left\{ \left\{ \begin{pmatrix} f_0 \\ f_1 \end{pmatrix}, \begin{pmatrix} g_0 \\ g_1 \end{pmatrix} \right\} : \{f_0, g_0\} \in S_0^*, \{f_1, g_1\} \in S_1^*, \right. \\ &\quad \left. b_0(f_0, g_0) + \Gamma b_1(f_1, g_1) = 0 \right\}. \end{aligned} \tag{5.13}$$

Conversely, if we assume that (5.2) holds, Lemma 3.4(d) implies that the adjoint of \tilde{A} is given by

$$\begin{aligned} \tilde{A}^* &= \left\{ \left\{ \begin{pmatrix} f_0 \\ f_1 \end{pmatrix}, \begin{pmatrix} g_0 \\ g_1 \end{pmatrix} \right\} : \{f_0, g_0\} \in S_0^*, \{f_1, g_1\} \in S_1^*, \right. \\ &\quad \left. Q_1^{-1} \Gamma^* Q_0 b_0(f_0, g_0) - b_1(f_1, g_1) = 0 \right\}. \end{aligned}$$

Since we assume that $Q_1 + \Gamma^* Q_0 \Gamma = 0$ it follows that $\tilde{A}^* = \tilde{A}$. The invertibility of Γ implies that $\tilde{A} \cap \mathcal{H}_j^2 = S_j, j = 0, 1$. Thus, \tilde{A} defined by (5.2) has all the properties stated in the theorem. \square

Lemma 5.2. *Let S be a symmetric relation in a Hilbert space \mathcal{H} and let \tilde{A} be a selfadjoint extension of S in $\tilde{\mathcal{H}}$. Let $\tilde{\mathcal{H}} = \mathcal{H} \oplus \mathcal{H}_1$ and set $S_1 = \tilde{A} \cap \mathcal{H}_1^2$. Then \tilde{A} is a minimal extension of S if and only if S_1 is simple.*

Proof. Let $S_1 = S_r + S_s$, where S_r is selfadjoint in a subspace $\mathcal{H}_r \subset \tilde{\mathcal{H}}_1$ and S_s is a simple symmetric operator in $\mathcal{H}_s = \mathcal{H}_1 \ominus \mathcal{H}_r$. Then $S_r \subset \tilde{A}$, hence $(S_r - z)^{-1} \subset (\tilde{A} - z)^{-1}$ and therefore, since both are operators,

$$(S_r - z)^{-1} = ((\tilde{A} - z)^{-1})|_{\mathcal{H}_r}, \quad z \in \rho(\tilde{A}) \cap \rho(S_r).$$

Hence, $\mathcal{H}_r \perp \mathcal{H}$ and \mathcal{H}_r are invariant under $(\tilde{A} - z)^{-1}$. The minimality of \tilde{A} implies that $\mathcal{H}_r = \{0\}$, that is S_1 is simple. Conversely, assume that S_1 is simple and let

$$\mathcal{H}_r = \tilde{\mathcal{H}} \ominus \text{span}\{\mathcal{H}, \text{ran}((\tilde{A} - z)^{-1}|_{\mathcal{H}}): z \in \mathbb{C} \setminus \mathbb{R}\}.$$

Then

$$\langle (\tilde{A} - z)^{-1} \mathcal{H}_r, \mathcal{H} \rangle = \langle \mathcal{H}_r, (\tilde{A} - \bar{z})^{-1} \mathcal{H} \rangle = \{0\},$$

$$\begin{aligned} \langle (\tilde{A} - z)^{-1} \mathcal{H}_r, (\tilde{A} - w)^{-1} \mathcal{H} \rangle &= \left\langle \mathcal{H}_r, \frac{(\tilde{A} - \bar{z})^{-1} - (\tilde{A} - w)^{-1}}{\bar{z} - w} \mathcal{H} \right\rangle \\ &= \{0\}, \quad w \neq \bar{z}, \end{aligned}$$

and, by continuity, letting $w \rightarrow \bar{z}$,

$$\langle (\tilde{A} - z)^{-1} \mathcal{H}_r, (\tilde{A} - \bar{z})^{-1} \mathcal{H} \rangle = \{0\},$$

and hence \mathcal{H}_r is invariant under $(\tilde{A} - z)^{-1}$. It follows that

$$\tilde{A} \cap \mathcal{H}_r^2 = \{ \{(\tilde{A} - z)^{-1}u, u + z(\tilde{A} - z)^{-1}u\} : u \in \mathcal{H}_r \}$$

is a selfadjoint operator which is a part of S_1 . Since S_1 is simple $\mathcal{H}_r = \{0\}$ and (2.4) is true. \square

Theorem 5.3. *Let S be a closed symmetric relation in a Hilbert space $(\mathcal{H}, \langle \cdot, \cdot \rangle_{\mathcal{H}})$ with defect index (d_+, d_-) , $d = d_+ + d_- < \infty$. Let \tilde{A} be a minimal selfadjoint extension of S in $\tilde{\mathcal{H}}$. Let $\tilde{\mathcal{H}} = \mathcal{H} \oplus \mathcal{H}_1$ and set $S_1 = \tilde{A} \cap \mathcal{H}_1^2$. Let b be a boundary mapping for S with Gram matrix Q .*

(a) *There exists a Q -boundary coefficient \mathcal{W} such that for each $z \in \mathbb{C} \setminus \mathbb{R}$ we have*

$$\tilde{P}_{\mathcal{H}}(\tilde{A} - z)^{-1}|_{\mathcal{H}} = (T(z) - z)^{-1},$$

with

$$T(z) := \{ \{f, g\} \in S^* : \mathcal{W}(z)b(f, g) = 0 \}.$$

(b) *Let \mathcal{U} be a Q -boundary coefficient with a minimal representation (3.2) and such that for each $z \in \mathbb{C} \setminus \mathbb{R}$ we have*

$$\tilde{P}_{\mathcal{H}}(\tilde{A} - z)^{-1}|_{\mathcal{H}} = (T(z) - z)^{-1},$$

with

$$T(z) = \{ \{f, g\} \in S^* : \mathcal{U}(z)b(f, g) = 0 \}.$$

Then $\tilde{A} \cap \mathcal{H}^2 = \{ \{f, g\} \in S^ : U_0b(f, g) = 0, B_0b(f, g) = 0 \}$ and the operator S_1 is isomorphic to the operator $S_{\mathcal{U}}$ of multiplication by the independent variable in $\mathcal{H}(K_{\mathcal{U}})$.*

(c) For $j = 1, 2$, let \tilde{A}_j be a minimal selfadjoint extension of S in a Hilbert space $\tilde{\mathcal{H}}_j$ and denote by $\tilde{P}_{\mathcal{H}}^j$ the orthogonal projection in $\tilde{\mathcal{H}}_j$ onto \mathcal{H} . The extensions \tilde{A}_j , $j = 1, 2$, are isomorphic under an isomorphism that when restricted to the space \mathcal{H} acts as the identity operator on \mathcal{H} if and only if

$$\tilde{P}_{\mathcal{H}}^1(\tilde{A}_1 - z)^{-1}|_{\mathcal{H}} = \tilde{P}_{\mathcal{H}}^2(\tilde{A}_2 - z)^{-1}|_{\mathcal{H}}.$$

Proof. Let \tilde{A} be a minimal selfadjoint extension of S in the Hilbert space $\tilde{\mathcal{H}}$. Put $\mathcal{H}_1 = \tilde{\mathcal{H}} \ominus \mathcal{H}$, $S_0 = \tilde{A} \cap \mathcal{H}^2$ and $S_1 = \tilde{A} \cap \mathcal{H}_1^2$. By Lemma 5.2 S_1 is a simple closed symmetric operator in \mathcal{H}_1 . Let b_1 be a fixed boundary mapping for S_1 with Gram matrix Q_1 and let $\Psi(z)$ be a fixed holomorphic basis of $\ker(S_1^* - z)$. The relation S_0 is a closed symmetric extension of S . Put $\dim(S_0/S) = \tau$. By Lemma 3.5 there exist a $\tau \times d$ matrix W_0 and, with $\omega = d - 2\tau$, an $\omega \times d$ matrix C_0 of maximal ranks such that

$$W_0 Q^{-1} \begin{pmatrix} W_0 \\ C_0 \end{pmatrix}^* = 0,$$

such that $C_0 Q^{-1} C_0^*$ is invertible and

$$S_0^* = \{ \{f, g\} \in S^* : W_0 b(f, g) = 0 \}. \tag{5.14}$$

The defect index of S_0 is (ω_+, ω_-) , $\omega_{\pm} = d_{\pm} - \tau$ and $c_0 := C_0 b|_{S_0^*}$ is a boundary mapping for S_0 with Gram matrix $P_0 := (C_0 Q^{-1} C_0^*)^{-1}$. The operator \tilde{A} is a canonical selfadjoint extension of $S_0 \oplus S_1$ in $\tilde{\mathcal{H}} = \mathcal{H} \oplus \mathcal{H}_1$ such that $S_0 = \tilde{A} \cap \mathcal{H}^2$ and $S_1 = \tilde{A} \cap \mathcal{H}_1^2$. By Theorem 5.1(a) the defect index of the operator S_1 is (ω_-, ω_+) and by Theorem 5.1(b)

$$\tilde{A} = \left\{ \left\{ \begin{pmatrix} f_0 \\ f_1 \end{pmatrix}, \begin{pmatrix} g_0 \\ g_1 \end{pmatrix} \right\} : \{f_0, g_0\} \in S_0^*, \{f_1, g_1\} \in S_1^*, \right. \\ \left. c_0(f_0, g_0) + \Gamma b_1(f_1, g_1) = 0 \right\}, \tag{5.15}$$

where Γ is a unique invertible $\omega \times \omega$ matrix with $Q_1 + \Gamma^* P_0 \Gamma = 0$.

Put

$$\mathcal{V}(z) := (Q_1 b_1(\widehat{\Psi}(z)))^* \quad \text{and} \quad \mathcal{W}_0(z) := \mathcal{V}(z) \Gamma^{-1}, \quad z \in \mathbb{C} \setminus \mathbb{R}.$$

By Proposition 4.2 $\mathcal{V}(z)$ is a minimal $(-Q_1)$ -boundary coefficient. It follows that $\mathcal{W}_0(z)$ is a minimal P_0 -boundary coefficient. Indeed, the properties (U1), (U2) and (U3') follow from the corresponding properties of $\mathcal{V}(z)$. To show the properties (U4) and (U5) we use the definition of $\mathcal{W}_0(z)$ and $P_0 = -\Gamma^{-*} Q_1 \Gamma^{-1}$ to calculate

$$\begin{aligned} \mathcal{W}_0(z) P_0^{-1} \mathcal{W}_0(w)^* &= \mathcal{V}(z) \Gamma^{-1} (-\Gamma^{-*} Q_1 \Gamma^{-1})^{-1} (\mathcal{V}(w) \Gamma^{-1})^* \\ &= -\mathcal{V}(z) \Gamma^{-1} \Gamma Q_1^{-1} \Gamma^* \Gamma^{-*} \mathcal{V}(w)^* \\ &= -\mathcal{V}(z) Q_1 \mathcal{V}(w)^*. \end{aligned} \tag{5.16}$$

Since $\mathcal{W}(z)$ is a minimal $(-Q_1)$ -boundary coefficient it follows from (5.16) that $\mathcal{W}_0(z)$ has properties (U4) and (U5). Thus, $\mathcal{W}_0(z)$ is a minimal P_0 -boundary coefficient.

Put

$$\mathcal{W}(z) = \begin{pmatrix} W_0 \\ \mathcal{W}_0(z)C_0 \end{pmatrix}.$$

Since

$$\begin{pmatrix} W_0 \\ \mathcal{W}_0(z)C_0 \end{pmatrix} Q^{-1} \begin{pmatrix} W_0 \\ \mathcal{W}_0(w)C_0 \end{pmatrix}^* = \begin{pmatrix} 0 & 0 \\ 0 & \mathcal{W}_0(z)P_0^{-1}\mathcal{W}(w)^* \end{pmatrix}$$

it follows that $\mathcal{W}(z)$ is a Q -boundary coefficient.

We now show that $\mathcal{W}(z)$ has the desired property. It follows from (5.15) that for $z \in \mathbb{C} \setminus \mathbb{R}$,

$$\begin{aligned} \tilde{P}_{\mathcal{H}}(\tilde{A} - z)^{-1}|_{\mathcal{H}} &= \{ \{g_0 - zf_0, f_0\}: \\ &\quad \{f_0, g_0\} \in S_0^*, c_0(f_0, g_0) + \Gamma b_1(f_1, g_1) = 0 \\ &\quad \text{for some } \{f_1, g_1\} \in S_1^* \cap zI \}. \end{aligned} \tag{5.17}$$

The condition on $\{f_0, g_0\} \in S_1^*$ appearing in (5.17), namely,

$$c_0(f_0, g_0) + \Gamma b_1(f_1, g_1) = 0 \quad \text{for some } \{f_1, g_1\} \in S_1^* \cap zI, \tag{5.18}$$

is equivalent to

$$Q_1 \Gamma^{-1} c_0(f_0, g_0) \in \text{ran} (Q_1 b_1(\hat{\Psi}(z))) = \text{ran}(\mathcal{W}(\bar{z})^*) = \text{ran}(\Gamma^* \mathcal{W}_0(\bar{z})^*)$$

or, equivalently,

$$P_0 c_0(f_0, g_0) = -\Gamma^{-*} Q_1 \Gamma^{-1} c_0(f_0, g_0) \in \text{ran}(\mathcal{W}_0(\bar{z})^*). \tag{5.19}$$

Since the P_0 -boundary coefficient $\mathcal{W}_0(z)$ satisfies (U4), (5.19) is equivalent to $\mathcal{W}_0(z)c_0(f_0, g_0) = 0$. Setting

$$T(z) := \{ \{f_0, g_0\} \in S_0^*: \mathcal{W}_0(z)c_0(f_0, g_0) = 0 \}, \tag{5.20}$$

we conclude that

$$\tilde{P}_{\mathcal{H}}(\tilde{A} - z)^{-1}|_{\mathcal{H}} = (T(z) - z)^{-1}.$$

The definitions of c_0 and \mathcal{W} , and (5.14) imply that

$$T(z) = \{ \{f_0, g_0\} \in S^*: \mathcal{W}(z)b(f_0, g_0) = 0 \}.$$

This proves (a).

To prove (b) note that, since $\mathcal{W}_0(z)$ is a minimal P_0 -boundary coefficient, definition (5.20) implies that

$$T(z) \cap T(\bar{z}) = \tilde{A} \cap \mathcal{H}^2 \quad \text{for all } z \in \mathbb{C} \setminus \mathbb{R}.$$

This was also observed in, for example, [12].

Let $\mathcal{U}(z)$ be a Q-boundary coefficient with a minimal representation (3.2) described in Theorem 3.2 and such that

$$T(z) = \{ \{f_0, g_0\} \in S^*: \mathcal{U}(z)b(f_0, g_0) = 0 \}.$$

The properties of the minimal representation (3.2) clearly imply that

$$T(z) = \{ \{f_0, g_0\} \in S^*: U_0b(f_0, g_0) = 0, \mathcal{U}_0(z)B_0b(f_0, g_0) = 0 \}.$$

Since the matrix

$$\begin{pmatrix} \mathcal{U}_0(z) \\ \mathcal{U}_0(\bar{z}) \end{pmatrix}$$

is invertible, for arbitrary $z \in \mathbb{C} \setminus \mathbb{R}$ we have

$$\begin{aligned} S_0 &= \tilde{A} \cap \mathcal{H}^2 \\ &= T(z) \cap T(\bar{z}) \\ &= \{ \{f, g\} \in S^*: U_0b(f, g) = 0, \mathcal{U}_0(z)B_0b(f, g) = 0, \mathcal{U}_0(\bar{z})B_0b(f, g) = 0 \} \\ &= \{ \{f, g\} \in S^*: U_0b(f, g) = 0, B_0b(f, g) = 0 \}. \end{aligned}$$

Since \mathcal{U} and \mathcal{W} are Q-boundary coefficients and since for each $z \in \mathbb{C}^\pm$ we have

$$\begin{aligned} T(z) &= \{ \{f_0, g_0\} \in S^*: \mathcal{W}(z)b(f_0, g_0) = 0 \} \\ &= \{ \{f_0, g_0\} \in S^*: \mathcal{U}(z)b(f_0, g_0) = 0 \}, \end{aligned}$$

that is, $\ker \mathcal{W}(z) = \ker \mathcal{U}(z)$, we conclude that there exists an invertible $d_\pm \times d_\pm$ matrix $\mathcal{A}(z)$ such that $\mathcal{U}(z) = \mathcal{A}(z)\mathcal{W}(z)$. Lemma 4.3 implies that there is an isomorphism from $\mathcal{H}(K_{\mathcal{U}})$ onto $\mathcal{H}(K_{\mathcal{W}})$ and under this isomorphism the operators $S_{\mathcal{U}}$ and $S_{\mathcal{W}}$ of multiplication by the independent variable z coincide. Note that the construction of \mathcal{W} , Lemma 4.3 and the proof of Corollary 4.5 imply that the operators $S_{\mathcal{W}}$ and S_1 are isomorphic. The combination of the last two statements completes the proof of (b).

Statement (c) follows from the theorem that minimal selfadjoint linearizations of the same Straus family are unitarily equivalent (see [11, Theorem 3.3] and [14, Proposition 3.1]). For the reader's convenience we sketch the proof of this result. Assume \tilde{A}_j in the Hilbert space $\tilde{\mathcal{H}}_j$, $j = 1, 2$, are minimal selfadjoint extensions of S in \mathcal{H} , such that

$$\tilde{P}_{\mathcal{H}}^1(\tilde{A}_1 - z)^{-1}|_{\mathcal{H}} = (T(z) - z)^{-1} = \tilde{P}_{\mathcal{H}}^2(\tilde{A}_2 - z)^{-1}|_{\mathcal{H}}, \quad z \in \mathbb{C} \setminus \mathbb{R}.$$

We show there is an isomorphism W from $\tilde{\mathcal{H}}_1$ onto $\tilde{\mathcal{H}}_2$ such that $W|_{\mathcal{H}}$ acts as the identity on \mathcal{H} and W intertwines \tilde{A}_1 and \tilde{A}_2 :

$$\tilde{A}_2 = \{ \{Wf, Wg\}: \{f, g\} \in \tilde{A}_1 \}.$$

Choose $\mu \in \mathbb{C} \setminus \mathbb{R}$. Using the resolvent identity, we obtain for $f, g \in \mathcal{H}$ and $z, w \in \mathbb{C} \setminus \mathbb{R}$,

$$\begin{aligned} & \langle (I + (z - \mu)(\tilde{A}_1 - z)^{-1})f, (I + (w - \mu)(\tilde{A}_1 - w)^{-1})g \rangle_{\tilde{\mathcal{H}}_1} \\ &= \langle f, g \rangle + \frac{(z - \mu)(z - \bar{\mu})}{z - \bar{w}} \langle (T(z) - z)^{-1}f, g \rangle \\ & \quad - \frac{(\bar{w} - \mu)(\bar{w} - \bar{\mu})}{z - \bar{w}} \langle f, (T(w) - w)^{-1}g \rangle \\ &= \langle (I + (z - \mu)(\tilde{A}_2 - z)^{-1})f, (I + (w - \mu)(\tilde{A}_2 - w)^{-1})g \rangle_{\tilde{\mathcal{H}}_2}. \end{aligned}$$

This shows that the relation

$$\text{span} \left\{ \left\{ (I + (z - \mu)(\tilde{A}_1 - z)^{-1})f, (I + (z - \mu)(\tilde{A}_2 - z)^{-1})f \right\} : f \in \mathcal{H}, z \in \mathbb{C} \setminus \mathbb{R} \right\}$$

in $\tilde{\mathcal{H}}_1 \times \tilde{\mathcal{H}}_2$ is isometric and has a dense domain and dense range, because \tilde{A}_1 and \tilde{A}_2 are minimal extensions. Hence, its closure is the graph of a unitary operator W from $\tilde{\mathcal{H}}_1$ onto $\tilde{\mathcal{H}}_2$ with the property

$$\begin{aligned} W[(I + (z - \mu)(\tilde{A}_1 - z)^{-1})f] &= (I + (z - \mu)(\tilde{A}_2 - z)^{-1})f, \\ f \in \mathcal{H}, z \in \mathbb{C} \setminus \mathbb{R}. \end{aligned}$$

In particular, $Wf = f$ for $f \in \mathcal{H}$ (set $z = \mu$) and

$$W[(\tilde{A}_1 - z)^{-1}f] = (\tilde{A}_2 - z)^{-1}f, \quad f \in \mathcal{H}, z \in \mathbb{C} \setminus \mathbb{R}.$$

These equalities and the resolvent identity imply for all $f \in \mathcal{H}$ and all $z, w \in \mathbb{C} \setminus \mathbb{R}$,

$$\begin{aligned} & W[(\tilde{A}_1 - w)^{-1}(I + (z - \mu)(\tilde{A}_1 - z)^{-1})f] \\ &= (\tilde{A}_2 - w)^{-1}[(I + (z - \mu)(\tilde{A}_2 - z)^{-1})f] \\ &= (\tilde{A}_2 - w)^{-1}W[(I + (z - \mu)(\tilde{A}_1 - z)^{-1})f] \end{aligned}$$

and so, by continuity, $W[(\tilde{A}_1 - w)^{-1}h] = (\tilde{A}_2 - w)^{-1}Wh$ for all $h \in \tilde{\mathcal{H}}_1$. From

$$\tilde{A}_j = \{ \{ (\tilde{A}_j - z)^{-1}h, h + z(\tilde{A}_j - z)^{-1}h \} : h \in \tilde{\mathcal{H}}_j \}, \quad j = 1, 2$$

(here the set on the right-hand side is independent of $z \in \mathbb{C} \setminus \mathbb{R}$), it follows that W intertwines \tilde{A}_1 and \tilde{A}_2 . \square

In the following theorem, we consider the following boundary eigenvalue problem.

$$\text{For } h \in \mathcal{H} \text{ find } \{f, g\} \in S^* \text{ with } g - zf = h \text{ and } \mathcal{U}(z)b(f, g) = 0. \quad (5.21)$$

By definition, a linearization of this problem is a selfadjoint extension \tilde{A} of S in $\tilde{\mathcal{H}}$ such that the unique solution of (5.21) for each $z \in \mathbb{C} \setminus \mathbb{R}$ is given by

$$f = \tilde{P}_{\mathcal{H}}(\tilde{A} - z)^{-1}h, \quad g = h + zf.$$

Theorem 5.4. *Let S be a closed symmetric linear relation in a Hilbert space \mathcal{H} with defect index (d_+, d_-) , $d = d_+ + d_- < \infty$, and let b be a boundary mapping for S with Gram matrix Q . Let \mathcal{U} be a Q -boundary coefficient and assume that it has a minimal representation (3.2). Let $S_{\mathcal{U}}$ be the operator of multiplication by the independent variable in the reproducing kernel Hilbert space $\mathcal{H}(K_{\mathcal{U}})$.*

(a) *There exists a boundary mapping $b_{\mathcal{U}}$ for $S_{\mathcal{U}}$ such that*

$$\tilde{A} := \left\{ \left\{ \begin{pmatrix} f \\ f_1 \end{pmatrix}, \begin{pmatrix} g \\ g_1 \end{pmatrix} \right\} : \{f, g\} \in S^*, \{f_1, g_1\} \in S_{\mathcal{U}}^*, \right. \\ \left. U_0b(f, g) = 0, B_0b(f, g) + b_{\mathcal{U}}(f_1, g_1) = 0 \right\}$$

is a minimal linearization of the boundary eigenvalue problem (5.21). The matrix $-(B_0Q^{-1}B_0^)^{-1}$ is Gram matrix of $b_{\mathcal{U}}$.*

(b) *If b_2 is an arbitrary boundary mapping for $S_{\mathcal{U}}$ with Gram matrix Q_2 , then there exists a unique $\omega \times \omega$ matrix Γ such that $Q_2 + \Gamma^*(B_0Q^{-1}B_0^*)^{-1}\Gamma = 0$ and*

$$\tilde{A} = \left\{ \left\{ \begin{pmatrix} f \\ f_1 \end{pmatrix}, \begin{pmatrix} g \\ g_1 \end{pmatrix} \right\} : \{f, g\} \in S^*, \{f_1, g_1\} \in S_{\mathcal{U}}^*, \right. \\ \left. U_0b(f, g) = 0, B_0b(f, g) + \Gamma b_2(f_1, g_1) = 0 \right\}.$$

(c) *Any minimal linearization of (5.21) is isomorphic to \tilde{A} , under an isomorphism that when restricted to the space \mathcal{H} acts as the identity operator on \mathcal{H} .*

Proof. Let S be a closed symmetric linear relation with the defect index (d_+, d_-) and let $d = d_+ + d_-$. Let $b : S^* \rightarrow \mathbb{C}^d$ be a boundary mapping for S with Gram matrix Q . Let $\mathcal{U}(z)$ be a Q -boundary coefficient with a minimal representation (3.2) described in Theorem 3.2. Further on in this proof we use the notation and results of Theorem 3.2. Let $S_0^* := \{\{f, g\} \in S^* : U_0b(f, g) = 0\}$. Then Lemma 3.5 implies that $S_0 = \{\{f, g\} \in S^* : U_0b(f, g) = 0, B_0b(f, g) = 0\}$, S_0 is a closed linear symmetric extension of S with defect index (ω_+, ω_-) and $\dim(S_0/S) = \tau$. Note that $B_0b|_{S_0^*}$ is a boundary mapping for S_0 with Gram matrix $(B_0Q^{-1}B_0^*)^{-1}$. By Theorem 4.4(b) we can choose a boundary mapping $b_{\mathcal{U}}$ for the operator $S_{\mathcal{U}}$ with Gram matrix $-(B_0Q^{-1}B_0^*)^{-1}$ and a holomorphic basis $\Phi(z)$ for $\ker(S_{\mathcal{U}}^* - z)$, $z \in \mathbb{C} \setminus \mathbb{R}$, in such a way that

$$\mathcal{U}_0(z) = \left(- (B_0Q^{-1}B_0^*)^{-1}b_{\mathcal{U}}(\widehat{\Phi}(\bar{z})) \right)^*.$$

We now can define \tilde{A} as given in the theorem:

$$\tilde{A} := \left\{ \left\{ \begin{pmatrix} f \\ f_1 \end{pmatrix}, \begin{pmatrix} g \\ g_1 \end{pmatrix} \right\} : \{f, g\} \in S^*, \{f_1, g_1\} \in S_{\mathcal{U}}^*, \right. \\ \left. \begin{aligned} &U_0b(f, g) = 0, B_0b(f, g) + b_{\mathcal{U}}(f_1, g_1) = 0 \end{aligned} \right\}.$$

It follows from Theorem 5.1(b) that \tilde{A} is a canonical selfadjoint extension of $S_0 \oplus S_{\mathcal{U}}$ in $\mathcal{H} \oplus \mathcal{H}(K_{\mathcal{U}})$ such that $\tilde{A} \cap \mathcal{H}^2 = S_0$ and $\tilde{A} \cap \mathcal{H}(K_{\mathcal{U}})^2 = S_{\mathcal{U}}$. Thus, \tilde{A} is an extension of S . Since by Theorem 4.4(a) the operator $S_{\mathcal{U}}$ is simple, Lemma 5.2 implies that \tilde{A} is a minimal selfadjoint extension of S . As in the proof of part (a) of Theorem 5.3 we have

$$\tilde{P}_{\mathcal{H}}(\tilde{A} - z)^{-1}|_{\mathcal{H}} = \{ \{g - zf, f\} : \{f, g\} \in S^*, U_0b(f, g) = 0 \\ B_0b(f, g) + b_{\mathcal{U}}(f_1, g_1) = 0 \\ \text{for some } \{f_1, g_1\} \in S_{\mathcal{U}}^* \cap zI \}.$$

Because of the special choice of the boundary mapping $b_{\mathcal{U}}$ and a holomorphic basis $\Phi(z)$ for $\ker(S_{\mathcal{U}}^* - z)$, as in the proof of the part (a) of Theorem 5.3, we conclude that

$$B_0b(f, g) + b_{\mathcal{U}}(f_1, g_1) = 0 \quad \text{for some } \{f_1, g_1\} \in S_{\mathcal{U}}^* \cap zI \tag{5.22}$$

is equivalent to $\mathcal{U}_0(z)B_0b(f, g) = 0$. Letting

$$T(z) := \{ \{f, g\} \in S^* : U_0b(f, g) = 0, \mathcal{U}_0(z)B_0b(f, g) = 0 \},$$

again as in the proof of (a) in Theorem 5.3, we conclude that

$$\tilde{P}_{\mathcal{H}}(\tilde{A} - z)^{-1}|_{\mathcal{H}} = (T(z) - z)^{-1}.$$

Theorem 3.2 yields that

$$T(z) = \{ \{f, g\} \in S^* : \mathcal{U}(z)b(f, g) = 0 \}.$$

Thus, \tilde{A} is a linearization of the boundary eigenvalue problem (5.21). This proves (a).

We now prove (b). Let b_2 be an arbitrary boundary mapping for $S_{\mathcal{U}}$ with Gram matrix Q_2 . Since the operator \tilde{A} is a canonical selfadjoint extension of $S_0 \oplus S_{\mathcal{U}}$, Theorem 5.1(b) applied to the boundary mappings b_0 , with Gram matrix $(B_0Q^{-1}B_0^*)^{-1}$, and b_2 implies that there exists a unique $\omega \times \omega$ matrix Γ such that $Q_2 + \Gamma^*(B_0Q^{-1}B_0^*)^{-1}\Gamma = 0$ and

$$\tilde{A} = \left\{ \left\{ \begin{pmatrix} f_0 \\ f_1 \end{pmatrix}, \begin{pmatrix} g_0 \\ g_1 \end{pmatrix} \right\} : \{f_0, g_0\} \in S_0^*, \{f_1, g_1\} \in S_{\mathcal{U}}^*, \right. \\ \left. b_0(f_0, g_0) + \Gamma b_2(f_1, g_1) = 0 \right\}$$

$$= \left\{ \left\{ \begin{pmatrix} f \\ f_1 \end{pmatrix}, \begin{pmatrix} g \\ g_1 \end{pmatrix} \right\} : \{f, g\} \in S^*, \{f_1, g_1\} \in S_{\mathcal{H}}^*, \right. \\ \left. \cup_0 b(f, g) = 0, B_0 b(f, g) + \Gamma b_2(f_1, g_1) = 0 \right\}.$$

Statement (c) follows from Theorem 5.3(c). \square

Appendix A. Extension theory in a Krein space environment

In this section, we study neutral subspaces of a Krein space $(\mathcal{H}, [\cdot, \cdot])$. The discussion at the beginning of Section 3 shows that the neutral subspaces of a Krein space are surrogate symmetric relations in a Hilbert space. In this section, we use Krein space terminology and notation. For similar results in symplectic language; see [16]; Table 1 is the dictionary.

First we describe a special Krein space in which the extension theory can be formulated using Krein space geometry. This idea goes back at least to Šmuljan [24]. Let $(\mathcal{H}, \langle \cdot, \cdot \rangle)$ be a Hilbert space. Then the Cartesian product \mathcal{H}^2 endowed with the indefinite product

$$[[\{x, y\}, \{u, v\}]] = \frac{1}{i}(\langle y, u \rangle - \langle x, v \rangle)$$

is a Krein space. Let $\text{Im}(\mu) > 0$. Then for arbitrary $\{x, \mu x\} \in \mu I$ we have

$$[[\{x, \mu x\}, \{x, \mu x\}]] = \frac{1}{i}(\langle \mu x, x \rangle - \langle x, \mu x \rangle) = 2\text{Im}(\mu)\langle x, x \rangle.$$

Thus, μI is a uniformly positive subspace of $(\mathcal{H}^2, [[\cdot, \cdot]])$. Similarly, $\overline{\mu} I$ is a uniformly negative subspace of $(\mathcal{H}^2, [[\cdot, \cdot]])$. The subspaces μI and $\overline{\mu} I$ are mutually orthogonal in $(\mathcal{H}^2, [[\cdot, \cdot]])$ and a simple calculation shows that $\mathcal{H}^2 = \mu I [+] \overline{\mu} I$ is a fundamental decomposition of $(\mathcal{H}^2, [[\cdot, \cdot]])$. The fundamental symmetry J_μ corresponding to this decomposition is given by (4.8). A linear relation is a closed subspace of \mathcal{H}^2 . The adjoint S^* of a linear relation S in \mathcal{H} is the orthogonal complement of S in $(\mathcal{H}^2, [[\cdot, \cdot]])$: $S^* = S^{\perp[[\cdot, \cdot]]}$. A relation S is symmetric if and only if S is a neutral subspace of $(\mathcal{H}^2, [[\cdot, \cdot]])$, that is, if $S \subset S^{\perp[[\cdot, \cdot]]}$. von Neumann’s formula is the following result about neutral subspaces of a general Krein space $(\mathcal{H}, [\cdot, \cdot])$.

Table 1

Relations in a Hilbert space \mathcal{H}	Subspaces of a Krein space \mathcal{H}^2
Adjoint	Orthogonal complement
Symmetric	Neutral
Selfadjoint	Equal to its orthogonal complement

Proposition A.1 (Generalized von Neumann’s formula). *Let $\mathcal{K} = \mathcal{K}_+[\dot{+}]\mathcal{K}_-$ be an arbitrary fundamental decomposition of a Krein space $(\mathcal{K}, [\cdot, \cdot])$. Let \mathcal{S} be a closed neutral subspace of $(\mathcal{K}, [\cdot, \cdot])$. Then*

$$\mathcal{S}^{[\perp]} = \mathcal{S}[\dot{+}](\mathcal{S}^{[\perp]} \cap \mathcal{K}_+)[\dot{+}](\mathcal{S}^{[\perp]} \cap \mathcal{K}_-). \tag{A.1}$$

Proof. Let J be the fundamental symmetry corresponding to $\mathcal{K} = \mathcal{K}_+[\dot{+}]\mathcal{K}_-$, let $P_{\pm} = \frac{1}{2}(I \pm J)$ be the orthogonal projection onto \mathcal{K}_{\pm} and let $\langle x, y \rangle = [Jx, y]$, $x, y \in \mathcal{K}$, be the corresponding Hilbert space inner product. For an arbitrary subspace \mathcal{L} of \mathcal{K} it is straightforward to verify that $J\mathcal{L} + \mathcal{L} = P_+\mathcal{L}[\dot{+}]P_-\mathcal{L}$. Since \mathcal{S} is a neutral subspace we have that $[P_+x, P_+y] = -[P_-x, P_-y]$ and therefore $\langle x, y \rangle = \pm 2[P_{\pm}x, P_{\pm}y] = 2\langle P_{\pm}x, P_{\pm}y \rangle$ for all $x, y \in \mathcal{S}$. Thus, $\frac{1}{\sqrt{2}}P_{\pm}|_{\mathcal{S}}$ is a unitary operator from $(\mathcal{S}, \langle \cdot, \cdot \rangle)$ to $(P_{\pm}(\mathcal{S}), \pm[\cdot, \cdot])$. Consequently, $P_{\pm}(\mathcal{S})$ is a closed subspace of \mathcal{K}_{\pm} . Denote by \mathcal{T}_{\pm} the orthogonal complement of $P_{\pm}(\mathcal{S})$ in $(\mathcal{K}_{\pm}, \pm[\cdot, \cdot])$. Since $0 = [P_{\pm}(\mathcal{S}), \mathcal{T}_{\pm}] = [\mathcal{S}, \mathcal{T}_{\pm}]$, it follows that $\mathcal{T}_{\pm} \subset \mathcal{S}^{[\perp]}$. Moreover, $\mathcal{T}_{\pm} = \mathcal{S}^{[\perp]} \cap \mathcal{K}_{\pm}$. Indeed, \subset is clear and if $x \in \mathcal{S}^{[\perp]} \cap \mathcal{K}_{\pm}$, then $[P_{\pm}(\mathcal{S}), x] = [\mathcal{S}, x] = 0$, which implies $x \in \mathcal{T}_{\pm}$. Thus, (A.1) can be restated as

$$\mathcal{S}^{[\perp]} = \mathcal{S}[\dot{+}]\mathcal{T}_+[\dot{+}]\mathcal{T}_-. \tag{A.2}$$

Clearly, $\mathcal{T}_+[\dot{+}]\mathcal{T}_- = (P_+(\mathcal{S})[\dot{+}]P_-(\mathcal{S}))^{[\perp]} = (J\mathcal{S}[\dot{+}]\mathcal{S})^{[\perp]}$. Therefore, (A.2) is equivalent to $\mathcal{S} = \mathcal{S}^{[\perp]} \cap (J\mathcal{S}[\dot{+}]\mathcal{S})$. As \mathcal{S} is neutral, $\mathcal{S} \subset \mathcal{S}^{[\perp]}$ and therefore $\mathcal{S} \subset \mathcal{S}^{[\perp]} \cap (J\mathcal{S}[\dot{+}]\mathcal{S})$. Since $\mathcal{S}^{[\perp]} = (J\mathcal{S})^{(\perp)}$, we have $J\mathcal{S} \cap \mathcal{S}^{[\perp]} = \{0\}$, and therefore $\mathcal{S}^{[\perp]} \cap (J\mathcal{S}[\dot{+}]\mathcal{S}) = \mathcal{S}$. This proves Proposition A.1. \square

The next proposition is an alternative way of stating von Neumann’s formula in which an emphasis is given to orthogonal complements of neutral subspaces.

Proposition A.2. *Let $(\mathcal{K}, [\cdot, \cdot])$ be a Krein space. Let \mathcal{L} be a closed subspace of $(\mathcal{K}, [\cdot, \cdot])$ and let $\mathcal{L}_0 := \mathcal{L} \cap \mathcal{L}^{[\perp]}$ be its isotropic part. Then $\mathcal{L}^{[\perp]}$ is a neutral subspace of \mathcal{K} if and only if there exists a fundamental symmetry J of \mathcal{K} with the corresponding fundamental decomposition $\mathcal{K} = \mathcal{K}_+[\dot{+}]\mathcal{K}_-$ such that*

$$\mathcal{L} = \mathcal{L}_0[\dot{+}](\mathcal{L} \cap \mathcal{K}_+)[\dot{+}](\mathcal{L} \cap \mathcal{K}_-) \quad \text{and} \quad J\mathcal{L} + \mathcal{L} = \mathcal{K}. \tag{A.3}$$

If (A.3) holds for one fundamental decomposition, then it holds for every fundamental decomposition.

Proof. Assume that $\mathcal{L}^{[\perp]}$ is a neutral subspace. Then $\mathcal{L}^{[\perp]} = \mathcal{L}_0$ and Proposition A.1 implies that the first equality in (A.3) holds for an arbitrary fundamental decomposition J . It follows from the proof of Proposition A.1 that $J\mathcal{L}_0[\dot{+}]\mathcal{L}_0 = P_+\mathcal{L}_0[\dot{+}]P_-\mathcal{L}_0$ is the orthogonal complement in $(\mathcal{K}, [\cdot, \cdot])$ of the regular subspace $(\mathcal{L} \cap \mathcal{K}_+)[\dot{+}](\mathcal{L} \cap \mathcal{K}_-)$, which corresponds to $\mathcal{T}_+[\dot{+}]\mathcal{T}_-$ in Proposition A.1. Therefore,

$$(J\mathcal{L}_0[\dot{+}]\mathcal{L}_0)[\dot{+}](\mathcal{L} \cap \mathcal{K}_+)[\dot{+}](\mathcal{L} \cap \mathcal{K}_-) = \mathcal{K}. \tag{A.4}$$

Since $\mathcal{L}_0 \subset \mathcal{L}$ we have $J\mathcal{L} + \mathcal{L} = (J\mathcal{L}_0 \dot{+} \mathcal{L}_0)[\dot{+}](\mathcal{L} \cap \mathcal{K}_+)[\dot{+}](\mathcal{L} \cap \mathcal{K}_-) = \mathcal{K}$.

Now assume that (A.3) holds for a fundamental symmetry J of \mathcal{K} and the corresponding fundamental decomposition $\mathcal{K} = \mathcal{K}_+[\dot{+}]\mathcal{K}_-$. Clearly, (A.3) implies (A.4). Let \mathcal{L}' denote the orthogonal complement of \mathcal{L}_0 in the Krein space $(J\mathcal{L}_0 \dot{+} \mathcal{L}_0, [\cdot, \cdot])$. Then (A.4) yields

$$\mathcal{L}'_0^{[\perp]} = \mathcal{L}'[\dot{+}](\mathcal{L} \cap \mathcal{K}_+)[\dot{+}](\mathcal{L} \cap \mathcal{K}_-). \quad (\text{A.5})$$

Since \mathcal{L}_0 is a maximal neutral subspace of $J\mathcal{L}_0 \dot{+} \mathcal{L}_0$, it follows that $\mathcal{L}' = \mathcal{L}_0$. Consequently, (A.5) and (A.3) imply $\mathcal{L}'_0^{[\perp]} = \mathcal{L}$. Therefore, $\mathcal{L}^{[\perp]} = \mathcal{L}_0$ is a neutral subspace of $(\mathcal{K}, [\cdot, \cdot])$. \square

It follows from von Neumann's formula (A.1) that the factor space $S^{[\perp]}/S$ is a Krein space. Since $S \cap \mathcal{K}_\pm = \{0\}$, the Krein space $S^{[\perp]}/S$ can be identified with $(S^{[\perp]} \cap \mathcal{K}_+)[\dot{+}](S^{[\perp]} \cap \mathcal{K}_-)$. Consequently, the numbers $\dim(S^{[\perp]} \cap \mathcal{K}_+)$ and $\dim(S^{[\perp]} \cap \mathcal{K}_-)$ do not depend on the choice of the fundamental decomposition $\mathcal{K}_+[\dot{+}]\mathcal{K}_-$.

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