On the negative squares of a class of self-adjoint extensions in Krein spaces

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A description of all exit space extensions with finitely many negative squares of a symmetric operator of defect one is given via Krein's formula. As one of the main results an exact characterization of the number of negative squares in terms of a fixed canonical extension and the behaviour of a function τ (that determines the exit space extension in Krein's formula) at zero and at infinity is obtained. To this end the class of matrix valued $\mathcal{D}_\kappa^{n\times n}$-functions is introduced and, in particular, the properties of the inverse of a certain $\mathcal{D}_\kappa^{2\times 2}$-function which is closely connected with the spectral properties of the exit space extensions with finitely many negative squares is investigated in detail. Among the main tools here are the analytic characterization of the degree of non-positivity of generalized poles of matrix valued generalized Nevanlinna functions and some extensions of recent factorization results.

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1 Introduction

It is a common feature in the theory of symmetric and self-adjoint operators that many spectral properties of the given operators are described in terms of locally analytic functions and their behavior close to singularities. For example, if $\widetilde{A}$ is a fixed self-adjoint extension of a closed simple symmetric A operator with defect one in a Hilbert space $\mathcal{K}$, then the corresponding Weyl function (or Q-function) $m : \mathbb{C}\backslash\mathbb{R} \to \mathbb{C}$ can be used to describe the spectrum of $\widetilde{A}$. Furthermore, the spectral properties of the self-adjoint extensions A_τ of A, labeled by a real parameter τ in Krein's formula for canonical extensions,

$$(A_\tau - \lambda)^{-1} = (\widetilde{A} - \lambda)^{-1} - \frac{1}{m(\lambda) + \tau}(\cdot, \varphi_{\overline{\lambda}})\varphi_\lambda, \qquad \lambda \in \rho(A_\tau) \cap \rho(\widetilde{A}),$$

where $\varphi_\lambda \in \ker\,(A^* - \lambda)$, are encoded in the functions

$$\lambda \mapsto -\frac{1}{m(\lambda) + \tau}.$$

When considering self-adjoint extensions $\widetilde{A}$ of A that act in larger Hilbert, Pontryagin or Krein spaces $\mathcal{K} \times \mathcal{H}$ the parameter τ in Krein's formula itself is a function. However, for the spectral analysis of these self-adjoint extensions it is not sufficient to consider the function $\lambda \mapsto -(m(\lambda) + \tau(\lambda))^{-1}$, as Krein's formula might suggest. Instead, it is necessary to investigate the structure of the singularities of the 2×2-matrix function

$$\widetilde{M}(\lambda) := -\begin{pmatrix} m(\lambda) & -1 \\ -1 & -\tau(\lambda)^{-1} \end{pmatrix}^{-1} = \frac{\tau(\lambda)}{m(\lambda) + \tau(\lambda)} \begin{pmatrix} -\tau(\lambda)^{-1} & 1 \\ 1 & m(\lambda) \end{pmatrix} \tag{1.1}$$

which, roughly speaking, can be viewed as a Weyl function (or Q-function) corresponding to the fixed self-adjoint extension $\widetilde{A}$ in $\mathcal{K} \times \mathcal{H}$.

The structure of the exit space $\mathcal{H}$ determines the properties of the function τ in Krein's formula and vice versa, e.g., a Hilbert or Pontryagin space will lead to a Nevanlinna or generalized Nevanlinna function, whereas a Krein space will lead to more general classes of locally meromorphic functions. The self-adjoint extensions in $\mathcal{K} \times \mathcal{H}$ in Krein's formula can also be regarded as linearizations or solution operators of certain boundary value problems in $\mathcal{K}$ with the function τ appearing in an eigenparameter dependent boundary condition. In this connection, functions of the form (1.1) have frequently appeared in the literature, see, e.g., [28, 30, 32, 33] for problems involving Sturm-Liouville operators and Hamiltonian systems, and [3, 6, 22, 24] for more abstract situations. As a concrete example one might think of a Sturm-Liouville problem of the form

$$-f'' + qf = r\lambda f \qquad \text{and} \qquad \tau(\lambda)f(0) = f'(0) \tag{1.2}$$

in $\mathcal{K} = L^2(\mathbb{R}^+)$, where q and $r > 0$ are real valued bounded functions, and $\tau : \mathbb{C}\backslash\mathbb{R} \to \mathbb{C}$ is locally meromorphic and symmetric with respect to $\mathbb{R}$. Then m can be identified with the usual Titchmarsh-Weyl coefficient, which under the above assumptions belongs to the class of Nevanlinna functions. The solvability properties of (1.2) are then encoded in the spectral structure of a self-adjoint operator in $L^2(\mathbb{R}^+) \times \mathcal{H}$ determined via Krein's formula as well as in the singularities of the function (1.1).

The main objective of the present paper is the investigation of a certain class of functions of the form (1.1) and the spectral structure of the corresponding self-adjoint exit space extension in Krein's formula in an indefinite setting. More precisely, our main interest is on functions m and τ belonging to the classes $\mathcal{D}_\kappa$, $\kappa \in \mathbb{N}_0$, introduced and studied in the scalar case in [9, 10, 11] in connection with indefinite Sturm-Liouville problems. Recall that a scalar function M belongs to the class $\mathcal{D}_\kappa$ if for some point λ_0 of holomorphy of M there exists a generalized Nevanlinna function $Q \in \mathcal{N}_\kappa$ holomorphic in λ_0 and a rational function G symmetric with respect to the real axis and holomorphic in $\overline{\mathbb{C}}\backslash\{\lambda_0, \overline{\lambda}_0\}$ such that

$$\frac{\lambda}{(\lambda - \lambda_0)(\lambda - \overline{\lambda}_0)} M(\lambda) = Q(\lambda) + G(\lambda);$$

cf. Definition 4.1. The classes $\mathcal{D}_\kappa$ are subclasses of the so-called definitizable functions which were comprehensively studied in [36, 37]. In particular, the general results in [37] imply that the functions from the class $\mathcal{D}_\kappa$ are connected with self-adjoint operators and relations with κ negative squares in Krein spaces in the same way as, e.g., Nevanlinna and generalized Nevanlinna functions are connected with self-adjoint operators and relations in Hilbert and Pontryagin spaces, respectively, see, e.g., [35, 41]. In other words, every function from the class $\mathcal{D}_\kappa$ admits a minimal representation

$$M(\lambda) = \operatorname{Re} M(\lambda_0) + \big[\big((\lambda - \operatorname{Re}\lambda_0) + (\lambda-\lambda_0)(\lambda-\overline{\lambda}_0)(A_0-\lambda)^{-1}\big)\gamma_{\lambda_0}, \gamma_{\lambda_0}\big]$$

via the resolvent of a self-adjoint operator (or relation) A_0 in a Krein space $(\mathcal{K}, [\cdot,\cdot])$ such that the Hermitian form $[A_0\cdot,\cdot]$ has κ negative squares. Here λ_0 is a fixed point in the domain of holomorphy of M and $\gamma_{\lambda_0} \in \mathcal{K}$. We mention that the class of self-adjoint operators with non-empty resolvent set and κ negative squares consists of operators which allow a rich spectral theory: There exists a spectral function with singularities and the non-real spectrum consists of at most κ pairs, symmetric with respect to the real line, see [43, 45] and, e.g., [11, Theorem 3.1].

The present paper is divided into two separate parts which are both of interest on their own: Part I deals with matrix valued $\mathcal{D}_\kappa$-functions and Part II is devoted to extensions of symmetric operators in Krein spaces and the number of their negative squares. In Part I the matrix valued analogue $\mathcal{D}_\kappa^{n\times n}$ of the classes $\mathcal{D}_\kappa$ are introduced and the answer for the following problem is found: Given scalar functions $m \in \mathcal{D}_{\kappa_m}$ and $\tau \in \mathcal{D}_{\kappa_\tau}$ describe $\widetilde{\kappa} \in \mathbb{N}_0$ such that the 2×2-matrix function $\widetilde{M}$ in (1.1) belongs to the class $\mathcal{D}_{\widetilde{\kappa}}^{2\times 2}$. It turns out in Theorem 4.5 that the index $\widetilde{\kappa}$ differs at most by one of the sum $\kappa_m + \kappa_\tau$ and the exact value of $\widetilde{\kappa}$ is determined in terms of the limiting behavior of the functions m and τ at the point 0 and ∞. For the special case that τ is a real constant this description can already be found in [11]. We point out that the solution of this seemingly simple problem does not only involve a sophisticated machinery of technical tools and nontrivial recent results from the theory of matrix valued generalized Nevanlinna functions, e.g., the purely analytic characterization of the degree of non-positivity for matrix valued generalized Nevanlinna functions from [48]; cf. Definition 2.13 and Theorem 2.15, but also requires an extension of certain factorization results for matrix valued generalized Nevanlinna functions from [48] and recent results on functions of the form (1.1) from [6].

Part II of this paper contains a variant of Krein's formula for the self-adjoint extensions $\widetilde{A}$ in $\mathcal{K}\times\mathcal{H}$ of a symmetric operator with finitely many negative squares and defect one in a Krein space $\mathcal{K}$. Here $\mathcal{H}$ is also allowed to be a Krein space and we give a parametrization of all extension $\widetilde{A}$ that also have finitely many negative squares. We remark that various other variants of the Krein-Naimark formula in an indefinite setting can be found in the literature. The case that A is a symmetric operator in a Pontryagin space $\mathcal{K}$ and $\mathcal{H}$ is a Hilbert space was investigated by M.G. Krein and H. Langer in [38]. Later V.A. Derkach considered both $\mathcal{K}$ and $\mathcal{H}$ to be Pontryagin or even Krein spaces; cf. [17, 18, 19, 20], other variants of (1.3) were proved in, e.g., [5, 7, 25, 27, 44].

For the purpose of the second part of the paper the abstract concept of boundary triplets and associated Weyl functions is a convenient tool. A boundary triplet $\{\mathbb{C}, \Gamma_0, \Gamma_1\}$ for a symmetric operator A of defect one consists of two linear mappings Γ_0, Γ_1 defined on the adjoint A^+ that satisfy an abstract Lagrange identity and a maximality condition, see Section 5 for details. Associated to $\{\mathbb{C}, \Gamma_0, \Gamma_1\}$ is the so-called Weyl function which is the abstract analog of the Titchmarsh-Weyl function from singular Sturm-Liouville theory. Denote by A_0 the self-adjoint restriction of A^+ onto $\ker \Gamma_0$ and let γ and m be the γ-field and Weyl function associated to $\{\mathbb{C}, \Gamma_0, \Gamma_1\}$. In Section 7 it will be shown that the formula

$$P_{\mathcal{K}}(\widetilde{A}-\lambda)^{-1}|_{\mathcal{K}} = (A_0-\lambda)^{-1} - \gamma(\lambda)\big(m(\lambda)+\tau(\lambda)\big)^{-1}\gamma(\overline{\lambda})^* \tag{1.3}$$

establishes a bijective correspondence between the compressed resolvents of minimal self-adjoint exit space extensions $\widetilde{A}$ of A that have finitely many negative squares and the functions τ belonging to the class $\bigcup_{\kappa\in\mathbb{N}_0} \mathcal{D}_\kappa \cup \{\infty\}$; see also [9]. Based on the coupling method from [22] and some technical tools from extension theory of symmetric operators in Krein spaces provided in Section 6 we show that $\widetilde{A}$ in (1.3) is the minimal representing operator or relation of the function $\widetilde{M}$ in (1.1), where now m is the Weyl function of the fixed boundary triplet $\{\mathbb{C}, \Gamma_0, \Gamma_1\}$ and τ is the parameter function in (1.3). The main result of the second part of the paper is now a consequence of this observation, Krein's formula and Theorem 4.5 from the first part of the paper: we obtain an exact characterization of the number of negative squares of $\widetilde{A}$ in (1.3) in terms of the negative index of the functions m and τ and the limiting behavior of the functions m and τ at the points 0 and ∞. This result can be regarded as generalization and improvement of [19] and earlier results by two of the authors in [9]. Moreover, this result can be applied to eigenparameter dependent boundary value problems. E.g., for Sturm-Liouville problems of the form (1.2) involving also a (possibly) indefinite weight function r and a function $\tau \in \mathcal{D}_{\kappa_\tau}$ in the boundary condition, sharp estimates for the number of non-real solutions can be easily obtained.

Part I. Generalized Nevanlinna and $\mathcal{D}_\kappa$-functions

In the first part of this paper we recall the notion of matrix valued generalized Nevanlinna functions. We present results from [48] which allow to retrieve the index κ of a given generalized Nevanlinna function in a purely analytic manner. Thereafter, we introduce the main class of functions under consideration: The class of matrix valued $\mathcal{D}_\kappa$-functions. These functions, multiplied with a simple rational function, allow a representation as the sum of a generalized Nevanlinna function and a simple rational term. The main result of the first part is Theorem 4.5; it provides an exact description of the index κ of the inverses of a special class of $\mathcal{D}_\kappa$-functions with 2×2 matrices as values.

2 Matrix valued generalized Nevanlinna functions

By $\mathbb{C}^+$ and $\mathbb{C}^-$ we denote the open upper and lower half plane, respectively. For the extended real line and the extended complex plane we write $\overline{\mathbb{R}}$ and $\overline{\mathbb{C}}$, respectively. We use the notation $\mathbb{N}=\{1,2,3,\dots\}$ and $\mathbb{N}_0=\{0,1,2,3,\dots\}$. Let $n\in\mathbb{N}$ and let Q be a matrix function with values in $\mathbb{C}^{n\times n}$ which is piecewise meromorphic in $\mathbb{C}\backslash\mathbb{R}$. The union of all points of holomorphy of Q in $\mathbb{C}\backslash\mathbb{R}$ and all points $\lambda\in\overline{\mathbb{R}}$ such that Q can be analytically continued to λ such that the continuations from $\mathbb{C}^+$ and $\mathbb{C}^-$ coincide is denoted by $\mathfrak{h}(Q)$. The $n\times n$-matrix function Q is said to be *symmetric* with respect to the real axis if $Q(\overline{\lambda})^*=Q(\lambda)$ holds for all $\lambda\in\mathfrak{h}(Q)$.

We recall the notion of generalized Nevanlinna functions which were introduced in [41, 42].

Definition 2.1 A matrix function Q with values in $\mathbb{C}^{n\times n}$ belongs to the *generalized Nevanlinna class* $\mathcal{N}_\kappa^{n\times n}$, if it is piecewise meromorphic in $\mathbb{C}\backslash\mathbb{R}$, symmetric with respect to the real axis and the kernel

$$N_Q(\lambda,w):=\frac{Q(\lambda)-Q(w)^*}{\lambda-\overline{w}},\qquad \lambda,w\in\mathfrak{h}(Q)\cap\mathbb{C}^+,$$

has $\kappa\in\mathbb{N}_0$ negative squares, that is, for any $N\in\mathbb{N}$, $\lambda_1,\dots,\lambda_N\in\mathfrak{h}(Q)\cap\mathbb{C}^+$ and $\vec{x}_1,\dots,\vec{x}_N\in\mathbb{C}^n$ the Hermitian matrix

$$\big(N_Q(\lambda_i,\lambda_j)\vec{x}_i,\vec{x}_j\big)_{i,j=1}^N$$

has at most κ negative eigenvalues, and κ is minimal with this property. The number κ of the generalized Nevanlinna class $\mathcal{N}_\kappa^{n\times n}$ is called *negative index*. The functions in the class $\mathcal{N}_0^{n\times n}$ are called *Nevanlinna functions*. For scalar functions we write $\mathcal{N}_\kappa$ instead of $\mathcal{N}_\kappa^{1\times 1}$.

It is a simple consequence of Definition 2.1 that $\mathcal{N}_\kappa^{n\times n}$ is closed under the following transformations.

Lemma 2.2 *Let $Q\in\mathcal{N}_\kappa^{n\times n}$. Then the function $\lambda\mapsto Q(-\frac{1}{\lambda})$ belongs to the same class $\mathcal{N}_\kappa^{n\times n}$. Furthermore, if $\det Q(\lambda_0)\neq 0$ for some $\lambda_0\in\mathfrak{h}(Q)\setminus\{\infty\}$, then also $\lambda\mapsto -Q(\lambda)^{-1}$ belongs to $\mathcal{N}_\kappa^{n\times n}$.*

It is well known that every rational function which is symmetric with respect to the real axis belongs to some generalized Nevanlinna class and that the sum Q_1+Q_2 of the generalized Nevanlinna functions $Q_1\in\mathcal{N}_{\kappa_1}^{n\times n}$ and $Q_2\in\mathcal{N}_{\kappa_2}^{n\times n}$ belongs to some generalized Nevanlinna class $\mathcal{N}_{\kappa'}^{n\times n}$, where $\kappa'\leq\kappa_1+\kappa_2$, see, e.g. [41]. In the next lemma we recall that the multiplication of a generalized Nevanlinna function with a rational function is again a generalized Nevanlinna function, only the negative index may change.

Lemma 2.3 *Let $Q \in \mathcal{N}_\kappa^{n\times n}$ and assume that r is a rational function with values in $\mathbb{C}^{n\times n}$. Then the function*

$$\lambda \mapsto Q_1(\lambda) := r(\overline{\lambda})^* Q(\lambda) r(\lambda)$$

belongs to $\mathcal{N}_{\kappa_1}^{n\times n}$ for some $\kappa_1 \in \mathbb{N}_0$.

P r o o f. It is clear that Q_1 is piecewise meromorphic in $\mathbb{C}\backslash\mathbb{R}$ and that $Q_1(\overline{\lambda})^* = Q_1(\lambda)$ holds for all $\lambda \in \mathfrak{h}(Q_1)$. Furthermore, the kernel N_{Q_1} can be rewritten as

$$N_{Q_1}(\lambda, w) = \frac{Q_1(\lambda) - Q_1(w)^*}{\lambda - \overline{w}} = \frac{r(\overline{\lambda})^* Q(\lambda) r(\lambda) - r(w)^* Q(\overline{w}) r(\overline{w})}{\lambda - \overline{w}} =$$

$$r(w)^* \frac{Q(\lambda) - Q(\overline{w})}{\lambda - \overline{w}} r(\lambda) + (I, r(w)^* Q(\overline{w})) \begin{pmatrix} 0 & \frac{r(\overline{\lambda})^* - r(w)^*}{\lambda - \overline{w}} \\ \frac{r(\lambda) - r(\overline{w})}{\lambda - \overline{w}} & 0 \end{pmatrix} \begin{pmatrix} I \\ Q(\lambda) r(\lambda) \end{pmatrix}.$$

Since r is a rational function it follows that the $2n \times 2n$ matrix

$$\begin{pmatrix} 0 & \frac{r(\overline{\lambda})^* - r(w)^*}{\lambda - \overline{w}} \\ \frac{r(\lambda) - r(\overline{w})}{\lambda - \overline{w}} & 0 \end{pmatrix}$$

is the kernel of a rational function which is symmetric with respect to the real axis, hence it has finitely many negative squares. As $Q \in \mathcal{N}_\kappa^{n\times n}$ also the first summand has finitely many negative squares and therefore the kernel N_{Q_1} has a finitely many negative squares. □

In the study of generalized Nevanlinna functions the so-called generalized poles and generalized zeros play a central role. Originally they have been defined with the help of a realization of the function, that is, a certain operator representation in a Pontryagin space, and have later also been characterized in terms of the asymptotic behavior of the function close to such a point, [13, 46, 48]. However in this section emphasis is put on the analytic point of view, and hence we are using these characterizations as definitions, cf. [48, Theorem 3.7]. In the following we denote by $\lambda \hat{\to} \alpha$ the usual limit $\lambda \to \alpha$ if $\alpha \in \mathbb{C}^+$, and the non-tangential limit in $\mathbb{C}^+$ if $\alpha \in \mathbb{R}$.

Definition 2.4 A point $\alpha \in \mathbb{C}^+ \cup \mathbb{R}$ is called a *generalized pole* of $Q \in \mathcal{N}_\kappa^{n\times n}$ if there exist an open neighbourhood $\mathcal{U}_\alpha$ of α and a holomorphic vector function $\vec{\eta} : \mathcal{U}_\alpha \cap \mathbb{C}^+ \to \mathbb{C}^n$ such that

(i) $\lim_{\lambda \hat{\to} \alpha} \vec{\eta}(\lambda) = 0$ and $\lim_{\lambda \hat{\to} \alpha} Q(\lambda)\vec{\eta}(\lambda) \neq 0$;

(ii) there exists an $n\times n$-matrix function H which is holomorphic at α such that $\lambda \mapsto (Q(\lambda) - H(\lambda))\vec{\eta}(\lambda)$ can be continued holomorphically into α;

(iii) $\lim_{\lambda, w \hat{\to} \alpha} \left(\frac{Q(\lambda) - Q(\overline{w})}{\lambda - \overline{w}} \vec{\eta}(\lambda), \vec{\eta}(w) \right)$ exists.

In this case $\vec{\eta}$ is called *pole cancellation function* of Q at α, the non-zero vector

$$\vec{\eta}_0 := \lim_{\lambda \hat{\to} \alpha} Q(\lambda)\vec{\eta}(\lambda)$$

is called *pole vector*, and $\vec{\eta}_0$ is said to be of *positive* (*negative, neutral*) *type* if the real number in (iii) is positive (negative and zero, respectively).

The point ∞ is called a *generalized pole* of Q if and only if the point 0 is a generalized pole of the function $\lambda \mapsto Q(-\frac{1}{\lambda})$. In this case, pole cancellation functions and pole vectors of positive (negative, neutral) type at the point 0 of the function $\lambda \mapsto Q(-\frac{1}{\lambda})$ are called *pole cancellation functions* and *pole vectors of positive (negative, neutral, respectively) type at* ∞ of the function Q.

For completeness we mention that a point $\alpha \in \mathbb{C}^-$ will be called a *generalized pole* of Q if $\overline{\alpha} \in \mathbb{C}^+$ is a generalized pole of Q and that pole cancellation functions, pole vectors and their sign types are defined analogously.

Remark 2.5 We note that different pole cancellation functions may lead to the same pole vector, but according to [48, Theorem 3.3] the type of the pole vector does not depend on the choice of the pole cancellation function. Furthermore, usual poles in $\mathbb{C}^+ \cup \mathbb{R}$ are also generalized poles in the sense of Definition 2.4. In this case there exists a pole cancellation function which is holomorphic even in a whole neighbourhood of the pole. In particular, it is easy to see, that for non-real poles all pole vectors are neutral.

The following well known fact on the sum of two generalized Nevanlinna functions can be found, for instance, in [16].

Lemma 2.6 *Let $Q_1 \in \mathcal{N}_{\kappa_1}^{n\times n}$ and $Q_2 \in \mathcal{N}_{\kappa_2}^{n\times n}$ be given such that there is no point $\alpha \in \mathbb{C}^+ \cup \overline{\mathbb{R}}$ which is a generalized pole of both Q_1 and Q_2. Then $Q_1 + Q_2 \in \mathcal{N}_{\kappa_1+\kappa_2}^{n\times n}$.*

Besides generalized poles also the notion of generalized zeros of generalized Nevanlinna functions will play an important role in the sequel.

Definition 2.7 A point $\beta \in \mathbb{C}^+ \cup \mathbb{R}$ is called a *generalized zero* of $Q \in \mathcal{N}_\kappa^{n\times n}$ if there exist an open neighbourhood $\mathcal{U}_\beta$ of β and a holomorphic vector function $\vec{\xi} : \mathcal{U}_\beta \cap \mathbb{C}^+ \to \mathbb{C}^n$ such that

(i) $\lim_{\lambda \hat{\to} \beta} \vec{\xi}(\lambda) \neq 0$ and $\lim_{\lambda \hat{\to} \beta} Q(\lambda)\vec{\xi}(\lambda) = 0$;

(ii) there exists an $n \times n$-matrix function H which is holomorphic at the point β such that $\lambda \mapsto \vec{\xi}(\lambda) + H(\lambda)Q(\lambda)\vec{\xi}(\lambda)$ can be continued holomorphically into β;

(iii) $\lim_{\lambda, w \hat{\to} \beta} \left(\frac{Q(\lambda) - Q(\overline{w})}{\lambda - \overline{w}} \vec{\xi}(\lambda), \vec{\xi}(w) \right)$ exists.

In this case $\vec{\xi}$ is called *root function* of Q at β, the non-zero vector

$$\vec{\xi}_0 := \lim_{\lambda \hat{\to} \beta} \vec{\xi}(\lambda)$$

is called *root vector*, and $\vec{\xi}_0$ is said to be of *positive* (*negative, neutral*) *type* if the real number in (iii) is positive (negative and zero, respectively).

The point ∞ is a generalized zero of Q if and only if the point 0 is a generalized zero of the function $\lambda \mapsto Q(-\frac{1}{\lambda})$. In this case, root functions and root vectors of positive (negative, neutral) type at the point 0 of the function $\lambda \mapsto Q(-\frac{1}{\lambda})$ are called *root functions* and *root vectors of positive (negative, neutral, respectively) type at* ∞ of the function Q.

Moreover, we note that $\beta \in \mathbb{C}^-$ is called a *generalized zero* of Q if $\overline{\beta} \in \mathbb{C}^+$ is a generalized zero of Q and root functions, pole vectors and their sign types are defined analogously.

Remark 2.8 If Q is holomorphic at β, then this point is a generalized zero in accordance with the above definition if and only if $\det Q(\beta) = 0$. In this case for every vector $\vec{\xi}_0 \in \ker Q(\beta)$ the constant function $\vec{\xi}(\lambda) := \vec{\xi}_0$ is a root function with root vector $\vec{\xi}_0$. Note also that if $\beta \in \mathbb{C}\backslash\mathbb{R}$ is a generalized zero of Q, then every root vector $\vec{\xi}_0$ is neutral.

Remark 2.9 Suppose that $Q \in \mathcal{N}_\kappa^{n\times n}$ is invertible for some $\mu \in \mathfrak{h}(Q)$. Then the generalized zeros and generalized poles of Q are connected as follows: A point $\alpha \in \overline{\mathbb{C}}$ is a generalized pole of Q with pole cancellation function $\vec{\eta}$ and pole vector $\vec{\eta}_0$ if and only if α is a generalized zero of the function $\lambda \mapsto -Q(\lambda)^{-1}$ with root function $\vec{\xi}(\lambda) := Q(\lambda)\vec{\eta}(\lambda)$ and root vector $\vec{\xi}_0 = \vec{\eta}_0$. Furthermore, it holds

$$\left(\frac{-Q(\lambda)^{-1} + Q(\overline{w})^{-1}}{\lambda - \overline{w}} \vec{\xi}(\lambda), \vec{\xi}(w) \right) = \left(\frac{Q(\lambda) - Q(\overline{w})}{\lambda - \overline{w}} \vec{\eta}(\lambda), \vec{\eta}(w) \right)$$

and hence also the types coincide.

Note that in the scalar case, given a generalized pole there is essential only one pole vector. Therefore, for a scalar function $q \in \mathcal{N}_\kappa$ a generalized pole of q with a pole vector of positive (negative, neutral) type is usually briefly called a *generalized pole of positive* (*resp. negative, neutral*) *type*. In a similar way the notion *generalized zero of positive* (*resp. negative, neutral*) *type* is used. In the case of scalar functions the above definitions simplify, cf., with a slightly different notation, [46].

Lemma 2.10 *For a scalar function $q \in \mathcal{N}_\kappa$ the following holds. A point $\beta \in \mathbb{R}$ is a generalized zero of q of positive (negative, neutral) type if and only if*

$$\lim_{\lambda \hat{\to} \beta} \frac{q(\lambda)}{(\lambda - \beta)}$$

is positive (negative and zero, respectively). A point $\alpha \in \mathbb{R}$ is a generalized pole of q of positive (negative, neutral) type if and only if

$$\lim_{\lambda \hat{\to} \alpha} -\frac{1}{(\lambda - \alpha) q(\lambda)}$$

is positive (negative and zero, respectively).

Proof. It suffices to verify the first assertion. The second statement follows from the first one and Remark 2.9. Assume first that $\lim_{\lambda \hat{\to} \beta} (\lambda - \beta)^{-1} q(\lambda)$ exists and is real. Then $\lim_{\lambda \hat{\to} \beta} q(\lambda) = 0$ and, by setting $\vec{\xi}(\lambda) = 1$ and $H(\lambda) = 0$ it follows that (i) and (ii) in Definition 2.7 are satisfied. The fact that the limit in (iii) exists and that it coincides with $\lim_{\lambda \hat{\to} \beta} (\lambda - \beta)^{-1} q(\lambda)$ can be shown by standard arguments, see, e.g., the proof of [6, Theorem 3.13].

Conversely, suppose now that $\beta \in \mathbb{R}$ is a generalized zero of q. Then (i) in Definition 2.7 implies $\lim_{\lambda \hat{\to} \beta} q(\lambda) = 0$ and by (iii) we have

$$\lim_{\lambda, w \hat{\to} \beta} \left(\frac{q(\lambda) - q(\overline{w})}{\lambda - \overline{w}} \vec{\xi}(\lambda), \vec{\xi}(w) \right) = \lim_{\lambda \hat{\to} \beta} \frac{q(\lambda)}{(\lambda - \beta)} |\vec{\xi}(\beta)|^2,$$

in particular, $\lim_{\lambda \hat{\to} \beta} (\lambda - \beta)^{-1} q(\lambda)$ exists and the sign of the limit of the right hand side is the type of the generalized zero at β. □

Roughly speaking the behaviour of a generalized Nevanlinna function close to a real point that is not a generalized pole of negative or neutral type is the same as that of a Nevanlinna function.

For later purposes we state the following lemma which is known for Nevanlinna functions.

Lemma 2.11 *Assume that $q_1 \in \mathcal{N}_{\kappa_1}$ and $q_2 \in \mathcal{N}_{\kappa_2}$ are scalar generalized Nevanlinna functions and that for some $\beta \in \mathbb{R}$*

$$\lim_{\lambda \hat{\to} \beta} q_1(\lambda) = 0 = \lim_{\lambda \hat{\to} \beta} q_2(\lambda) \quad \textit{and} \quad \lim_{\lambda \hat{\to} \beta} \frac{q_1(\lambda) + q_2(\lambda)}{\lambda - \beta} = \nu \in \mathbb{R}$$

holds. Then β is a generalized zero of q_1 and q_2; in particular, the limits

$$\lim_{\lambda \hat{\to} \beta} \frac{q_1(\lambda)}{\lambda - \beta} \qquad \textit{and} \qquad \lim_{\lambda \hat{\to} \beta} \frac{q_2(\lambda)}{\lambda - \beta}$$

exist and are real.

Proof. As β is not a generalized pole of q_1 and of q_2, it is well known from [41] that there exist functions h_1, h_2 holomorphic in a neighbourhood of β with $q_1(\lambda) = m_1(\lambda) + h_1(\lambda)$ and $q_2(\lambda) = m_2(\lambda) + h_2(\lambda)$, and $\lim_{\lambda \hat{\to} \beta} m_1(\lambda) = \lim_{\lambda \hat{\to} \beta} m_2(\lambda) = 0$, where m_1 and m_2 are Nevanlinna functions, that can be written in the form

$$m_1(\lambda) = \eta_1 + \int_\Delta \frac{d\sigma_1(t)}{t - \lambda} \quad \text{and} \quad m_2(\lambda) = \eta_2 + \int_\Delta \frac{d\sigma_2(t)}{t - \lambda}, \quad \eta_1, \eta_2 \in \mathbb{R},$$

where Δ is a bounded interval which contains β and σ_1, σ_2 are finite measures with support in Δ. Then

$$\lim_{\lambda \hat{\to} \beta} \frac{q_1(\lambda) + q_2(\lambda)}{\lambda - \beta} = \nu \in \mathbb{R}$$

implies

$$\lim_{\lambda \hat{\to} \beta} \frac{m_1(\lambda) + m_2(\lambda)}{\lambda - \beta} = \nu - (h_1'(\beta) + h_2'(\beta))$$

and, as

$$m_1(\lambda) + m_2(\lambda) = \eta_1 + \eta_2 + \int_\Delta \frac{d(\sigma_1+\sigma_2)(t)}{t-\lambda},$$

it follows from [6, Theorem 3.13 (iii)] that $\int_\Delta \frac{d(\sigma_1+\sigma_2)(t)}{(t-\beta)^2} < \infty$. Hence,

$$\int_\Delta \frac{d\sigma_1(t)}{(t-\beta)^2} < \infty \quad \text{and} \quad \int_\Delta \frac{d\sigma_2(t)}{(t-\beta)^2} < \infty,$$

and the assertion follows from [6, Theorem 3.13 (iii)], see also [21, 39]. □

As in the scalar case a special role in the investigation of generalized Nevanlinna functions is played by those generalized poles which are *not of positive type*. To such a pole there is associated the so-called *degree of non-positivity*, see [48, Section 3]. The precise definition of this quantity is given in Definition 2.13 below.

Definition 2.12 Let $Q \in \mathcal{N}_\kappa^{n\times n}$ and let $\alpha \in \mathbb{C}$ be a generalized pole of Q and $\vec{\eta}$ a pole cancellation function of Q at α. The *order* of the pole cancellation function $\vec{\eta}$ is defined as the maximal number $l_0 \in \mathbb{N} \cup \{\infty\}$ such that for $0 \le j < l_0$ the limits

$$\lim_{\lambda \hat{\to} \alpha} \vec{\eta}^{(j)}(\lambda) = \vec{0} \quad \text{and} \quad \lim_{\lambda, w \hat{\to} \alpha} \frac{d^{2j}}{d\lambda^j d\overline{w}^j}\left(\frac{Q(\lambda)-Q(\overline{w})}{\lambda - \overline{w}}\vec{\eta}(\lambda), \vec{\eta}(w)\right)$$

exist. The order of the pole cancellation function $\vec{\eta}$ is denoted by $\operatorname{ord}\vec{\eta}$.

Definition 2.13 Let $Y = \{\vec{\eta}_1, \dots, \vec{\eta}_m\}$ be a system of pole cancellation functions of $Q \in \mathcal{N}_\kappa^{n\times n}$ at the point $\alpha \in \mathbb{C}$ such that the corresponding pole vectors are linearly independent. Let d_i be integers with $1 \le d_i \le \operatorname{ord}\vec{\eta}_i$ for $1 \le i \le m$, respectively. We define $H_{d_1,\dots,d_m}$ via

$$H_{d_1,\dots,d_m} := (G_{i,j})_{1\le i,j\le m} \quad \text{with} \quad G_{i,j} := \left(g^{i,j}_{k_i,l_j}\right)_{0\le k_i \le d_i-1,\, 0\le l_j\le d_j-1}$$

where

$$g^{i,j}_{k_i,l_j} := \lim_{\lambda \hat{\to} \alpha} \lim_{w \hat{\to} \alpha} \frac{1}{k_i! l_j!} \frac{d^{k_i+l_j}}{d\lambda^{k_i} d\overline{w}^{l_j}} \left(\frac{Q(\lambda)-Q(\overline{w})}{\lambda-\overline{w}} \vec{\eta}_i(\lambda), \vec{\eta}_j(w)\right).$$

If $H_{1,\dots,1} = (g^{i,j}_{0,0})_{1\le i,j\le m}$ is negative semi-definite, we denote by $\vartheta(Y)$ the maximal integer for which there exists a choice $d_1, \dots, d_m$ with $\sum_{i=1}^m d_i = \vartheta(Y)$ such that $H_{d_1,\dots,d_m}$ is negative semi-definite, otherwise we set $\vartheta(Y) := 0$. We say that $\vartheta(Y)$ is the *degree of non-positivity of the system* Y.

We remark that the existence of the above iterated limits is assured by [48, Theorem 3.3].

Definition 2.14 A system Y of pole cancellation functions of $Q \in \mathcal{N}_\kappa^{n\times n}$ at the point α such that the corresponding pole vectors are linearly independent is said to have *maximal degree of non-positivity* if there does not exist a system of pole cancellation functions at the point α such that the corresponding pole vectors are linearly independent whose degree of non-positivity is larger. In this case we set

$$\kappa_\alpha(Q) := \vartheta(Y)$$

and we set $\kappa_\alpha(Q) := 0$ if α is not a generalized pole of Q.

If the point ∞ is a generalized pole of Q we define $\kappa_\infty(Q)$ to be the maximal degree of non-positivity at the point 0 of the function defined by $\lambda \mapsto Q(-\frac{1}{\lambda})$.

Generalized poles of $Q \in \mathcal{N}_\kappa^{n\times n}$ are eigenvalues of the self-adjoint relation in a minimal realization of Q in some Pontryagin space Π_κ, see, e.g., [48]. In particular, it is shown in [48, Theorem 3.7] that $\kappa_\alpha(Q)$ coincides with the dimension of a maximal non-positive invariant subspace of the algebraic eigenspace at the eigenvalue α. However, the well known weaker statement in Theorem 2.15 below is sufficient for our purpose.

Theorem 2.15 *Let $Q \in \mathcal{N}_\kappa^{n\times n}$ be given. Then it holds*

$$\sum_{\alpha\in\mathbb{C}^+\cup\mathbb{R}\cup\{\infty\}} \kappa_\alpha(Q) = \kappa.$$

The following special case will be useful.

Lemma 2.16 *Let $Q \in \mathcal{N}_\kappa^{n\times n}$ be given and assume that $\alpha \in \mathbb{C}\backslash\mathbb{R}$ is a generalized pole of Q. If for every pole cancellation function $\vec{\eta}$ of Q at α*

$$\lim_{\lambda\to\alpha} \frac{d}{d\lambda}\vec{\eta}(\lambda) \neq 0 \tag{2.1}$$

holds, then the degree of non-positivity $\kappa_\alpha(Q)$ of the generalized pole α is equal to the maximal number of linearly independent pole vectors of Q at α.

P r o o f. It is easily computed that the matrix $H_{1,\dots,1}$ from Definition 2.13 for every system Y of pole cancellation functions is the zero matrix. Because of (2.1) all the pole cancellation functions of Q at α have order 1, hence the degree of non-positivity $\vartheta(Y)$ of the system Y coincides with the number of linearly independent pole vectors of the system Y of pole cancellation functions. □

Remark 2.17 We mention that the maximal degree of non-positivity coincides in the case of scalar generalized Nevanlinna functions with the notion of multiplicity of a generalized pole of non-positive type, as used in [46]. See also [48, Section 2] for a detailed motivation for the introduction of the above notion.

3 Factorization of matrix valued generalized Nevanlinna functions

In this section we collect and slightly extend some results on factorizations of generalized Nevanlinna functions from [21, 29, 47]. Proposition 3.1 below will play an important role in the proof of one of our main results. Although we are in particularly interested in factorization results for matrix valued generalized Nevanlinna functions we briefly review the scalar case for the convenience of the reader.

Let $G \in \mathfrak{N}_\kappa$, $\kappa \in \mathbb{N}_0$ be a scalar generalized Nevanlinna function. Denote by α_j (β_i), $j = 1,\dots,r$ $(i = 1,\dots,s)$ the generalized poles (generalized zeros) of non-positive type in $\mathbb{R}\cup\mathbb{C}^+$ with multiplicities ν_j (τ_i) of G. By [29] (see also [21]) there exists a scalar Nevanlinna function $G_0 \in \mathcal{N}_0$ such that

$$G(\lambda) = \frac{\prod_{i=1}^{s}(\lambda-\beta_i)^{\tau_i}(\lambda-\overline{\beta}_i)^{\tau_i}}{\prod_{j=1}^{r}(\lambda-\alpha_j)^{\nu_j}(\lambda-\overline{\alpha}_j)^{\nu_j}} G_0(\lambda) \qquad \text{and} \qquad \max\left\{\sum_{i=1}^{s}\tau_i, \sum_{j=1}^{r}\nu_j\right\} = \kappa. \tag{3.1}$$

Equation (3.1) shows the following simple fact: Multiplying a scalar Nevanlinna function with an expression of the form $\frac{(\lambda-\delta)(\lambda-\overline{\delta})}{(\lambda-\gamma)(\lambda-\overline{\gamma})}$, where $\gamma, \delta \in \mathbb{C}$, $\gamma \notin \{\delta, \overline{\delta}\}$, increases the index $\kappa = 0$ by one. If we multiply a scalar generalized Nevanlinna function $G \in \mathfrak{N}_\kappa$, $\kappa \geq 1$, with the same expression, then the negative index $\kappa + \Delta$ of the resulting function

$$\widetilde{G}(\lambda) = \frac{(\lambda-\delta)(\lambda-\overline{\delta})}{(\lambda-\gamma)(\lambda-\overline{\gamma})} G(\lambda) \in \mathfrak{N}_{\kappa+\Delta} \tag{3.2}$$

depends on the fact whether generalized poles and zeros cancel (and whether the function has a generalized pole at infinity) or not. More precisely, for the number Δ the following holds:

$$\begin{array}{ll}(1) & \left.\begin{array}{l}\delta \text{ generalized pole of non-positive type of } G\\ \gamma \text{ generalized zero of non-positive type of } G\end{array}\right\} \Rightarrow \Delta = -1,\\[2ex] (2) & \left.\begin{array}{l}\delta \text{ generalized pole of non-positive type of } G\\ \gamma \text{ no generalized zero of non-positive type of } G\end{array}\right\} \Rightarrow \Delta = 0,\\[2ex] (3) & \left.\begin{array}{l}\delta \text{ no generalized pole of non-positive type of } G\\ \gamma \text{ generalized zero of non-positive type of } G\end{array}\right\} \Rightarrow \Delta = 0,\\[2ex] (4) & \left.\begin{array}{l}\delta \text{ no generalized pole of non-positive type of } G\\ \gamma \text{ no generalized zero of non-positive type of } G\end{array}\right\} \Rightarrow \Delta = 1.\end{array}$$

Let us now consider matrix valued generalized Nevanlinna functions. In contrast to the scalar case here also the pole and root vectors and their sign types have to be taken into account. In what follows we will write $\kappa(Q)$, if we want to emphasize that this number is the negative index of the generalized Nevanlinna function Q. The next proposition extends [47, Theorems 3.1 and 4.1].

Proposition 3.1 *Let $Q \in \mathcal{N}^{n\times n}_{\kappa(Q)}$ and $\gamma, \delta \in \mathbb{C}$ with $\gamma \notin \{\delta, \overline{\delta}\}$. Let $\vec{\psi}, \vec{\varphi} \in \mathbb{C}^n$ such that $(\vec{\psi}, \vec{\varphi}) \neq 0$ and define the projection $P := \frac{(\,\cdot\,,\vec{\varphi})}{(\vec{\psi},\vec{\varphi})}\vec{\psi}$ in $\mathbb{C}^n$. Then*

$$\widetilde{Q}(\lambda) := \left(I - P^* + \frac{\lambda-\delta}{\lambda-\overline{\gamma}}P^*\right) Q(\lambda) \left(I - P + \frac{\lambda-\overline{\delta}}{\lambda-\gamma}P\right) \in \mathcal{N}^{n\times n}_{\kappa(\widetilde{Q})} \tag{3.3}$$

is a generalized Nevanlinna function with negative index $\kappa(\widetilde{Q}) = \kappa(Q) + \Delta$, where

$$\begin{array}{ll}\text{(1a)} & \left.\begin{array}{l}\delta \textit{ gen. pole of } Q \textit{ and } \vec{\varphi} \textit{ a corr. non-positive pole vector}\\ \gamma \textit{ gen. zero of } Q \textit{ and } \vec{\psi} \textit{ a corr. non-positive root vector}\end{array}\right\} \Rightarrow \Delta = -1,\\[2ex] \text{(1b)} & \left.\begin{array}{l}\delta \textit{ gen. pole of } Q \textit{ and } \vec{\varphi} \textit{ a corr. non-positive pole vector}\\ \gamma \textit{ gen. zero of } Q \textit{ and } \vec{\psi} \textit{ a corr. positive root vector}\end{array}\right\} \Rightarrow \Delta = 0,\\[2ex] \text{(1c)} & \left.\begin{array}{l}\delta \textit{ gen. pole of } Q \textit{ and } \vec{\varphi} \textit{ a corr. positive pole vector}\\ \gamma \textit{ gen. zero of } Q \textit{ and } \vec{\psi} \textit{ a corr. non-positive root vector}\end{array}\right\} \Rightarrow \Delta = 0,\\[2ex] \text{(2)} & \left.\begin{array}{l}\delta \textit{ gen. pole of } Q \textit{ and } \vec{\varphi} \textit{ a corr. non-positive pole vector}\\ \gamma \in \mathbb{C}\backslash\mathbb{R} \textit{ neither zero nor pole of } Q,\ \vec{\psi} \textit{ arbitrary}\end{array}\right\} \Rightarrow \Delta = 0,\\[2ex] \text{(3a)} & \left.\begin{array}{l}\delta \in \mathbb{C}\backslash\mathbb{R} \textit{ neither zero nor pole of } Q,\ \vec{\varphi} \textit{ arbitrary}\\ \gamma \textit{ gen. zero of } Q \textit{ and } \vec{\psi} \textit{ a corr. non-positive root vector}\end{array}\right\} \Rightarrow \Delta = 0,\\[2ex] \text{(3b)} & \left.\begin{array}{l}\delta \in \mathbb{C}\backslash\mathbb{R} \textit{ neither zero nor pole of } Q,\ \vec{\varphi} \textit{ arbitrary}\\ \gamma \textit{ gen. zero of } Q \textit{ and } \vec{\psi} \textit{ a corr. positive root vector}\end{array}\right\} \Rightarrow \Delta = 1.\end{array}$$

Roughly speaking in case (1a) a generalized pole and a generalized zero not of positive type cancel (since the directions fit) and hence the negative index is reduced by 1. In (1b), (2), and (3a) a generalized pole or zero not of positive type cancels but at the same time a new one appears, hence the negative index is preserved. Although the number Δ in the above proposition could be calculated also in other cases than (1a)-(1c), (2), and (3a)-(3b), we have restricted ourselves to those which are relevant for us.

Sketch of Proof. Case (1a) is Theorem 3.1 in [47], whereas (1c) can be obtained by a slight modification of the rather technical proof of (1a), which uses the operator representation of the function Q.

More precisely, let A be a minimal representing self-adjoint relation for the function Q in a Pontryagin space $\mathcal{K}$ and define the self-adjoint relation $\widetilde{A}$ in the Pontryagin space $\widetilde{\mathcal{K}} := \mathcal{K}[+]\mathbb{C}$ via its resolvent by

$$(\widetilde{A}-\lambda)^{-1} := \begin{pmatrix} (A-\lambda)^{-1} & 0 \\ 0 & \frac{1}{\gamma-\lambda} \end{pmatrix}.$$

Minimality of the realization for $\widetilde{Q}$ is obtained by factoring out the eigenvector corresponding to the generalized pole δ of Q, which is positive (for the detailed arguments see page 336 in [47]). This yields a minimal representation of $\widetilde{Q}$ in a Pontryagin space with again κ negative squares, which proves $\widetilde{Q} \in \mathcal{N}_\kappa^{n\times n}$. Case (1b) follows from (1c) by taking inverses. Case (2) is precisely [47, Theorem 4.1] and (3a) is obtained from (2) by taking inverses. Case (3b) follows from applying [47, Remark below Theorem 4.1] to the reciprocal function. □

One expects that in the situation of Proposition 3.1 new generalized poles and zeros for $\widetilde{Q}$ are created in case that they do not cancel with generalized zeros and poles of Q. The following lemma makes this more precise.

Lemma 3.2 *Let the functions Q, $\widetilde{Q}$, the points γ, δ the vectors $\vec{\psi}, \vec{\varphi} \in \mathbb{C}^n$ and the projection P be as in Proposition* 3.1. *If $\gamma \in \mathbb{R}$ is not a generalized zero of Q, then γ is a generalized pole of $\widetilde{Q}$ with non-positive pole vector $\vec{\varphi}$.*

Proof. We show that the function

$$\vec{\eta}(\lambda) := \frac{\lambda-\gamma}{\lambda-\delta}\big(I-P+\frac{\lambda-\gamma}{\lambda-\overline{\delta}}P\big)\,Q(\lambda)^{-1}\vec{\varphi}$$

is a pole cancellation function of $\widetilde{Q}$ at γ. Note that since γ is not a generalized zero of Q the function $-Q(\lambda)^{-1}$ has no generalized pole at γ. It is well-known that for a Nevanlinna function R with no generalized pole at γ we have $\lim_{\lambda \hat{\to} \gamma}(\lambda-\gamma)(R(\lambda)\vec{x},\vec{x}) = 0$ for all vectors $\vec{x} \in \mathbb{C}^n$; cf. [39]. Hence $\lim_{\lambda \hat{\to} \gamma}(\lambda-\gamma)R(\lambda) = 0 \in \mathbb{C}^{n\times n}$. Now, with [47, Section 5], the function $-Q(\lambda)^{-1}$ can be written as a product of a Nevanlinna function R_0 and a rational function B, $-Q(\lambda)^{-1} = B(\overline{\lambda})^* R_0(\lambda)B(\lambda)$, such that B has no pole in γ. Hence it holds $\lim_{\lambda \hat{\to} \gamma}(\lambda-\gamma)Q(\lambda)^{-1} = 0$ and thus $\lim_{\lambda \hat{\to} \gamma}\vec{\eta}(\lambda) = \vec{0}$. Furthermore, with $P^* = \frac{(\cdot,\vec{\psi})}{(\vec{\varphi},\vec{\psi})}\vec{\varphi}$ we have

$$\begin{aligned}\widetilde{Q}(\lambda)\vec{\eta}(\lambda) &= \frac{\lambda-\gamma}{\lambda-\delta}\left(I-P^*+\frac{\lambda-\delta}{\lambda-\gamma}P^*\right)Q(\lambda)\left(I-P+\frac{\lambda-\overline{\delta}}{\lambda-\gamma}P\right)\left(I-P+\frac{\lambda-\gamma}{\lambda-\overline{\delta}}P\right)Q(\lambda)^{-1}\vec{\varphi} \\ &= \frac{\lambda-\gamma}{\lambda-\delta}\left(I-P^*+\frac{\lambda-\delta}{\lambda-\gamma}P^*\right)\vec{\varphi} = \vec{\varphi},\end{aligned}$$

which implies

$$-\big(\widetilde{Q}(\lambda)\vec{\eta}(\lambda),\vec{\eta}(w)\big) = \frac{\overline{w}-\gamma}{\overline{w}-\overline{\delta}}\cdot\frac{\overline{w}-\gamma}{\overline{w}-\delta}\big(-Q(\overline{w})^{-1}\vec{\varphi},\vec{\varphi}\big).$$

We define the function N via

$$N(z) := \frac{z-\gamma}{z-\overline{\delta}}\cdot\frac{z-\gamma}{z-\delta}\big(-Q(z)^{-1}\vec{\varphi},\vec{\varphi}\big) = -\big(\widetilde{Q}(\lambda)\vec{\eta}(\lambda),\vec{\eta}(\overline{z})\big). \tag{3.4}$$

By assumption, the function $z \mapsto (-Q(z)^{-1}\vec{\varphi},\vec{\varphi})$ is a scalar generalized Nevanlinna function which has no generalized pole at γ. Hence the function N in (3.4) is a generalized Nevanlinna function with generalized zero γ of non-positive type (see (3.2)) and this implies,

$$\lim_{\lambda,w \hat{\to} \gamma}\left(\frac{\widetilde{Q}(\lambda)-\widetilde{Q}(\overline{w})}{\lambda-\overline{w}}\vec{\eta}(\lambda),\vec{\eta}(w)\right) = \lim_{\lambda,w \hat{\to} \gamma}\frac{N(\lambda)-N(\overline{w})}{\lambda-\overline{w}} \leq 0.$$

Moreover, as $\widetilde{Q}(\lambda)\vec{\eta}(\lambda) = \vec{\varphi}$, (ii) of Definition 2.4 is satisfied with $H \equiv 0$. This finally gives that $\vec{\eta}$ is a pole cancellation function of $\widetilde{Q}$ at γ with non-positive pole vector $\vec{\varphi}$. □

In the proof of Theorem 4.5 below special matrix functions appear. Functions of this type have been studied in [6]. We recall those results which are of interest for us here.

Proposition 3.3 *Let q_m and q_τ, $q_\tau \not\equiv 0$ be scalar generalized Nevanlinna functions with $q_m + q_\tau \not\equiv 0$ and define*

$$\Omega(\lambda) := \begin{pmatrix} q_m(\lambda) & -1 \\ -1 & -\frac{1}{q_\tau(\lambda)} \end{pmatrix}.$$

Then the point $w_0 \in \mathbb{C}$ is a generalized zero of the generalized Nevanlinna function Ω if and only if it is either a generalized zero of $q_m + q_\tau$ or it is a generalized pole of both q_m and q_τ. Moreover, the following hold:

1. *If w_0 is a generalized zero of Ω and if q_τ has a generalized pole at w_0 then there exists (up to scalar multiples) only one root vector $\vec{\xi_0} = (0,1)^\top$ of Ω at w_0 and its type coincides with the the sign of*

$$\lim_{\lambda \hat{\to} w_0} \frac{-\frac{1}{q_m(\lambda)} - \frac{1}{q_\tau(\lambda)}}{\lambda - w_0}.$$

2. *If w_0 is a generalized zero of Ω and if q_τ has no generalized pole at the point w_0 then the limits $\lim_{\lambda \hat{\to} w_0} q_\tau(\lambda) = -\lim_{\lambda \hat{\to} w_0} q_m(\lambda) =: q_\tau(w_0)$ exist and there exists (up to scalar multiples) only one root vector $\vec{\xi_0} = (1, -q_\tau(w_0))^\top$ of Ω at w_0 and its type coincides with the the sign of*

$$\lim_{\lambda \hat{\to} w_0} \frac{q_m(\lambda) + q_\tau(\lambda)}{\lambda - w_0}.$$

The proof can be found in [6, Propositions 4.7 (ii) and 4.9 (iii)]. However, the particular form of the root vectors and the existence of the limit $\lim_{\lambda \hat{\to} w_0} q_\tau(\lambda)$ appear only within the proof of [6, Proposition 4.9 (iii)].

4 Matrix valued $\mathcal{D}_\kappa$-functions

In this section we introduce a class of matrix valued functions that play an important role throughout this paper. In the scalar case this class of functions was defined and investigated in [10] and [11] in connection with indefinite Sturm-Liouville operators.

Definition 4.1 A matrix function M with values in $\mathbb{C}^{n\times n}$ belongs to the class $\mathcal{D}_\kappa^{n\times n}$ if it is piecewise meromorphic in $\mathbb{C}\backslash\mathbb{R}$, symmetric with respect to the real axis and there exists a point $\lambda_0 \in \mathfrak{h}(M)\backslash\{\infty\}$, a function $Q \in \mathcal{N}_\kappa^{n\times n}$ holomorphic in λ_0 and a rational function G holomorphic in $\overline{\mathbb{C}}\backslash\{\lambda_0, \overline{\lambda}_0\}$ such that

$$\frac{\lambda}{(\lambda-\lambda_0)(\lambda-\overline{\lambda}_0)} M(\lambda) = Q(\lambda) + G(\lambda) \tag{4.1}$$

holds for all points λ where M, Q and G are holomorphic. The class $\mathcal{D}_\kappa^{1\times 1}$ will be denoted by $\mathcal{D}_\kappa$.

We note that the classes $\mathcal{D}_\kappa^{n\times n}$, $\kappa \in \mathbb{N}_0$, are subclasses of the class of definitizable functions, see [36, 37]. The next lemma ensures that the definition of the classes $\mathcal{D}_\kappa^{n\times n}$ does not depend on the choice of the point λ_0. Moreover, it implies $\mathcal{D}_\kappa^{n\times n} \cap \mathcal{D}_{\kappa'}^{n\times n} = \emptyset$, if $\kappa \neq \kappa'$.

Lemma 4.2 *Let M be a $\mathbb{C}^{n\times n}$-valued function meromorphic in $\mathbb{C}\backslash\mathbb{R}$, let $\lambda_0 \in \mathfrak{h}(M)\backslash\{\infty\}$, $Q \in \mathcal{N}_\kappa^{n\times n}$ and G be as in Definition 4.1 such that (4.1) holds. Then for every $z \in \mathfrak{h}(M)\backslash\{\infty\}$ there exists $Q_z \in \mathcal{N}_\kappa^{n\times n}$ holomorphic in z and a rational function G_z holomorphic in $\overline{\mathbb{C}}\backslash\{z, \overline{z}\}$ such that*

$$\frac{\lambda}{(\lambda-z)(\lambda-\overline{z})} M(\lambda) = Q_z(\lambda) + G_z(\lambda) \tag{4.2}$$

holds for all points λ where M, Q_z and G_z are holomorphic.

P r o o f. Let us show that (4.1) implies (4.2). For this let $z \in \mathfrak{h}(M)\backslash\{\infty\}$ such that $z \notin \{\lambda_0, \overline{\lambda}_0\}$. From (4.1) we conclude $z \in \mathfrak{h}(Q)$ and

$$\frac{\lambda}{(\lambda - z)(\lambda - \overline{z})} M(\lambda) = h(\lambda)\overline{h(\overline{\lambda})}\big(Q(\lambda) + G(\lambda)\big), \tag{4.3}$$

where $h(\lambda) := \frac{\lambda-\lambda_0}{\lambda-z}$. The function $\lambda \mapsto h(\lambda)\overline{h(\overline{\lambda})}Q(\lambda)$ is either holomorphic in z and $\overline{z}$ or it has an isolated singularity at z and at $\overline{z}$. Moreover, by Lemma 2.3, this function belongs to $\mathcal{N}_{\widetilde{\kappa}}^{n\times n}$ for some $\widetilde{\kappa} \in \mathbb{N}_0$. Obviously, there exists a rational function r_z holomorphic in $\overline{\mathbb{C}}\backslash\{z, \overline{z}\}$ which is symmetric with respect to the real line such that

$$Q_z(\lambda) := h(\lambda)\overline{h(\overline{\lambda})}Q(\lambda) - r_z(\lambda) \tag{4.4}$$

is holomorphic in z. Then the function Q_z belongs to $\mathcal{N}_{\kappa_z}^{n\times n}$ for some $\kappa_z \in \mathbb{N}_0$; cf. [41] or the text below Lemma 2.2. We set $G_z(\lambda) := r_z(\lambda) + h(\lambda)\overline{h(\overline{\lambda})}G(\lambda)$. Then the rational function G_z is holomorphic in $\overline{\mathbb{C}}\backslash\{z, \overline{z}\}$ and from (4.3) we see that (4.2) holds. Observe that by (4.1) and (4.4) we have

$$\mathfrak{h}(Q) = \mathfrak{h}(Q_z) \qquad \text{and} \qquad \{\lambda_0, \overline{\lambda}_0, z, \overline{z}\} \subset \mathfrak{h}(Q). \tag{4.5}$$

It remains to show $Q_z \in \mathcal{N}_{\kappa}^{n\times n}$, i.e., we have to verify $\kappa_z = \kappa$. To this end, it is sufficient to show

$$\kappa_\alpha(Q_z) = \kappa_\alpha(Q) \quad \text{for all } \alpha \in \mathbb{C} \cup \{\infty\};$$

cf. Theorem 2.15. Note that only points $\alpha \in \overline{\mathbb{C}}$ which do not belong to $\mathfrak{h}(Q)$ are of interest since $\kappa_\alpha(Q) = \kappa_\alpha(Q_z) = 0$ holds for $\alpha \in \mathfrak{h}(Q) = \mathfrak{h}(Q_z)$; cf. (4.5).

Let $\alpha \in \mathbb{C}\backslash\mathfrak{h}(Q)$ and let us show that a function $\vec{\eta}$ is a pole cancellation function of Q at α of positive (negative, neutral) type if and only if it is a pole cancellation function of Q_z at α of positive (negative, neutral) type. Indeed, assume that $\vec{\eta}$ is a pole cancellation function of Q at α. We have $h(\alpha)\overline{h(\overline{\alpha})} \neq 0$ by (4.5) and with (4.4) we obtain

$$\lim_{\lambda \hat{\to} \alpha} Q_z(\lambda)\vec{\eta}(\lambda) = \lim_{\lambda \hat{\to} \alpha} \Big(h(\lambda)\overline{h(\overline{\lambda})}Q(\lambda)\vec{\eta}(\lambda) - r_z(\lambda)\vec{\eta}(\lambda)\Big) \neq 0. \tag{4.6}$$

Furthermore, if H denotes the function from (ii) of Definition 2.4 which is holomorphic at α such that $\lambda \mapsto (Q(\lambda) - H(\lambda))\vec{\eta}(\lambda)$ can be continued holomorphically into α, then the function $H_z(\lambda) := h(\lambda)\overline{h(\overline{\lambda})}H(\lambda) - r_z(\lambda)$ is holomorphic at α and

$$\lambda \mapsto (Q_z(\lambda) - H_z(\lambda))\vec{\eta}(\lambda) = h(\lambda)\overline{h(\overline{\lambda})}(Q(\lambda) - H(\lambda))\vec{\eta}(\lambda)$$

can be continued holomorphically into α. Moreover, we have

$$\begin{aligned}
&\left(\frac{Q_z(\lambda) - Q_z(\overline{w})}{\lambda - \overline{w}}\vec{\eta}(\lambda), \vec{\eta}(w)\right) = \\
&\quad h(\lambda)\frac{\overline{h(\overline{\lambda})} - \overline{h(w)}}{\lambda - \overline{w}}\,(Q(\lambda)\vec{\eta}(\lambda), \vec{\eta}(w)) + h(\lambda)\overline{h(w)}\left(\frac{Q(\lambda) - Q(\overline{w})}{\lambda - \overline{w}}\vec{\eta}(\lambda), \vec{\eta}(w)\right) \\
&\quad + \overline{h(w)}\frac{h(\lambda) - h(\overline{w})}{\lambda - \overline{w}}\,(\vec{\eta}(\lambda), Q(w)\vec{\eta}(w)) - \left(\frac{r_z(\lambda) - r_z(\overline{w})}{\lambda - \overline{w}}\vec{\eta}(\lambda), \vec{\eta}(w)\right)
\end{aligned} \tag{4.7}$$

and, using the properties of the pole cancellation function $\vec{\eta}$, we conclude

$$\lim_{\lambda, w \hat{\to} \alpha} \left(\frac{Q_z(\lambda) - Q_z(\overline{w})}{\lambda - \overline{w}}\vec{\eta}(\lambda), \vec{\eta}(w)\right) = |h(\alpha)|^2 \lim_{\lambda, w \hat{\to} \alpha} \left(\frac{Q(\lambda) - Q(\overline{w})}{\lambda - \overline{w}}\vec{\eta}(\lambda), \vec{\eta}(w)\right),$$

i.e., $\vec{\eta}$ is a pole cancellation function of Q_z at α and its type coincides with the type of the pole cancellation function $\vec{\eta}$ of Q at α. Moreover, a similar reasoning applies when changing the roles of Q and Q_z.

It remains to investigate the degree of non-positivity. Let $Y = \{\vec{\eta}_1, \dots, \vec{\eta}_m\}$ be a system of pole cancellation functions of $Q \in \mathcal{N}_\kappa^{n\times n}$ at the point $\alpha \in \mathbb{C}$ such that the corresponding pole vectors are linearly independent. We define for $0 \le k_i <\operatorname{ord}\vec{\eta}_i$, $0 \le l_j <\operatorname{ord}\vec{\eta}_j$ for $1 \le i, j \le m$ the numbers

$$g^{i,j}_{k_i,l_j} := \lim_{\lambda \hat{\to} \alpha} \lim_{w \hat{\to} \alpha} \frac{1}{k_i! l_j!} \frac{d^{k_i+l_j}}{d\lambda^{k_i} d\overline{w}^{l_j}} \left(\frac{Q(\lambda) - Q(\overline{w})}{\lambda - \overline{w}} \vec{\eta}_i(\lambda), \vec{\eta}_j(w) \right);$$

cf. Definition 2.13. As the function h and r_z are holomorphic at α (and, hence, their derivatives) and as $Q\vec{\eta}_i$, $i = 1, \dots, m$, can be decomposed (see Definition 2.4) in a neighbourhood of α into the sum of two functions, $Q\vec{\eta}_i = (Q - H_i)\vec{\eta}_i + H_i\vec{\eta}_i$ (and, hence, their derivatives), holomorphic in α, we see that by (4.7) and by the properties of the pole cancellation functions $\vec{\eta}_i$,

$$\begin{aligned}
&\lim_{\lambda \hat{\to} \alpha} \lim_{w \hat{\to} \alpha} \frac{1}{k_i! l_j!} \frac{d^{k_i+l_j}}{d\lambda^{k_i} d\overline{w}^{l_j}} \left(\frac{Q_z(\lambda) - Q_z(\overline{w})}{\lambda - \overline{w}} \vec{\eta}_i(\lambda), \vec{\eta}_j(w) \right) \\
&= \lim_{\lambda \hat{\to} \alpha} \lim_{w \hat{\to} \alpha} \frac{1}{k_i! l_j!} \frac{d^{k_i+l_j}}{d\lambda^{k_i} d\overline{w}^{l_j}} h(\lambda)\overline{h(w)} \left(\frac{Q(\lambda) - Q(\overline{w})}{\lambda - \overline{w}} \vec{\eta}_i(\lambda), \vec{\eta}_j(w) \right) \\
&= \lim_{\lambda \hat{\to} \alpha} \lim_{w \hat{\to} \alpha} \sum_{r=0}^{k_i} \sum_{s=0}^{l_j} \frac{1}{k_i! l_j!} \binom{k_i}{r} \binom{l_j}{s} \frac{d^{r+s}}{d\lambda^r d\overline{w}^s} \left(\frac{Q(\lambda) - Q(\overline{w})}{\lambda - \overline{w}} \vec{\eta}_i(\lambda), \vec{\eta}_j(w) \right) \frac{d^{k_i-r}}{d\lambda^{k_i-r}} h(\lambda) \frac{d^{l_j-s}}{d\overline{w}^{l_j-s}} \overline{h(w)} \\
&= \sum_{r=0}^{k_i} \sum_{s=0}^{l_j} g^{i,j}_{r,s} \frac{1}{(k_i - r)!} h^{(k_i-r)}(\alpha) \overline{\frac{1}{(l_j - s)!} h^{(l_j-s)}(\alpha)}.
\end{aligned}$$

Hence, the order of every pole cancellation function from the system $Y = \{\vec{\eta}_1, \dots, \vec{\eta}_m\}$ considered as a pole cancellation function of Q at α is equal to its order considered as a pole cancellation function of Q_z at α. Let $H_{d_1,\dots,d_m}$ be the matrix in Definition 2.13 and denote by $H^z_{d_1,\dots,d_m}$ the analogous matrix with entries defined via Q_z instead of Q. For $p \in \mathbb{N}$ we define the matrix

$$C_p := \begin{pmatrix}
h(\alpha) & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\
h'(\alpha) & h(\alpha) & 0 & \cdots & \cdots & \cdots & 0 \\
\frac{1}{2!} h''(\alpha) & h'(\alpha) & h(\alpha) & & 0 & \cdots & 0 \\
\vdots & & & & & & \vdots \\
\vdots & & & & & & 0 \\
\frac{1}{(p-1)!} h^{(p-1)}(\alpha) & \cdots & \cdots & \cdots & \cdots & h'(\alpha) & h(\alpha)
\end{pmatrix}$$

and we obtain

$$H^z_{d_1,\dots,d_m} = \begin{pmatrix}
C_{d_1} & 0 & \cdots & 0 \\
0 & C_{d_2} & 0 & \vdots \\
\vdots & & & 0 \\
0 & \cdots & 0 & C_{d_m}
\end{pmatrix} H_{d_1,\dots,d_m} \begin{pmatrix}
C^*_{d_1} & 0 & \cdots & 0 \\
0 & C^*_{d_2} & 0 & \vdots \\
\vdots & & & 0 \\
0 & \cdots & 0 & C^*_{d_m}
\end{pmatrix}.$$

The first and the third matrix on the right hand side of the above equation are invertible, hence $H_{d_1,\dots,d_m}$ is negative semi-definite if and only if $H^z_{d_1,\dots,d_m}$ is negative semi-definite. Therefore $\kappa_\alpha(Q) = \kappa_\alpha(Q_z)$ for $\alpha \in \mathbb{C}\backslash\mathfrak{h}(Q)$.

If $\alpha = \infty$, we apply the above reasoning to the functions $\lambda \mapsto Q(-\frac{1}{\lambda})$ and $\lambda \mapsto Q_z(-\frac{1}{\lambda})$. □

Recall (see Lemma 2.2) that for generalized Nevanlinna functions Q with $\det Q(\mu_0) \neq 0$ for some $\mu_0 \in \mathfrak{h}(Q)\backslash\{\infty\}$ we have $Q \in \mathcal{N}_\kappa^{n\times n}$ if and only if $-Q^{-1} \in \mathcal{N}_\kappa^{n\times n}$, in particular, the index κ does not change. The next remark, and Theorem 4.4 and 4.5 below show that, in general, for functions M from the class $\mathcal{D}_\kappa^{n\times n}$ the index κ changes when considering $-M^{-1}$.

Remark 4.3 Let $M \in \mathcal{D}_\kappa^{n\times n}$ and assume that $\det M(\mu_0) \neq 0$ holds for some $\mu_0 \in \mathfrak{h}(M)\backslash\{\infty\}$. Choose $Q \in \mathcal{N}_\kappa^{n\times n}$ and G as in Definition 4.1. Then

$$\frac{\lambda}{(\lambda-\lambda_0)(\lambda-\overline{\lambda}_0)}\left(-M(\lambda)^{-1}\right) = \frac{\lambda^2}{(\lambda-\lambda_0)^2(\lambda-\overline{\lambda}_0)^2}\left(-(Q(\lambda)+G(\lambda))^{-1}\right)$$

together with Lemma 2.3 and Lemma 2.6 show $-M^{-1} \in \mathcal{D}_{\widehat{\kappa}}^{n\times n}$ for some $\widehat{\kappa} \in \mathbb{N}_0$. We note for completeness that with the help of minimal operator representations of the functions M and $-M^{-1}$ and a perturbation argument it can be shown that $|\kappa-\widehat{\kappa}| \leq n$ holds; cf. [10, Theorem 9] and [37, Theorem 3.9].

For scalar functions $m \in \mathcal{D}_\kappa$ a full description of the index $\widehat{\kappa}$ for $-m^{-1} \in \mathcal{D}_{\widehat{\kappa}}$ was given in [11, Theorem 3.3], which we present here in a slightly different form.

Theorem 4.4 *Let $m \in \mathcal{D}_\kappa$, $\kappa \geq 1$, and assume $m \not\equiv 0$. Then $-m^{-1} \in \mathcal{D}_{\widehat{\kappa}}$ with $\widehat{\kappa} = \kappa + \Delta_0 + \Delta_\infty$, where*

$$\Delta_0 = \begin{cases} -1 & \text{if } \lim\limits_{\lambda \hat{\to} 0} m(\lambda) \leq 0, \\ 0 & \textit{otherwise} \end{cases} \quad \textit{and} \quad \Delta_\infty = \begin{cases} 0 & \text{if } \lim\limits_{\lambda \hat{\to} \infty} m(\lambda) \geq 0, \\ 1 & \textit{otherwise.} \end{cases}$$

The main result of this section is the following theorem where the index of a certain function $\widetilde{M} \in \mathcal{D}_\kappa^{2\times 2}$, that will play an essential role in part II of the present paper, is given in terms of the local behavior of m and τ at the points 0 and ∞.

Theorem 4.5 *Let the functions $m \in \mathcal{D}_{\kappa_m}$ and $\tau \in \mathcal{D}_{\kappa_\tau}$ be given, $\tau \not\equiv 0$, and assume $m + \tau \not\equiv 0$. Then*

$$\widetilde{M} = -\begin{pmatrix} m & -1 \\ -1 & -\frac{1}{\tau} \end{pmatrix}^{-1} \in \mathcal{D}_\kappa^{2\times 2}$$

with $\kappa = \kappa_m + \kappa_\tau + \Delta_0 + \Delta_\infty$, where

$$\Delta_0 = \begin{cases} -1 & \textit{if } \lim\limits_{\lambda \hat{\to} 0} m(\lambda) \textit{ and } \lim\limits_{\lambda \hat{\to} 0} \tau(\lambda) \textit{ exist and } \lim\limits_{\lambda \hat{\to} 0} (m(\lambda)+\tau(\lambda)) \leq 0, \\ 0 & \textit{otherwise,} \end{cases}$$

and

$$\Delta_\infty = \begin{cases} 0 & \textit{if } \lim\limits_{\lambda \hat{\to} \infty} m(\lambda) \textit{ and } \lim\limits_{\lambda \hat{\to} \infty} \tau(\lambda) \textit{ exist and } \lim\limits_{\lambda \hat{\to} \infty} (m(\lambda)+\tau(\lambda)) \geq 0, \\ 1 & \textit{otherwise.} \end{cases}$$

Proof. In the special case $m \equiv 0$ we have

$$\widetilde{M} = \begin{pmatrix} -\frac{1}{\tau} & 1 \\ 1 & 0 \end{pmatrix}$$

and therefore $\widetilde{M} \in \mathcal{D}_\kappa^{2\times 2}$ if and only if $-\frac{1}{\tau} \in \mathcal{D}_\kappa$. Hence the claim follows directly from the result for scalar functions, see Theorem 4.4, and in what follows we assume $m \not\equiv 0$.

Since $m \in \mathcal{D}_{\kappa_m}$ and $\tau \in \mathcal{D}_{\kappa_\tau}$ are meromorphic in $\mathbb{C}^+$, and it was assumed that $m + \tau \not\equiv 0$, one can choose a λ_0 with

$$\lambda_0 \in \mathbb{C}^+ \cap \mathfrak{h}(m) \cap \mathfrak{h}(m^{-1}) \cap \mathfrak{h}(\tau) \cap \mathfrak{h}(\tau^{-1}) \cap \mathfrak{h}\big((m+\tau)^{-1}\big). \tag{4.8}$$

Recall that by Lemma 4.2 and by definition $\widetilde{M} \in \mathcal{D}_\kappa^{2\times 2}$ if and only if

$$\frac{\lambda}{(\lambda-\lambda_0)(\lambda-\overline{\lambda}_0)}\widetilde{M}(\lambda) = \widetilde{Q}(\lambda) + \widetilde{G}(\lambda) \quad \text{with } \widetilde{Q} \in \mathcal{N}_\kappa^{2\times 2}, \tag{4.9}$$

where the rational function $\widetilde{G}$ is holomorphic in $\overline{\mathbb{C}}\backslash\{\lambda_0, \overline{\lambda}_0\}$ and $\widetilde{Q}$ is holomorphic in λ_0. By assumption (4.8), the function $\widetilde{M}$ is holomorphic at λ_0. We claim that here $\widetilde{G}$ belongs to $\mathcal{N}_2^{2\times 2}$. In fact, $\widetilde{G}$ has only one generalized pole λ_0 in $\mathbb{C}^+ \cup \mathbb{R} \cup \{\infty\}$ which is an usual pole. Hence it suffices to show that its degree of non-positivity is 2. Since $\widetilde{M}$ is holomorphic and invertible in λ_0, we see with (4.8) and (4.9) that $\lambda \mapsto (\lambda-\lambda_0)(x_0,y_0)^\top$ is a pole cancellation function of $\widetilde{G}$ at λ_0 for every $x_0, y_0 \in \mathbb{C}\backslash\{0\}$. Assume now that there exists a pole cancellation function $\vec{\eta}$ such that

$$\lim_{\lambda\to\lambda_0} \frac{d}{d\lambda}\vec{\eta}(\lambda) = 0.$$

As $\vec{\eta}$ is holomorphic in λ_0, there exists a function $\vec{\eta}_0$, holomorphic in λ_0, with $\vec{\eta}(\lambda) = (\lambda-\lambda_0)^2\vec{\eta}_0(\lambda)$. But this, together with (4.9), gives $\lim_{\lambda\to\lambda_0} \widetilde{G}(\lambda)\vec{\eta}(\lambda) = 0$, a contradiction to the fact that $\vec{\eta}$ a pole cancellation function. Hence, according to Lemma 2.16, the degree of non-positivity of the generalized pole λ_0 of $\widetilde{G}$ is indeed 2, that is, $\widetilde{G} \in \mathcal{N}_2^{2\times 2}$.

Next we show that instead of considering $\widetilde{Q}$ directly one can also count the negative squares of a different generalized Nevanlinna function Q, which turns out to be more convenient. For this, consider the functions

$$q_m(\lambda) := \frac{\lambda}{(\lambda-\lambda_0)(\lambda-\overline{\lambda}_0)}\, m(\lambda) \in \mathcal{N}_{\kappa_m+1} \tag{4.10}$$

and

$$q_\tau(\lambda) := \frac{\lambda}{(\lambda-\lambda_0)(\lambda-\overline{\lambda}_0)}\, \tau(\lambda) \in \mathcal{N}_{\kappa_\tau+1}. \tag{4.11}$$

That $q_m \in \mathcal{N}_{\kappa_m+1}$ and $q_\tau \in \mathcal{N}_{\kappa_\tau+1}$ can be seen as follows: Since $m \in \mathcal{D}_{\kappa_m}$ there exists a function $\widetilde{q}_m \in \mathcal{N}_{\kappa_m}$ holomorphic in λ_0 and a rational function g_m holomorphic in $\overline{\mathbb{C}}\backslash\{\lambda_0, \overline{\lambda}_0\}$ such that

$$\frac{\lambda}{(\lambda-\lambda_0)(\lambda-\overline{\lambda}_0)}\, m(\lambda) = \widetilde{q}_m(\lambda) + g_m(\lambda).$$

Since $\lambda_0 \in \mathfrak{h}(m^{-1})$ the rational function g_m has a simple pole at the non-real point λ_0. Hence it belongs to $\mathcal{N}_1$ and according to Lemma 2.6 it holds $\widetilde{q}_m + g_m = q_m \in \mathcal{N}_{\kappa_m+1}$. The same reasoning applies to $q_\tau \in \mathcal{D}_{\kappa_\tau}$.

Define Q via the functions q_m and q_τ from (4.10) and (4.11) by

$$Q(\lambda) := \begin{pmatrix} \lambda-\overline{\lambda}_0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{\lambda-\lambda_0}{\lambda} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} q_m(\lambda) & -1 \\ -1 & -\frac{1}{q_\tau(\lambda)} \end{pmatrix} \begin{pmatrix} \frac{\lambda-\overline{\lambda}_0}{\lambda} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \lambda-\lambda_0 & 0 \\ 0 & 1 \end{pmatrix}. \tag{4.12}$$

Multiplying the factors on the right side of (4.12) gives

$$Q(\lambda) = \begin{pmatrix} \frac{(\lambda-\lambda_0)^2(\lambda-\overline{\lambda}_0)^2}{\lambda^2} q_m(\lambda) & -\frac{(\lambda-\lambda_0)(\lambda-\overline{\lambda}_0)}{\lambda} \\ -\frac{(\lambda-\lambda_0)(\lambda-\overline{\lambda}_0)}{\lambda} & -\frac{1}{q_\tau(\lambda)} \end{pmatrix} = \frac{(\lambda-\lambda_0)(\lambda-\overline{\lambda}_0)}{\lambda} \begin{pmatrix} m(\lambda) & -1 \\ -1 & -\frac{1}{\tau(\lambda)} \end{pmatrix}$$

and hence (4.9) implies $-Q^{-1} = \widetilde{Q} + \widetilde{G}$. Since $\widetilde{Q} \in \mathcal{N}_\kappa^{2\times 2}$ is holomorphic in λ_0 and $\widetilde{G} \in \mathcal{N}_2^{2\times 2}$ is holomorphic in $\overline{\mathbb{C}}\backslash\{\lambda_0, \overline{\lambda}_0\}$ it follows from Lemma 2.6 that $-Q^{-1} = \widetilde{Q} + \widetilde{G}$ belongs to the class $\mathcal{N}_{\kappa+2}^{2\times 2}$ and by Lemma 2.2 this is equivalent to $Q \in \mathcal{N}_{\kappa+2}^{2\times 2}$, i.e.

$$\widetilde{Q} \in \mathcal{N}_\kappa^{2\times 2} \quad \text{if and only if} \quad Q \in \mathcal{N}_{\kappa+2}^{2\times 2}.$$

The idea for obtaining the negative index of Q is now the following: From (4.10) and (4.11) we see directly that the function

$$\Omega(\lambda) := \begin{pmatrix} q_m(\lambda) & -1 \\ -1 & -\frac{1}{q_\tau(\lambda)} \end{pmatrix} \tag{4.13}$$

belongs to the class $\mathcal{N}^{2\times 2}_{\kappa_m+\kappa_\tau+2}$. With the help of Proposition 3.1 we are going to calculate the numbers Δ_0 and Δ_∞, which describe the change of the negative index induced by the multiplication with the factors

$$\begin{pmatrix} \frac{\lambda-\lambda_0}{\lambda} & 0 \\ 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} \frac{\lambda-\overline{\lambda}_0}{\lambda} & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \lambda-\overline{\lambda}_0 & 0 \\ 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} \lambda-\lambda_0 & 0 \\ 0 & 1 \end{pmatrix},$$

respectively. Then

$$\kappa = \kappa(\widetilde{Q}) = \kappa(Q) - 2 = \kappa_m + \kappa_\tau + 2 + \Delta_0 + \Delta_\infty - 2 = \kappa_m + \kappa_\tau + \Delta_0 + \Delta_\infty.$$

It remains to show the formulas for Δ_0 and Δ_∞ given as in the formulation of Theorem 4.5. This is done in Lemma 4.6 below for Δ_0 and for Δ_∞ in Lemma 4.7 below. □

Lemma 4.6 *Let $m \in \mathcal{D}_{\kappa_m}$ and $\tau \in \mathcal{D}_{\kappa_\tau}$ be as in the assumptions of Theorem 4.5, let $\Omega \in \mathcal{N}^{2\times 2}_{\kappa_m+\kappa_\tau+2}$ be the generalized Nevanlinna function in (4.13) and let $\lambda_0 \in \mathbb{C}^+$ be as in (4.8) . Then*

$$\widetilde{\Omega}(\lambda) := \begin{pmatrix} \frac{\lambda-\lambda_0}{\lambda} & 0 \\ 0 & 1 \end{pmatrix} \Omega(\lambda) \begin{pmatrix} \frac{\lambda-\overline{\lambda}_0}{\lambda} & 0 \\ 0 & 1 \end{pmatrix} \in \mathcal{N}^{2\times 2}_{\kappa(\Omega)+\Delta_0}, \tag{4.14}$$

where

$$\Delta_0 = \begin{cases} -1 & \text{if } \lim\limits_{\lambda \hat{\to} 0} m(\lambda) \text{ and } \lim\limits_{\lambda \hat{\to} 0} \tau(\lambda) \text{ exist and } \lim\limits_{\lambda \hat{\to} 0} (m(\lambda)+\tau(\lambda)) \le 0, \\ 0 & \text{otherwise.} \end{cases}$$

P r o o f. In view of Proposition 3.1 we first calculate the index shift Δ_0 in different cases depending on the behavior of Ω at the point zero. Then these results will be summarized in terms of the behavior of m and τ.

Note first that the product in (4.14) is of the form (3.3) with $\vec{\varphi} = \vec{\psi} = (1,0)^\top$ and the points $\delta = \lambda_0$ and $\gamma = 0$. Since

$$\Omega(\lambda) = \begin{pmatrix} \frac{\lambda}{(\lambda-\lambda_0)(\lambda-\overline{\lambda}_0)}\, m(\lambda) & -1 \\ -1 & -\frac{(\lambda-\lambda_0)(\lambda-\overline{\lambda}_0)}{\lambda} \frac{1}{\tau(\lambda)} \end{pmatrix}$$

we see that assumption (4.8) on the choice of the point λ_0 implies that $\delta = \lambda_0$ is a pole of Ω with pole vector $\vec{\varphi} = (1,0)^\top$, which is neutral since $\lambda_0 \in \mathbb{C} \setminus \mathbb{R}$. For $\gamma = 0$ we are going to discuss the different cases separately.

(a) If 0 is a generalized zero of Ω with non-positive root vector $(1,0)^\top$, then Proposition 3.1 (1a) gives directly $\Delta_0 = -1$.

(b) If 0 is a generalized zero of Ω with positive root vector $(1,0)^\top$, then Proposition 3.1 (1b) yields $\Delta_0 = 0$.

In the remaining cases, where 0 is either a generalized zero of Ω but $(1,0)^\top$ is not a corresponding root vector or 0 is no generalized zero of Ω, Proposition 3.1 cannot be applied directly. Due to this fact we rewrite (4.14) as the product

$$\Omega(\lambda) = \begin{pmatrix} \frac{\lambda}{\lambda-\lambda_0} & 0 \\ 0 & 1 \end{pmatrix} \widetilde{\Omega}(\lambda) \begin{pmatrix} \frac{\lambda}{\lambda-\overline{\lambda}_0} & 0 \\ 0 & 1 \end{pmatrix} \tag{4.15}$$

and note

$$\widetilde{\Omega}(\lambda) = \begin{pmatrix} \frac{m(\lambda)}{\lambda} & -\frac{\lambda-\lambda_0}{\lambda} \\ -\frac{\lambda-\overline{\lambda}_0}{\lambda} & -\frac{(\lambda-\lambda_0)(\lambda-\overline{\lambda}_0)}{\lambda} \frac{1}{\tau(\lambda)} \end{pmatrix}. \tag{4.16}$$

Obviously, also (4.15) is of the form (3.3), now with the points $\gamma = \overline{\lambda}_0$, $\delta = 0$ and again the vectors $\vec{\varphi} = \vec{\psi} = (1,0)^\top$. In order to avoid dealing with the fact that $\gamma = \overline{\lambda}_0$ is a generalized zero of $\widetilde{\Omega}$ (as $\det \widetilde{\Omega}(\overline{\lambda}_0) = 0$, cf. Remark 2.8) we introduce the function

$$\widetilde{\Omega}^{(1)}(\lambda) := \widetilde{\Omega}(\lambda) + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \tag{4.17}$$

which leads to

$$\Omega^{(1)}(\lambda) := \begin{pmatrix} \frac{\lambda}{\lambda-\lambda_0} & 0 \\ 0 & 1 \end{pmatrix} \widetilde{\Omega}^{(1)}(\lambda) \begin{pmatrix} \frac{\lambda}{\lambda-\overline{\lambda}_0} & 0 \\ 0 & 1 \end{pmatrix} = \Omega(\lambda) + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \tag{4.18}$$

Now $\gamma = \overline{\lambda}_0 \in \mathbb{C}\backslash\mathbb{R}$ is neither a pole nor a zero of $\widetilde{\Omega}^{(1)}$ since it belongs to the domain of holomorphy and $\widetilde{\Omega}^{(1)}(\overline{\lambda}_0)$ is invertible. After this preparation we are ready to deal with the remaining cases.

(c) If 0 is not a generalized zero of Ω, then Lemma 3.2 and (4.14) imply that 0 is a generalized pole of $\widetilde{\Omega}$ with non-positive pole vector $(1,0)^\top$ and hence also of $\widetilde{\Omega}^{(1)}$. Then Proposition 3.1 (2) applied to (4.18) gives $\kappa(\widetilde{\Omega}^{(1)}) = \kappa(\Omega^{(1)})$ and together with (4.17) and (4.18) we obtain $\kappa(\widetilde{\Omega}) = \kappa(\Omega)$, that is, $\Delta_0 = 0$.

(d) Finally, assume that 0 is a generalized zero of Ω, but $(1,0)^\top$ is not a root vector. We claim that then the function $\Omega^{(1)}$ in (4.18) has no generalized zero at 0. In fact, write $\Omega^{(1)}$ as

$$\Omega^{(1)}(\lambda) = \begin{pmatrix} q_m(\lambda) & -1 \\ -1 & -\frac{1}{q_\tau^{(1)}(\lambda)} \end{pmatrix} \quad \text{with} \quad q_\tau^{(1)}(\lambda) := -\frac{1}{-\frac{1}{q_\tau(\lambda)} + 1}, \tag{4.19}$$

where q_m and q_τ are as in (4.10) and (4.11), respectively. In what follows we are making frequent use of Proposition 3.3. The assumption that 0 is a generalized zero of Ω splits into two further subcases in Proposition 3.3. In the first case 0 is a generalized pole of both q_m and q_τ, but then $q_\tau^{(1)}$ obviously has no generalized pole at 0 and Proposition 3.3 applied to $\Omega^{(1)}$ implies that 0 cannot be a generalized zero of $\Omega^{(1)}$. In the second case 0 is a generalized zero of $q_m + q_\tau$ and the limits $\lim_{\lambda \hat{\to} 0} q_\tau(\lambda) = -\lim_{\lambda \hat{\to} 0} q_m(\lambda)$ exist and are not equal to zero since by assumption $(1,0)^\top$ is not a corresponding root vector of Ω at 0. Hence, from (4.19) we have that if $\lim_{\lambda \hat{\to} 0} q_\tau^{(1)}(\lambda)$ exists, then $\lim_{\lambda \hat{\to} 0} q_m(\lambda) + \lim_{\lambda \hat{\to} 0} q_\tau^{(1)}(\lambda) \neq 0$. Therefore, Proposition 3.3 yields that also in this case 0 is not a generalized zero of $\Omega^{(1)}$. As 0 is not a generalized zero of $\Omega^{(1)}$, Lemma 3.2 and

$$\widetilde{\Omega}^{(1)}(\lambda) = \begin{pmatrix} \frac{\lambda-\lambda_0}{\lambda} & 0 \\ 0 & 1 \end{pmatrix} \Omega^{(1)}(\lambda) \begin{pmatrix} \frac{\lambda-\overline{\lambda}_0}{\lambda} & 0 \\ 0 & 1 \end{pmatrix}.$$

imply that 0 is a generalized pole of $\widetilde{\Omega}^{(1)}$ with non-positive pole vector $(1,0)^\top$. As in the preceding case **(c)** we obtain from Proposition 3.1 (2) that $\Delta_0 = 0$.

Summing up, we have shown $\Delta_0 = 0$ in all cases except when 0 is a generalized zero of Ω and $(1,0)^\top$ is a corresponding non-positive root vector, in which case $\Delta_0 = -1$. In the latter case, taking into account the particular root vector and Proposition 3.3 (ii), it follows that

$$\lim_{\lambda \hat{\to} 0} q_m(\lambda) = 0 = \lim_{\lambda \hat{\to} 0} q_\tau(\lambda) \qquad \text{and} \qquad \lim_{\lambda \hat{\to} 0} \frac{q_m(\lambda) + q_\tau(\lambda)}{\lambda} \leq 0 \tag{4.20}$$

holds. From (4.10), (4.11), and Lemma 2.11 we conclude that also the limits

$$\lim_{\lambda \hat{\to} 0} m(\lambda) = \lim_{\lambda \hat{\to} 0} (\lambda - \lambda_0)(\lambda - \overline{\lambda}_0)\frac{q_m(\lambda)}{\lambda} \quad \text{and} \quad \lim_{\lambda \hat{\to} 0} \tau(\lambda) = \lim_{\lambda \hat{\to} 0} (\lambda - \lambda_0)(\lambda - \overline{\lambda}_0)\frac{q_\tau(\lambda)}{\lambda}$$

exist. Furthermore, the inequality in (4.20) implies

$$\lim_{\lambda \hat{\to} 0} m(\lambda) + \tau(\lambda) = \lim_{\lambda \hat{\to} 0} \big((\lambda - \lambda_0)(\lambda - \overline{\lambda}_0)\big)\frac{q_m(\lambda) + q_\tau(\lambda)}{\lambda} \leq 0,$$

which completes the proof of Lemma 4.6. □

Finally we prove the statement on Δ_∞.

Lemma 4.7 *Let $m \in \mathcal{D}_{\kappa_m}$ and $\tau \in \mathcal{D}_{\kappa_\tau}$ be as in the assumptions of Theorem 4.5, let $\widetilde{\Omega}$ be the generalized Nevanlinna function in (4.14) and let $\lambda_0 \in \mathbb{C}^+$ be as in (4.8). Then*

$$\begin{pmatrix} \lambda-\overline{\lambda}_0 & 0 \\ 0 & 1 \end{pmatrix} \widetilde{\Omega}(\lambda) \begin{pmatrix} \lambda-\lambda_0 & 0 \\ 0 & 1 \end{pmatrix} \in \mathcal{N}^{2\times 2}_{\kappa(\widetilde{\Omega})+\Delta_\infty}, \tag{4.21}$$

where

$$\Delta_\infty = \begin{cases} 0 & \text{if } \lim\limits_{\lambda \hat{\to} \infty} m(\lambda) \text{ and } \lim\limits_{\lambda \hat{\to}\infty} \tau(\lambda) \text{ exist and } \lim\limits_{\lambda\hat{\to}\infty}(m(\lambda)+\tau(\lambda)) \geq 0, \\ 1 & \text{otherwise.} \end{cases}$$

P r o o f. In order to use Proposition 3.1 we rewrite (4.21) by setting $w = -\frac{1}{\lambda}$ and $w_0 = -\frac{1}{\lambda_0}$. Then

$$\lambda - \overline{\lambda}_0 = \frac{w-\overline{w}_0}{w\overline{w}_0} \qquad \text{and} \qquad \lambda-\lambda_0 = \frac{w-w_0}{ww_0}$$

and, due to Lemma 2.2, the statement of Lemma 4.7 is equivalent to

$$\begin{pmatrix} \frac{1}{\overline{w}_0} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{w-\overline{w}_0}{w} & 0 \\ 0 & 1 \end{pmatrix} \widetilde{\Omega}\left(-\frac{1}{w}\right) \begin{pmatrix} \frac{w-w_0}{w} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{w_0} & 0 \\ 0 & 1 \end{pmatrix} \in \mathcal{N}^{2\times 2}_{\kappa(\widetilde{\Omega})+\Delta_\infty}.$$

It follows from (4.16) that

$$\Lambda(w) := \widetilde{\Omega}\left(-\frac{1}{w}\right) = \begin{pmatrix} -wm\left(-\frac{1}{w}\right) & \frac{w-w_0}{w_0} \\ \frac{w-\overline{w}_0}{\overline{w}_0} & \frac{(w-w_0)(w-\overline{w}_0)}{ww_0\overline{w}_0} \cdot \frac{1}{\tau\left(-\frac{1}{w}\right)} \end{pmatrix}, \tag{4.22}$$

and since these constant factors do not change the negative index the above statement is equivalent to

$$\widetilde{\Lambda}(w) := \begin{pmatrix} \frac{w-\overline{w}_0}{w} & 0 \\ 0 & 1 \end{pmatrix} \Lambda(w) \begin{pmatrix} \frac{w-w_0}{w} & 0 \\ 0 & 1 \end{pmatrix} \in \mathcal{N}^{n\times n}_{\kappa(\Lambda)+\Delta_\infty}. \tag{4.23}$$

With (4.22) and (4.8) the function Λ is analytic in $\delta = \overline{w}_0 = -\frac{1}{\overline{\lambda}_0}$ and $\det \Lambda(\overline{w}_0) = 0$, hence $\overline{w}_0$ is a generalized zero of Λ; cf. Remark 2.8. In order to apply Proposition 3.1, we introduce the functions

$$\Lambda^{(1)}(w) := \Lambda(w) + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \tag{4.24}$$

and

$$\widetilde{\Lambda}^{(1)}(w) := \begin{pmatrix} \frac{w-\overline{w}_0}{w} & 0 \\ 0 & 1 \end{pmatrix} \Lambda^{(1)}(w) \begin{pmatrix} \frac{w-w_0}{w} & 0 \\ 0 & 1 \end{pmatrix} = \widetilde{\Lambda}(w) + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \tag{4.25}$$

Observe that

$$\kappa(\Lambda) = \kappa(\Lambda^{(1)}) \quad \text{and} \quad \kappa(\widetilde{\Lambda}) = \kappa(\widetilde{\Lambda}^{(1)}). \tag{4.26}$$

In the notation of Proposition 3.1 we again have $\vec{\varphi} = \vec{\psi} = (1,0)^\top$, $\gamma = 0$ and $\delta = \overline{w}_0$ for both (4.23) and (4.25). The point $\delta = \overline{w}_0$ is neither a pole nor a zero of the function $\Lambda^{(1)}$. Again we are going to discuss the different cases for $\gamma = 0$.

(a) If 0 is a generalized zero of Λ with non-positive root vector $(1,0)^\top$, then 0 is also a generalized zero of $\Lambda^{(1)}$ with non-positive root vector $(1,0)^\top$ and hence (4.26) and Proposition 3.1 (3a) applied to (4.25) yield $\Delta_\infty = 0$.

(b) If 0 is a generalized zero of Λ with positive root vector $(1,0)^\top$, then Proposition 3.1 (3b) yields $\Delta_\infty = 1$.

(c) If 0 is not a generalized zero of Λ, then Lemma 3.2 and (4.23) imply that 0 is a generalized pole of $\widetilde{\Lambda}$ with non-positive pole vector $(1,0)^\top$ and hence also of $\widetilde{\Lambda}^{(1)}$. Furthermore, since $\widetilde{\Lambda}(w_0) = 0$ we have

$$\widetilde{\Lambda}^{(1)}(w_0) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},$$

that is w_0 is a generalized zero of $\widetilde{\Lambda}^{(1)}$ with (neutral) root vector $(1,0)^\top$; cf. Remark 2.8. Therefore, Proposition 3.1 (1a) applied to

$$\Lambda^{(1)}(w) = \begin{pmatrix} \frac{w}{w-\overline{w}_0} & 0 \\ 0 & 1 \end{pmatrix} \widetilde{\Lambda}^{(1)}(w) \begin{pmatrix} \frac{w}{w-w_0} & 0 \\ 0 & 1 \end{pmatrix},$$

where $\vec{\varphi} = \vec{\psi} = (1,0)^\top$, $\gamma = w_0$ and $\delta = 0$, yields together with (4.26)

$$\kappa(\Lambda) = \kappa(\Lambda^{(1)}) = \kappa(\widetilde{\Lambda}^{(1)}) - 1 = \kappa(\widetilde{\Lambda}) - 1,$$

and hence in this case $\Delta_\infty = 1$.

(d) Finally, assume that 0 is a generalized zero of Λ, but $(1,0)^\top$ is not a root vector. We claim that then the function $\Lambda^{(1)}$ in (4.24) has no generalized zero at 0. To this end we rewrite Λ and $\Lambda^{(1)}$ in such a way that Proposition 3.3 can be applied. We set

$$h_m(w) := -wm\left(-\frac{1}{w}\right) \quad \text{and} \quad h_\tau(w) := \frac{-ww_0\overline{w}_0}{(w-w_0)(w-\overline{w}_0)}\,\tau\left(-\frac{1}{w}\right). \tag{4.27}$$

Then the functions h_m and h_τ are scalar generalized Nevanlinna functions, which follows directly from applying the Möbius transform $w = -\frac{1}{\lambda}$, Lemma 2.2 and Lemma 2.3, and the fact that $m \in \mathcal{D}_{\kappa_m}$ and $\tau \in \mathcal{D}_{\kappa_\tau}$. We have

$$\Lambda(w) = \Lambda_0(w) + w\begin{pmatrix} 0 & \frac{1}{w_0} \\ \frac{1}{\overline{w}_0} & 0 \end{pmatrix} \quad \text{and} \quad \Lambda^{(1)}(w) = \Lambda_0^{(1)}(w) + w\begin{pmatrix} 0 & \frac{1}{w_0} \\ \frac{1}{\overline{w}_0} & 0 \end{pmatrix}, \tag{4.28}$$

where

$$\Lambda_0(w) := \begin{pmatrix} h_m(w) & -1 \\ -1 & -\frac{1}{h_\tau(w)} \end{pmatrix}, \quad \Lambda_0^{(1)}(w) := \begin{pmatrix} h_m(w) & -1 \\ -1 & -\frac{1}{h_\tau^{(1)}(w)} \end{pmatrix}, \quad h_\tau^{(1)}(w) := \frac{-1}{-\frac{1}{h_\tau(w)}+1}.$$

Observe that $\vec{\xi}$ is a root function of Λ ($\Lambda^{(1)}$) at $w=0$ if and only if it is a root function of Λ_0 ($\Lambda_0^{(1)}$, respectively) at $w=0$, where the type of the root vector may have changed. Hence it suffices to show that if 0 is a generalized zero of Λ_0 but $(1,0)^\top$ is not a root vector, then 0 is not a generalized zero of $\Lambda_0^{(1)}$. As in part **(d)** of the proof of Lemma 4.6, due to Proposition 3.3, the assumption splits into two subcases. If 0 is a generalized pole of h_m and h_τ, then $h_\tau^{(1)}$ has no generalized pole at 0 and Proposition 3.3 applied to $\Lambda_0^{(1)}$ implies that 0 cannot be a generalized zero of $\Lambda_0^{(1)}$. In the second case 0 is a generalized zero of $h_m + h_\tau$ and the limits $\lim_{w \hat{\to} 0} h_m(w) = -\lim_{w \hat{\to} 0} h_\tau(w)$ exist and are not equal to zero since by assumption $(1,0)^\top$ is not a corresponding root vector of Λ_0 at 0. Hence, from (4.28) we have that if $\lim_{w \hat{\to} 0} h_\tau^{(1)}(w)$ exists, then $\lim_{w \hat{\to} 0} h_m(w) + \lim_{w \hat{\to} 0} h_\tau^{(1)}(\lambda) \neq 0$. Therefore, Proposition 3.3 yields that also in this case 0 is not a generalized zero of $\Lambda_0^{(1)}$. Thus, 0 is not a generalized zero of $\Lambda^{(1)}$ and the above claim is proved.

Lemma 3.2 and (4.25) imply that the point 0 is a generalized pole of

$$\widetilde{\Lambda}^{(1)}(w) = \begin{pmatrix} \frac{w-\overline{w}_0}{w} & 0 \\ 0 & 1 \end{pmatrix} \Lambda^{(1)}(w) \begin{pmatrix} \frac{w-w_0}{w} & 0 \\ 0 & 1 \end{pmatrix},$$

with non-positive pole vector $(1,0)^\top$. As in case **(c)** it follows $\Delta_\infty = 1$.

Summing up, we have shown $\Delta_\infty = 1$ in all cases except when 0 is a generalized zero of Λ and $(1,0)^\top$ is a corresponding non-positive root vector, in which case $\Delta_\infty = 0$. As

$$\left(\begin{pmatrix} 0 & \frac{1}{w_0} \\ \frac{1}{\overline{w}_0} & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \end{pmatrix}\right) = 0,$$

one concludes with (4.28) that in the latter case 0 is a generalized zero of Λ_0 with non-positive root vector $(1,0)^\top$. Hence, taking into account the particular root vector and Proposition 3.3 (ii), it follows that

$$\lim_{w \hat{\to} 0} h_m(w) = 0 = \lim_{w \hat{\to} 0} h_\tau(w) \qquad \text{and} \qquad \lim_{w \hat{\to} 0} \frac{h_m(w) + h_\tau(w)}{w} \leq 0 \tag{4.29}$$

holds. From (4.27) and Lemma 2.11 we conclude that also the limits

$$\lim_{\lambda \hat{\to} \infty} m(\lambda) = \lim_{w \hat{\to} 0} m\left(-\frac{1}{w}\right) = -\lim_{w \hat{\to} 0} \frac{h_m(w)}{w} \tag{4.30}$$

and

$$\lim_{\lambda \hat{\to} \infty} \tau(\lambda) = \lim_{w \hat{\to} 0} \tau\left(-\frac{1}{w}\right) = -\lim_{w \hat{\to} 0} \frac{(w - w_0)(w - \overline{w}_0)}{w_0 \overline{w}_0} \frac{h_\tau(w)}{w} \tag{4.31}$$

exist. Furthermore, the inequality in (4.29) together with (4.30) and (4.31) implies

$$\lim_{\lambda \hat{\to} \infty} m(\lambda) + \tau(\lambda) = \lim_{w \hat{\to} 0} m\left(-\frac{1}{w}\right) + \tau\left(-\frac{1}{w}\right) = -\lim_{w \hat{\to} 0} \frac{h_m(w) + h_\tau(w)}{w} \geq 0,$$

which completes the proof of Lemma 4.7. □

Remark 4.8 For the sake of completeness we mention that $\kappa_m = \kappa_\tau = 0$ in Theorem 4.5 implies $\Delta_0 + \Delta_\infty \geq 0$. That is, we have always $\kappa \geq 0$ in Theorem 4.5. Indeed, choose λ_0 as in (4.8), then, with (4.10) and (4.11),

$$q_m + q_\tau \in \mathcal{N}_0 \cup \mathcal{N}_1.$$

Hence, at least one point in $\{0, \infty\}$ is not a generalized zero of non-positive type of $q_m + q_\tau$ and $\Delta_0 + \Delta_\infty \geq 0$ follows.

Remark 4.9 Note that only in the special case of $m \equiv 0$ we made use of the corresponding statement for scalar $\mathcal{D}_\kappa$-functions in Theorem 4.4 from [11]. However, alternatively this result would also follow from investigating the case $m = \tau$.

Part II. Self-adjoint exit space extensions of symmetric operators in Krein spaces

In this second part of the paper we first briefly recall the concept of boundary triplets and associated Weyl functions of symmetric operators and relations in Krein spaces; cf. [18, 20], and then we investigate direct products of symmetric relations in different Krein spaces in a similar manner as in [22]. These considerations will be useful in the proofs of our main results on the negative squares of self-adjoint exit space extensions of symmetric operators of defect one with finitely many negative squares in Section 7. First a Krein-type formula in the indefinite setting will be proved and then the negative squares of the extensions will be described with the help of the main result Theorem 4.5 in Part I.

5 Boundary triplets and Weyl functions

Let $(\mathcal{K}, [\cdot,\cdot])$ be a separable Krein space with fundamental symmetry J. For the basic theory of Krein spaces and operators acting therein we refer to [2] and [12]. We study linear relations in $\mathcal{K}$, that is, linear subspaces of $\mathcal{K} \times \mathcal{K}$. The set of all closed linear relations in $\mathcal{K}$ will be denoted by $\widetilde{\mathcal{C}}(\mathcal{K})$. For a linear relation A we write $\operatorname{dom} A$, $\operatorname{ran} A$, $\ker A$ and $\operatorname{mul} A$ for the domain, range, kernel and multivalued part of A, respectively. The elements in a linear relation A will usually be written in the form $\{x, x'\}$, where $x \in \operatorname{dom} A$ and $x' \in \operatorname{ran} A$. For the usual definitions of the linear operations with relations, the inverse etc., we refer to [1, 14]. Linear operators are identified with linear relations via their graphs.

Let A be a linear relation in the Krein space $\mathcal{K}$. Then the *adjoint relation* $A^+ \in \widetilde{\mathcal{C}}(\mathcal{K})$ is defined by

$$A^+ := \big\{\{y, y'\} : [x', y] = [x, y'] \text{ for all } \{x, x'\} \in A\big\}.$$

Note that this definition extends the usual definition of the adjoint of a densely defined operator in a Krein space, see, e.g. [2]. If $\mathcal{L}$ is an arbitrary subset of the Krein space $\mathcal{K}$ we set $\mathcal{L}^{[\perp]} := \{x \in \mathcal{K} : [x, y] = 0 \text{ for all } y \in \mathcal{L}\}$. As $\operatorname{mul} A = (\operatorname{dom} A^+)^{[\perp]}$ and $\operatorname{mul} A^+ = (\operatorname{dom} A)^{[\perp]}$ it is clear that A (A^+) is an operator if and only if $\operatorname{dom} A^+$ ($\operatorname{dom} A$, respectively) is dense. If A is a linear relation in the Krein space $(\mathcal{K}, [\cdot,\cdot])$, then A is said to be *symmetric* (*self-adjoint*) if $A \subset A^+$ ($A = A^+$, respectively).

Let $A \in \widetilde{\mathcal{C}}(\mathcal{K})$ be a closed symmetric relation in $\mathcal{K}$. We say that A is of *defect* $m \in \mathbb{N}_0 \cup \{\infty\}$, if both deficiency indices

$$n_\pm(JA) = \dim \ker\, ((JA)^* - \overline{\lambda}), \qquad \lambda \in \mathbb{C}^\pm,$$

of the symmetric relation JA in the Hilbert space $(\mathcal{K}, [J\cdot,\cdot])$ are equal to m; here * stands for the Hilbert space adjoint. This is equivalent to the fact that there exist self-adjoint extensions of A in $\mathcal{K}$ and that each self-adjoint extension $\hat{A}$ of A in $\mathcal{K}$ satisfies $\dim(\hat{A}/A) = m$.

We shall use the so-called boundary triplets for the description of the self-adjoint extensions of closed symmetric relations in Krein spaces. The following definition is taken from [20].

Definition 5.1 Let A be a closed symmetric relation in the Krein space $\mathcal{K}$. We say that $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is a *boundary triplet* for A^+ if $(\mathcal{G}, (\cdot,\cdot))$ is a Hilbert space and there exist mappings $\Gamma_0, \Gamma_1 : A^+ \to \mathcal{G}$ such that $\Gamma := \binom{\Gamma_0}{\Gamma_1} : A^+ \to \mathcal{G} \times \mathcal{G}$ is surjective and the identity

$$[f', g] - [f, g'] = (\Gamma_1 \hat{f}, \Gamma_0 \hat{g}) - (\Gamma_0 \hat{f}, \Gamma_1 \hat{g}) \tag{5.1}$$

holds for all $\hat{f} = \{f, f'\}, \hat{g} = \{g, g'\} \in A^+$.

In the following we recall some basic facts on boundary triplets which can be found in, e.g., [18] and [20]. For the Hilbert space case we refer to [25, 26, 34]. Let A be a closed symmetric relation in $\mathcal{K}$. Note first that each boundary triplet $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ for A^+ is also a boundary triplet for the adjoint $(JA)^*$ of the closed symmetric relation in the Hilbert space $(\mathcal{K}, [J\cdot,\cdot])$ and vice versa. This allows to translate many facts from the Hilbert to the Krein space case. E.g., it follows that a boundary triplet for A^+ exists if and only if A admits self-adjoint extensions in the Krein space $(\mathcal{K}, [\cdot,\cdot])$. Let in the following $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ and $\Gamma = (\Gamma_0, \Gamma_1)^\top$ be as in Definition 5.1. Then $A = \ker \Gamma$, the mappings Γ_0 and Γ_1 are continuous and the self-adjoint extensions $A_0 := \ker \Gamma_0$ and $A_1 := \ker \Gamma_1$ of A are transversal, that is, $A_0 \cap A_1 = A$ and $A_0 \,\widehat{+}\, A_1 = A^+$, where $\widehat{+}$ denotes the sum of subspaces. The mapping Γ induces, via

$$A_\Theta := \Gamma^{(-1)}\Theta = \big\{\hat{f} \in A^+ \,|\, \Gamma \hat{f} \in \Theta\big\} = \ker\, (\Gamma_1 - \Theta\Gamma_0), \quad \Theta \in \widetilde{\mathcal{C}}(\mathcal{G}), \tag{5.2}$$

a bijective correspondence $\Theta \mapsto A_\Theta$ between the set of closed linear relations $\widetilde{\mathcal{C}}(\mathcal{G})$ in $\mathcal{G}$ and the set of closed extensions $A_\Theta \subset A^+$ of A. Note that the product and sum in the expression $\ker\, (\Gamma_1 - \Theta\Gamma_0)$ in (5.2) are understood in the sense of linear relations. Moreover, $A_{\Theta^*} = (A_\Theta)^+$ holds and, hence, (5.2) gives a one-to-one correspondence between the closed symmetric (self-adjoint) extensions of A in the Krein space $(\mathcal{K}, [\cdot,\cdot])$ and the closed symmetric (self-adjoint, respectively) relations in $\mathcal{G}$ in the Hilbert space $(\mathcal{G}, (\cdot,\cdot))$.

For a closed symmetric relation A the defect subspace at the point λ is defined as

$$\mathcal{N}_{\lambda, A^+} := \ker\, (A^+ - \lambda) = \operatorname{ran}(A - \overline{\lambda})^{[\perp]}$$

and we set

$$\hat{\mathcal{N}}_{\lambda, A^+} = \big\{\{f_\lambda, \lambda f_\lambda\} : f_\lambda \in \mathcal{N}_{\lambda, A^+}\big\}.$$

When no confusion can arise we will simply write $\mathcal{N}_\lambda$ and $\hat{\mathcal{N}}_\lambda$ instead of $\mathcal{N}_{\lambda, A^+}$ and $\hat{\mathcal{N}}_{\lambda, A^+}$, respectively.

Let again $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^+ and assume, in addition, that the resolvent set of the self-adjoint relation $A_0 = \ker \Gamma_0$ is nonempty, i.e., there exist $\lambda \in \mathbb{C}$ such that $(A_0 - \lambda)^{-1}$ is an everywhere defined bounded operator in $\mathcal{K}$. Then we have

$$A^+ = A_0 \,\widehat{+}\, \hat{\mathcal{N}}_\lambda, \quad \text{direct sum},$$

for all $\lambda \in \rho(A_0)$. If π_1 denotes the projection onto the first component of $\mathcal{K} \times \mathcal{K}$, then for every $\lambda \in \rho(A_0)$ the operators

$$\gamma(\lambda) = \pi_1\big(\Gamma_0 \upharpoonright \hat{\mathcal{N}}_\lambda\big)^{-1} \quad \text{and} \quad m(\lambda) = \Gamma_1\big(\Gamma_0 \upharpoonright \hat{\mathcal{N}}_\lambda\big)^{-1}$$

are well defined and belong to $\mathcal{L}(\mathcal{G}, \mathcal{K})$ and $\mathcal{L}(\mathcal{G})$, respectively. Here $\mathcal{L}(\mathcal{G}, \mathcal{K})$ stands for the space of bounded everywhere defined linear operators mapping from $\mathcal{G}$ into $\mathcal{K}$ and $\mathcal{L}(\mathcal{G})$ is used instead of $\mathcal{L}(\mathcal{G}, \mathcal{G})$. The functions $\lambda \mapsto \gamma(\lambda)$ and $\lambda \mapsto m(\lambda)$ are called the *γ-field* and the *Weyl function* corresponding to A and $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$. The functions γ and m are holomorphic on $\rho(A_0)$ and the relations

$$\gamma(\zeta) = \big(1 + (\zeta - \lambda)(A_0 - \zeta)^{-1}\big)\gamma(\lambda) \tag{5.3}$$

and

$$m(\lambda) - m(\zeta)^* = (\lambda - \overline{\zeta})\gamma(\zeta)^+\gamma(\lambda) \tag{5.4}$$

hold for $\lambda, \zeta \in \rho(A_0)$; cf. [20]. It is important to note that in general the set $\rho(A_0)$ can be a proper subset of $\mathfrak{h}(m)\backslash\{\infty\}$; note that ∞ may belong to $\mathfrak{h}(m)$ whereas by definition $\rho(A_0) \subset \mathbb{C}$. Let $\lambda_0 \in \rho(A_0)$. Then (5.4), (5.3) and $\operatorname{Im} m(\lambda_0) = (\operatorname{Im} \lambda_0)\, \gamma(\lambda_0)^+\gamma(\lambda_0)$ imply

$$m(\lambda) = \operatorname{Re}\, m(\lambda_0) + \gamma(\lambda_0)^+\big((\lambda - \operatorname{Re}\lambda_0) + (\lambda - \lambda_0)(\lambda - \overline{\lambda}_0)(A_0 - \lambda)^{-1}\big)\gamma(\lambda_0) \tag{5.5}$$

for all $\lambda \in \rho(A_0)$. If, in addition, the symmetric relation A has the property

$$\mathcal{K} = \operatorname{clsp}\big\{\mathcal{N}_\lambda \,|\, \lambda \in \rho(A_0)\big\}, \tag{5.6}$$

then A is automatically an operator and A_0 fulfils the minimality condition

$$\mathcal{K} = \operatorname{clsp}\big\{\big(1 + (\lambda - \lambda_0)(A_0 - \lambda)^{-1}\big)\gamma(\lambda_0)x \,|\, \lambda \in \rho(A_0),\, x \in \mathcal{G}\big\}. \tag{5.7}$$

In this case we have

$$\mathfrak{h}(m)\backslash\{\infty\} = \rho(A_0) \quad \text{and} \quad \mathfrak{h}(m^{-1})\backslash\{\infty\} = \rho(A_1). \tag{5.8}$$

The following well-known variant of Krein's formula for canonical extensions shows how the resolvents of closed extensions A_Θ of A can be described with the help of the resolvent of the fixed extension A_0, the parameter Θ and the Weyl function. For a proof see, e.g., [20].

Theorem 5.2 *Let A be a closed symmetric relation in the Krein space $\mathcal{K}$, let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^+ and assume that $A_0 = \ker \Gamma_0$ has a nonempty resolvent set. Denote by γ and m the corresponding γ-field and Weyl function, let $\Theta \in \widetilde{\mathcal{C}}(\mathcal{G})$ and let A_Θ be the corresponding extension via* (5.2)*. Then $\lambda \in \rho(A_0)$ belongs to $\rho(A_\Theta)$ if and only if $0 \in \rho(\Theta - m(\lambda))$ and*

$$(A_\Theta - \lambda)^{-1} = (A_0 - \lambda)^{-1} + \gamma(\lambda)\big(\Theta - m(\lambda)\big)^{-1}\gamma(\overline{\lambda})^+$$

holds for all $\lambda \in \rho(A_\Theta) \cap \rho(A_0)$. In particular, for $A_1 = \ker \Gamma_1$ the inclusion $\rho(A_1) \cap \rho(A_0) \subset \mathfrak{h}(m^{-1})$ holds and

$$(A_1 - \lambda)^{-1} = (A_0 - \lambda)^{-1} - \gamma(\lambda)m(\lambda)^{-1}\gamma(\overline{\lambda})^+$$

is valid for all $\lambda \in \rho(A_1) \cap \rho(A_0)$.

6 Direct products of symmetric relations

In this section we collect some results on boundary triplets and Weyl functions for direct products of symmetric linear relations in Krein spaces. The following notation will be useful: If $(\mathcal{K}, [\cdot,\cdot]_{\mathcal{K}})$ and $(\mathcal{H}, [\cdot,\cdot]_{\mathcal{H}})$ are Krein spaces the elements of $\mathcal{K}\times\mathcal{H}$ will be written in the form $\{k,h\}$, $k\in\mathcal{K}$, $h\in\mathcal{H}$. The space $\mathcal{K}\times\mathcal{H}$ equipped with the inner product $[\cdot,\cdot]$ defined by

$$[\{k,h\},\{k',h'\}] := [k,k']_{\mathcal{K}} + [h,h']_{\mathcal{H}}, \quad k,k'\in\mathcal{K},\ \ h,h'\in\mathcal{H},$$

is a Krein space. If A is a relation in $\mathcal{K}$ and T is a relation in $\mathcal{H}$ we shall write $A\times T$ for the direct product of A and T which is a relation in $\mathcal{K}\times\mathcal{H}$,

$$A\times T = \left\{ \begin{pmatrix} \{f,g\} \\ \{f',g'\} \end{pmatrix} \,\middle|\, \{f,f'\}\in A,\ \{g,g'\}\in T \right\}. \tag{6.1}$$

For the pair $\begin{pmatrix} \{f,g\} \\ \{f',g'\} \end{pmatrix}$ on the right hand side of (6.1) we shall also write $\{\hat f,\hat g\}$, where $\hat f = \{f,f'\}$ and $\hat g = \{g,g'\}$.

Let A and T be closed symmetric relations of equal defect $n\le\infty$ in the Krein spaces $\mathcal{K}$ and $\mathcal{H}$ and let $\{\mathcal{G},\Gamma_0,\Gamma_1\}$ and $\{\mathcal{G},\Gamma_0',\Gamma_1'\}$ be boundary triplets for A^+ and T^+, respectively. The corresponding γ-fields and Weyl functions are denoted by γ, γ', m and τ, respectively. The elements in $\mathcal{G}\times\mathcal{G}$ will be written as column vectors. It is easy to see that $A\times T$ is a closed symmetric relation in $\mathcal{K}\times\mathcal{H}$, $(A\times T)^+ = A^+\times T^+$, and $\{\mathcal{G}\times\mathcal{G},\Gamma_0'',\Gamma_1''\}$, where Γ_0'' and Γ_1'' are the mappings from $A^+\times T^+$ into $\mathcal{G}\times\mathcal{G}$ defined by

$$\Gamma_0''\{\hat f,\hat g\} := \begin{pmatrix} \Gamma_0\hat f \\ \Gamma_0'\hat g \end{pmatrix} \quad\text{and}\quad \Gamma_1''\{\hat f,\hat g\} := \begin{pmatrix} \Gamma_1\hat f \\ \Gamma_1'\hat g \end{pmatrix}, \tag{6.2}$$

$\{\hat f,\hat g\}\in A^+\times T^+$, is a boundary triplet for $A^+\times T^+$. Assume that for the self-adjoint relations $A_0 := \ker\Gamma_0$ and $T_0 := \ker\Gamma_0'$ the condition $\rho(A_0)\cap\rho(T_0)\neq\emptyset$ is fulfilled. Then, for $\lambda\in\rho(A_0)\cap\rho(T_0) = \rho(A_0\times T_0)$ the corresponding γ-field γ'' is given by

$$\lambda\mapsto\gamma''(\lambda) = \begin{pmatrix} \gamma(\lambda) & 0 \\ 0 & \gamma'(\lambda) \end{pmatrix} \in \mathcal{L}(\mathcal{G}\times\mathcal{G},\mathcal{K}\times\mathcal{H})$$

and the Weyl function M'' corresponding to $A\times T$ and the boundary triplet $\{\mathcal{G}\times\mathcal{G},\Gamma_0'',\Gamma_1''\}$ is given by

$$\lambda\mapsto M''(\lambda) = \begin{pmatrix} m(\lambda) & 0 \\ 0 & \tau(\lambda) \end{pmatrix} \in \mathcal{L}(\mathcal{G}\times\mathcal{G}), \quad \lambda\in\rho(A_0\times T_0).$$

In Proposition 6.1 below we introduce another boundary triplet $\{\mathcal{G}\times\mathcal{G},\widetilde\Gamma_0,\widetilde\Gamma_1\}$ for $A^+\times T^+$; cf. [22, §3.3]. The self-adjoint relation $\ker\widetilde\Gamma_0$ will play an important role in Section 7. The simple proof of Proposition 6.1 is left to the reader.

Proposition 6.1 *Let A and T be closed symmetric relations of equal defect $n\le\infty$ in the Krein spaces $\mathcal{K}$ and $\mathcal{H}$, let $\{\mathcal{G},\Gamma_0,\Gamma_1\}$ and $\{\mathcal{G},\Gamma_0',\Gamma_1'\}$ be boundary triplets for A^+ and T^+, respectively, and assume $\rho(A_0)\cap\rho(T_0)\neq\emptyset$. Denote the corresponding γ-fields and Weyl functions by γ, γ', m and τ, respectively. Then the following holds:*

(i) *$\{\mathcal{G}\times\mathcal{G},\widetilde\Gamma_0,\widetilde\Gamma_1\}$, where $\widetilde\Gamma_0$ and $\widetilde\Gamma_1$ are mappings from $A^+\times T^+$ into $\mathcal{G}\times\mathcal{G}$ defined by*

$$\widetilde\Gamma_0\{\hat f,\hat g\} := \begin{pmatrix} -\Gamma_1\hat f + \Gamma_1'\hat g \\ \Gamma_0\hat f + \Gamma_0'\hat g \end{pmatrix} \quad\textit{and}\quad \widetilde\Gamma_1\{\hat f,\hat g\} := \begin{pmatrix} \Gamma_0\hat f \\ \Gamma_1'\hat g \end{pmatrix},$$

$\{\hat f,\hat g\}\in A^+\times T^+$, is a boundary triplet for $A^+\times T^+$.

(ii) *If $\rho(\ker \widetilde{\Gamma}_0) \cap \rho(\ker \widetilde{\Gamma}_1) \cap \rho(T_0)$ is nonempty, then the Weyl function $\widetilde{M}$ and the γ-field $\widetilde{\gamma}$ corresponding to $\{\mathcal{G} \times \mathcal{G}, \widetilde{\Gamma}_0, \widetilde{\Gamma}_1\}$ are given for $\lambda \in \rho(\ker \widetilde{\Gamma}_0) \cap \rho(\ker \widetilde{\Gamma}_1) \cap \rho(T_0)$ by*

$$\widetilde{M}(\lambda) = -\begin{pmatrix} m(\lambda) & -1 \\ -1 & -\tau(\lambda)^{-1} \end{pmatrix}^{-1} \quad \text{and} \quad \widetilde{\gamma}(\lambda) = \begin{pmatrix} \gamma(\lambda) & 0 \\ 0 & \gamma'(\lambda)\tau(\lambda)^{-1} \end{pmatrix} \widetilde{M}(\lambda).$$

In the next proposition we define a symmetric extension H of $A \times T$ such that

$$H \subset \ker \widetilde{\Gamma}_0 \subset H^+ \quad \text{and} \quad H \subset A_0 \times T_0 \subset H^+$$

holds, and by restricting the boundary triplet $\{\mathcal{G} \times \mathcal{G}, \widetilde{\Gamma}_0, \widetilde{\Gamma}_1\}$ from Proposition 6.1 we obtain a boundary triplet $\{\mathcal{G}, \widehat{\Gamma}_0, \widehat{\Gamma}_1\}$ for H^+ where the corresponding Weyl function $\widehat{M}$ has the form

$$\lambda \mapsto \widehat{M}(\lambda) = -\big(m(\lambda) + \tau(\lambda)\big)^{-1}.$$

The proof of Proposition 6.2 is straightforward and therefore left to the reader. The assertions can be deduced from Proposition 6.1 and [22, Proposition 4.1].

Proposition 6.2 *Let A and T be closed symmetric relations of equal defect $n \leq \infty$ in the Krein spaces $\mathcal{K}$ and $\mathcal{H}$, let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ and $\{\mathcal{G}, \Gamma_0', \Gamma_1'\}$ be boundary triplets for A^+ and T^+, respectively, and assume $\rho(A_0) \cap \rho(T_0) \neq \emptyset$. Denote the corresponding γ-fields and Weyl functions by γ, γ', m and τ, respectively. Then the following holds:*

(i) *The closed linear relation*

$$H := \big\{\{\hat{f}, \hat{g}\} \in A^+ \times T^+ : \Gamma_0 \hat{f} = \Gamma_0' \hat{g} = \Gamma_1 \hat{f} - \Gamma_1' \hat{g} = 0\big\}$$

is symmetric in $\mathcal{K} \times \mathcal{H}$ with $A \times T \subset H$. Its adjoint $H^+ \subset A^+ \times T^+$ is given by

$$H^+ = \big\{\{\hat{f}, \hat{g}\} \in A^+ \times T^+ : \Gamma_0 \hat{f} + \Gamma_0' \hat{g} = 0\big\}.$$

(ii) *$\{\mathcal{G}, \widehat{\Gamma}_0, \widehat{\Gamma}_1\}$, where $\widehat{\Gamma}_0$ and $\widehat{\Gamma}_1$ are linear mappings from H^+ into $\mathcal{G}$ defined by*

$$\widehat{\Gamma}_0\{\hat{f}, \hat{g}\} := -\Gamma_1 \hat{f} + \Gamma_1' \hat{g} \quad \text{and} \quad \widehat{\Gamma}_1\{\hat{f}, \hat{g}\} := \Gamma_0 \hat{f},$$

$\{\hat{f}, \hat{g}\} \in H^+$, is a boundary triplet for H^+.

(iii) *For all $\lambda \in \rho(\ker \widehat{\Gamma}_0) \cap \rho(\ker \widehat{\Gamma}_1)$ the Weyl function $\widehat{M}$ and the γ-field $\widehat{\gamma}$ corresponding to $\{\mathcal{G}, \widehat{\Gamma}_0, \widehat{\Gamma}_1\}$ are given by*

$$\widehat{M}(\lambda) = -\big(m(\lambda) + \tau(\lambda)\big)^{-1} \quad \text{and} \quad \widehat{\gamma}(\lambda) = \begin{pmatrix} \gamma(\lambda)\widehat{M}(\lambda) \\ -\gamma'(\lambda)\widehat{M}(\lambda) \end{pmatrix}.$$

7 Negative squares of self-adjoint extensions in exit spaces

A closed symmetric relation A in the Krein space $(\mathcal{K}, [\cdot,\cdot])$ is said to have κ *negative squares*, $\kappa \in \mathbb{N}_0$, if the Hermitian form $\langle \cdot, \cdot \rangle$ on A, defined by

$$\big\langle \{f, f'\}, \{g, g'\} \big\rangle := [f, g'] = [f', g], \quad \{f, f'\}, \{g, g'\} \in A,$$

has κ negative squares, that is, there exists a κ-dimensional subspace $\mathcal{M}$ in A, such that $\langle \hat{f}, \hat{f} \rangle < 0$ if $\hat{f} = \{f, f'\} \in \mathcal{M}$, $\hat{f} \neq 0$, but no $\kappa + 1$-dimensional subspace with this property. Suppose, in addition, that the symmetric relation A is of finite defect n and let $\{\mathbb{C}^n, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^+.

Then the self-adjoint relation $A_0 = \ker \Gamma_0$ has κ', $\kappa \le \kappa' \le \kappa + n$ negative squares and if $\rho(A_0)$ is nonempty this is equivalent to the fact that the form

$$\big[\big(1 + \lambda(A_0 - \lambda)^{-1}\big)\cdot, (A_0 - \lambda)^{-1}\cdot\big], \quad \lambda \in \rho(A_0),$$

defined on $\mathcal{K}$ has κ' negative squares. Then the corresponding Weyl function belongs to the classes of matrix valued functions introduced in Section 4. The following lemma can be proved in the same way as [10, Lemma 7].

Lemma 7.1 *Let A be a closed symmetric relation of finite defect n in $\mathcal{K}$, let $\{\mathbb{C}^n, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^+ and assume that the self-adjoint relation $A_0 = \ker \Gamma_0$ has κ' negative squares and $\rho(A_0) \neq \emptyset$. Then the corresponding Weyl function m belongs to some class $\mathcal{D}^{n\times n}_{\kappa''}$, $\kappa'' \le \kappa'$. If, in addition, the condition*

$$\mathcal{K} = \operatorname{clsp}\big\{\mathcal{N}_\lambda : \lambda \in \rho(A_0)\big\} = \operatorname{clsp}\big\{\operatorname{ran}\gamma(\lambda) : \lambda \in \rho(A_0)\big\} \tag{7.1}$$

is fulfilled, then $\kappa'' = \kappa'$, i.e., $m \in \mathcal{D}^{n\times n}_{\kappa'}$

Remark 7.2 We note that it can be shown that also the converse in Lemma 7.1 holds, that is, every function $m \in \mathcal{D}^{n\times n}_{\kappa}$, $\kappa \in \mathbb{N}_0$, can be realized as the Weyl function of a certain boundary triplet; cf. [3, 4] and [10, Theorem 8].

From now on it will be assumed that the closed symmetric operator or relation A is of defect one. Clearly, in this case the Weyl function m is a scalar function. The statements from the next lemma will be used in the following.

Lemma 7.3 *Let A be a closed symmetric operator of defect one with finitely many negative squares in the Krein space $\mathcal{K}$ and assume that $\operatorname{ran}(A-\lambda)$ is closed for all $\lambda \in \mathcal{O} \cup \mathcal{O}^*$, where $\mathcal{O}$ is an open subset in $\mathbb{C}^+$ and $\mathcal{O}^* = \{\lambda \in \mathbb{C} : \overline{\lambda} \in \mathcal{O}\}$. Then the following holds:*

(i) *If $\operatorname{dom} A$ is dense, then all self-adjoint extensions of A in $\mathcal{K}$ are operators and have a nonempty resolvent set.*

(ii) *If $\mathcal{K} = \operatorname{clsp}\{\ker(A^+ - \lambda) : \lambda \in \mathcal{O} \cup \mathcal{O}^*\}$ holds, then all self-adjoint extensions of A in $\mathcal{K}$ have a nonempty resolvent set.*

Furthermore, if A has $\kappa \in \mathbb{N}_0$ negative squares and A' is a self-adjoint extension of A in $\mathcal{K}$ with $\rho(A') \neq \emptyset$, then A' has κ or $\kappa+1$ negative squares and $\sigma(A') \cap (\mathbb{C}\backslash\mathbb{R})$ consists of at most $\kappa+1$ pairs of eigenvalues $\{\mu_j, \overline{\mu}_j\}$, $j = 1, \dots, n+1$.

Proof. Assertions (i) and the last statement on the number of non-real eigenvalues are known from [15, 45], see also [11]. Assertion (ii) is essentially a consequence of the fact that the condition $\mathcal{K} = \operatorname{clsp}\{\mathcal{N}_\lambda : \lambda \in \mathcal{O} \cup \mathcal{O}^*\}$ together with (5.6)-(5.7) implies that the Weyl function of any boundary triplet $\{\mathbb{C}, \Gamma_0, \Gamma_1\}$ of A^+ is not equal to a constant. Thus, by Theorem 5.2 each self-adjoint extension of A in $\mathcal{K}$ has a nonempty resolvent set. □

Remark 7.4 There exist closed symmetric non-densely defined operators which satisfy the assumptions of Lemma 7.3 and possess self-adjoint extensions with an empty resolvent set.

Let A be a closed symmetric operator or relation of defect one in the Krein space $\mathcal{K}$, let $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^+ and let $\mathcal{H}$ be a further Krein space. A self-adjoint extension $\widetilde{A}$ of A in $\mathcal{K} \times \mathcal{H}$ is said to be an *exit space extension of* A and $\mathcal{H}$ is called the *exit space*. The exit space extension $\widetilde{A}$ of A is said to be *minimal* if $\rho(\widetilde{A})$ is nonempty and

$$\mathcal{K} \times \mathcal{H} = \operatorname{clsp}\big\{\mathcal{K},\ \operatorname{ran}\big((\widetilde{A} - \lambda)^{-1} \upharpoonright_{\mathcal{K}}\big) : \lambda \in \rho(\widetilde{A})\big\} \tag{7.2}$$

holds. Clearly (7.2) is equivalent to

$$\mathcal{H} = \operatorname{clsp}\big\{\operatorname{ran}\big(P_{\mathcal{H}}(\widetilde{A} - \lambda)^{-1} \upharpoonright_{\mathcal{K}}\big) : \lambda \in \rho(\widetilde{A})\big\}.$$

Assume that $\widetilde{B}$ is another minimal self-adjoint exit space extension of A in a Krein space $\mathcal{K} \times \mathcal{H}'$ and that the set $\mathbb{C}\backslash\mathbb{R}$ up to at most finitely many points is contained in $\rho(\widetilde{A}) \cap \rho(\widetilde{B})$. Then $\widetilde{A}$ and $\widetilde{B}$ are said to be *weakly isomorphic* if there exists an operator

$$V : \mathrm{sp}\left\{\mathcal{K},\ \mathrm{ran}\left((\widetilde{A}-\lambda)^{-1}\restriction_{\mathcal{K}}\right) : \lambda \in \rho(\widetilde{A})\right\} \to \mathrm{sp}\left\{\mathcal{K},\ \mathrm{ran}\left((\widetilde{B}-\lambda)^{-1}\restriction_{\mathcal{K}}\right) : \lambda \in \rho(\widetilde{B})\right\}$$

which preserves the inner product, $[Vx, Vy] = [x, y]$, $x, y \in \mathrm{dom}\, V$, such that

$$V(\widetilde{A}-\lambda)^{-1}x = (\widetilde{B}-\lambda)^{-1}Vx, \quad x \in \mathrm{dom}\, V, \quad \lambda \in \rho(\widetilde{A}) \cap \rho(\widetilde{B}),$$

holds; cf. [31].

In the next theorem we verify Krein's formula for the generalized resolvents of a symmetric operator of defect one with finitely many negative squares; cf. [9]. The proof is based on the coupling method from [22, 24] and the observations in Section 6. We refer the reader to the classical papers [40, 49, 50] and [5, 7, 8, 17, 18, 19, 20, 38, 44] for Krein's formula in Hilbert, Pontryagin and Krein space cases. In the special case where $\mathcal{K}$ and $\mathcal{H}$ are Hilbert spaces and the symmetric operator A is nonnegative a bijective correspondence between the self-adjoint extensions with finitely many negative eigenvalues (that is, negative squares) and a corresponding generalized class of Stieltjes functions was obtained in [25, 27]. In the following we use the notation

$$\widetilde{\mathcal{D}} := \bigcup_{\kappa=0}^{\infty} \mathcal{D}_\kappa \ \cup \left\{\left(\begin{smallmatrix} 0 \\ c \end{smallmatrix}\right) \,\middle|\, c \in \mathbb{C}\right\}.$$

Theorem 7.5 *Let A be a closed symmetric operator of defect one in the Krein space $\mathcal{K}$ and let $\{\mathbb{C}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^+ with corresponding γ-field γ and Weyl function m. Assume that $A_0 = \ker \Gamma_0$ has finitely many negative squares and $\rho(A_0) \neq \emptyset$. Then*

$$P_{\mathcal{K}}(\widetilde{A}-\lambda)^{-1}\restriction_{\mathcal{K}} = (A_0-\lambda)^{-1} - \gamma(\lambda)\big(m(\lambda)+\tau(\lambda)\big)^{-1}\gamma(\overline{\lambda})^+ \tag{7.3}$$

establishes (up to weak isomorphy) a one-to-one correspondence between minimal self-adjoint extensions $\widetilde{A}$ of A with finitely many negative squares in Krein spaces $\mathcal{K} \times \mathcal{H}$ and functions τ from the class $\widetilde{\mathcal{D}}$ with $\tau \neq -m$. The formula (7.3) *holds for all points λ belonging to the set*

$$\rho(\widetilde{A}) \cap \rho(A_0) \cap \mathfrak{h}(\tau) = \mathfrak{h}\big((m+\tau)^{-1}\big) \cap \rho(A_0) \cap \mathfrak{h}(\tau). \tag{7.4}$$

P r o o f. Let $\mathcal{H}$ be a Krein space and let $\widetilde{A}$ be a minimal self-adjoint extension of A in $\mathcal{K} \times \mathcal{H}$ which has a finite number of negative squares. Observe that by definition this in particular means $\rho(\widetilde{A}) \neq \emptyset$. Obviously the symmetric relation $\widetilde{A} \cap \mathcal{K}^2$ in $\mathcal{K}$ is an extension of the operator A, and as A is of defect one $\widetilde{A} \cap \mathcal{K}^2$ is either self-adjoint in $\mathcal{K}$ or coincides with A.

In the case $\widetilde{A} \cap \mathcal{K}^2 = (\widetilde{A} \cap \mathcal{K}^2)^+$ it follows that $\widetilde{A} \cap \mathcal{H}^2 = (\widetilde{A} \cap \mathcal{H}^2)^+$ and $\widetilde{A} = \widetilde{A} \cap \mathcal{K}^2 \times \widetilde{A} \cap \mathcal{H}^2$; cf. [22, Remark 5.3]. Therefore $(\widetilde{A}-\lambda)^{-1}$ maps elements from $\mathcal{K}$ into $\mathcal{K}$ and, by the minimality of $\widetilde{A}$,

$$\mathcal{H} = \mathrm{clsp}\left\{P_{\mathcal{H}}(\widetilde{A}-\lambda)^{-1}\restriction_{\mathcal{K}} : \lambda \in \rho(\widetilde{A})\right\} = \{0\}$$

and therefore $\widetilde{A}$ is a self-adjoint extension of A in $\mathcal{K} = \mathcal{K} \times \{0\}$. Hence by Theorem 5.2 there exists a constant $\tau \in \overline{\mathbb{R}}$ such that

$$(\widetilde{A}-\lambda)^{-1} = (A_0-\lambda)^{-1} - \gamma(\lambda)\big(m(\lambda)+\tau\big)^{-1}\gamma(\overline{\lambda})^+$$

and (7.4) hold.

Suppose now $A = \widetilde{A} \cap \mathcal{K}^2$ and let $T := \widetilde{A} \cap \mathcal{H}^2$. Then the same arguments as in [22, Lemma 5.1 and Theorem 5.4] show that T is of defect one and the adjoints of A and T are given by

$$A^+ = \widehat{P}_{\mathcal{K}}\widetilde{A} := \left\{\{k, k'\} : \begin{pmatrix} \{k, h\} \\ \{k', h'\} \end{pmatrix} \in \widetilde{A}\right\} \subset \mathcal{K} \times \mathcal{K}$$

and

$$T^+ = \widehat{P}_{\mathcal{H}}\widetilde{A} := \left\{\{h,h'\} : \begin{pmatrix}\{k,h\}\\ \{k',h'\}\end{pmatrix} \in \widetilde{A}\right\} \subset \mathcal{H}\times\mathcal{H},$$

respectively. Here $\widehat{P}_{\mathcal{K}} : \widetilde{A} \to A^+$ and $\widehat{P}_{\mathcal{H}} : \widetilde{A} \to T^+$ denote the mappings given by

$$\begin{pmatrix}\{k,h\}\\ \{k',h'\}\end{pmatrix} \mapsto \{k,k'\} \quad \text{and} \quad \begin{pmatrix}\{k,h\}\\ \{k',h'\}\end{pmatrix} \mapsto \{h,h'\},$$

respectively. Furthermore, it was proved in [22, Theorem 5.4] that $\{\mathbb{C},\Gamma_0',\Gamma_1'\}$, where

$$\Gamma_0'\hat{g} := -\Gamma_0\widehat{P}_{\mathcal{K}}\widehat{P}_{\mathcal{H}}^{-1}\hat{g} \quad \text{and} \quad \Gamma_1'\hat{g} := \Gamma_1\widehat{P}_{\mathcal{K}}\widehat{P}_{\mathcal{H}}^{-1}\hat{g}, \tag{7.5}$$

is a boundary triplet for T^+. Observe that Γ_0' and Γ_1' are well defined since $\operatorname{mul}\widehat{P}_{\mathcal{K}}\widehat{P}_{\mathcal{H}}^{-1} = A = \ker\Gamma_0 \cap \ker\Gamma_1$. From

$$\operatorname{ran}\big(P_{\mathcal{H}}(\widetilde{A}-\lambda)^{-1}\restriction_{\mathcal{K}}\big) = \ker\,(T^+-\lambda), \qquad \lambda\in\rho(\widetilde{A}),$$

(see, e.g., [23, Lemma 2.14]) it follows together with the minimality of $\widetilde{A}$, see (7.2), that

$$\mathcal{H} = \operatorname{clsp}\big\{\mathcal{N}_{\lambda,T^+} : \lambda\in\rho(\widetilde{A})\big\} \tag{7.6}$$

holds. In particular this implies that T is an operator. Since $\widetilde{A}$ has finitely many negative squares also $T = \widetilde{A}\cap\mathcal{H}^2$ has finitely many negative squares and $\operatorname{ran}(T-\lambda)$ is closed for all $\lambda\in\rho(\widetilde{A})$. Hence by Lemma 7.3 the self-adjoint extension $T_0 = \ker\Gamma_0'$ of T has a nonempty resolvent set and the γ-field γ' and the Weyl function τ corresponding to the boundary triplet $\{\mathbb{C},\Gamma_0',\Gamma_1'\}$ are defined on $\rho(T_0)$. Furthermore, T_0 also has finitely many negative squares and therefore τ belongs to the some class $\mathcal{D}_\kappa$, $\kappa\in\mathbb{N}_0$, see Lemma 7.1. Since (7.6) holds we have $\rho(T_0) = \mathfrak{h}(\tau)\backslash\{\infty\}$.

Define the closed symmetric relation H in $\mathcal{K}\times\mathcal{H}$ by

$$H := \big\{\{\hat{f},\hat{g}\}\in A^+\times T^+ : \Gamma_0\hat{f} = \Gamma_0'\hat{g} = \Gamma_1\hat{f} - \Gamma_1'\hat{g} = 0\big\} \tag{7.7}$$

as in Proposition 6.2 (i) and let $\{\mathbb{C},\widehat{\Gamma}_0,\widehat{\Gamma}_1\}$ be the boundary triplet from Proposition 6.2 (ii),

$$\widehat{\Gamma}_0\{\hat{f},\hat{g}\} = -\Gamma_1\hat{f} + \Gamma_1'\hat{g}, \quad \widehat{\Gamma}_1\{\hat{f},\hat{g}\} = \Gamma_0\hat{f}, \qquad \{\hat{f},\hat{g}\}\in H^+, \tag{7.8}$$

where $H^+ = \{\{\hat{f},\hat{g}\}\in A^+\times T^+ : \Gamma_0\hat{f} + \Gamma_0'\hat{g} = 0\}$. Observe that $A_0\times T_0 = \ker\widehat{\Gamma}_1$ holds. We claim that $\ker\widehat{\Gamma}_0$ coincides with the self-adjoint relation $\widetilde{A}$. In fact, an element $\{\hat{f},\hat{g}\}\in\ker\widehat{\Gamma}_0$ satisfies

$$\Gamma_0\hat{f} = -\Gamma_0'\hat{g} = \Gamma_0\widehat{P}_{\mathcal{K}}\widehat{P}_{\mathcal{H}}^{-1}\hat{g} \quad \text{and} \quad \Gamma_1\hat{f} = \Gamma_1'\hat{g} = \Gamma_1\widehat{P}_{\mathcal{K}}\widehat{P}_{\mathcal{H}}^{-1}\hat{g}. \tag{7.9}$$

Observe that (7.9) implies $\hat{f} - \widehat{P}_{\mathcal{K}}\widehat{P}_{\mathcal{H}}^{-1}\hat{g}\in\ker\Gamma_0\cap\ker\Gamma_1 = A$. Therefore $\{\hat{f} - \widehat{P}_{\mathcal{K}}\widehat{P}_{\mathcal{H}}^{-1}\hat{g}, 0\}\in\widetilde{A}$ and as $\{\widehat{P}_{\mathcal{K}}\widehat{P}_{\mathcal{H}}^{-1}\hat{g},\hat{g}\}\in\widetilde{A}$ we conclude $\{\hat{f},\hat{g}\}\in\widetilde{A}$. Conversely, $\{\hat{f},\hat{g}\}\in\widetilde{A}$ yields $\{\hat{f} - \widehat{P}_{\mathcal{K}}\widehat{P}_{\mathcal{H}}^{-1}\hat{g}, 0\}\in\widetilde{A}$, i.e., $\hat{f} - \widehat{P}_{\mathcal{K}}\widehat{P}_{\mathcal{H}}^{-1}\hat{g}\in A$, and hence

$$\Gamma_0\hat{f} + \Gamma_0'\hat{g} = \Gamma_0\big(\hat{f} - \widehat{P}_{\mathcal{K}}\widehat{P}_{\mathcal{H}}^{-1}\hat{g}\big) = 0, \qquad \Gamma_1\hat{f} - \Gamma_1'\hat{g} = \Gamma_1\big(\hat{f} - \widehat{P}_{\mathcal{K}}\widehat{P}_{\mathcal{H}}^{-1}\hat{g}\big) = 0.$$

Therefore $\{\hat{f},\hat{g}\}\in H^+$ and $\widehat{\Gamma}_0\{\hat{f},\hat{g}\} = 0$, that is, $\widetilde{A} = \ker\widehat{\Gamma}_0$, i.e.,

$$\widetilde{A} = \big\{\{\hat{f},\hat{g}\}\in A^+\times T^+ : \Gamma_0\hat{f} + \Gamma_0'\hat{g} = \Gamma_1\hat{f} - \Gamma_1'\hat{g} = 0\big\}. \tag{7.10}$$

Each of the relations $\widetilde{A}$, A_0 and T_0 has finitely many negative squares and a nonempty resolvent set. Hence, there are at most finitely many points in $\mathbb{C}\backslash\mathbb{R}$ which do not belong to

$$\rho(\widetilde{A})\cap\rho(A_0\times T_0) = \rho(\ker\widehat{\Gamma}_0)\cap\rho(\ker\widehat{\Gamma}_1).$$

Let $\widehat{\gamma}$ and $\widehat{M}$ be the γ-field and Weyl function corresponding to the boundary triplet $\{\mathbb{C},\widehat{\Gamma}_0,\widehat{\Gamma}_1\}$, i.e.,

$$\widehat{\gamma}(\lambda)=\begin{pmatrix}-\gamma(\lambda)(m(\lambda)+\tau(\lambda))^{-1}\\ \gamma'(\lambda)(m(\lambda)+\tau(\lambda))^{-1}\end{pmatrix},\qquad \lambda\in\rho(\widetilde{A})\cap\rho(A_0\times T_0), \tag{7.11}$$

and

$$\widehat{M}(\lambda)=-\big(m(\lambda)+\tau(\lambda)\big)^{-1},\qquad \lambda\in\rho(\widetilde{A})\cap\rho(A_0\times T_0); \tag{7.12}$$

cf. Proposition 6.2. Then it follows from Theorem 5.2 that

$$(\widetilde{A}-\lambda)^{-1}=\big((A_0\times T_0)-\lambda\big)^{-1}+\widehat{\gamma}(\lambda)\widehat{M}(\lambda)^{-1}\widehat{\gamma}(\overline{\lambda})^{+} \tag{7.13}$$

holds and that $\lambda\in\rho(\widetilde{A})$ belongs to $\rho(A_0\times T_0)=\rho(A_0)\cap\mathfrak{h}(\tau)$ if and only if $0\in\rho(\widehat{M}(\lambda))$, i.e., $m(\lambda)+\tau(\lambda)\neq 0$. Therefore

$$\rho(\widetilde{A})\cap\rho(A_0)\cap\mathfrak{h}(\tau)=\mathfrak{h}\big((m+\tau)^{-1}\big)\cap\rho(A_0)\cap\mathfrak{h}(\tau)$$

and as

$$\widehat{\gamma}(\lambda)\widehat{M}(\lambda)^{-1}\widehat{\gamma}(\overline{\lambda})^{+}=\begin{pmatrix}-\gamma(\lambda)(m(\lambda)+\tau(\lambda))^{-1}\gamma(\overline{\lambda})^{+} & \gamma(\lambda)(m(\lambda)+\tau(\lambda))^{-1}\gamma'(\overline{\lambda})^{+}\\ \gamma'(\lambda)(m(\lambda)+\tau(\lambda))^{-1}\gamma(\overline{\lambda})^{+} & -\gamma'(\lambda)(m(\lambda)+\tau(\lambda))^{-1}\gamma'(\overline{\lambda})^{+}\end{pmatrix} \tag{7.14}$$

for $\lambda\in\rho(\widetilde{A})\cap\rho(A_0)\cap\mathfrak{h}(\tau)$ the compression of (7.13) onto $\mathcal{K}$ is given by (7.3).

Now we verify the converse direction, that is, for a given function $\tau\in\widetilde{\mathcal{D}}$ we construct a minimal self-adjoint extension $\widetilde{A}$ such that the compressed resolvent of $\widetilde{A}$ onto $\mathcal{K}$ is given by (7.3). In the special case $\tau\in\overline{\mathbb{R}}$ one chooses the canonical extension $\widetilde{A}=A_{-\tau}=\ker\,(\Gamma_1+\tau\Gamma_0)$, so that by Theorem 5.2 formulas (7.3) and (7.4) hold. Let now $\tau\in\widetilde{\mathcal{D}}$ be a function which is not equal to a constant. With the help of the operator representation [37, Theorem 3.9] of τ it was proved in [10, Theorem 8] that there exists a Krein space $\mathcal{H}$, a closed symmetric operator T of defect one with finitely many negative squares in $\mathcal{H}$ and a boundary triplet $\{\mathbb{C},\Gamma_0',\Gamma_1'\}$ for T^+ such that $T_0=\ker\,\Gamma_0'$ has a nonempty resolvent set and τ coincides with the corresponding Weyl function on $\rho(T_0)$. Moreover, the condition

$$\mathcal{H}=\operatorname{clsp}\big\{\mathcal{N}_{\lambda,T^+}:\lambda\in\rho(T_0)\big\} \tag{7.15}$$

holds. Now we make again use of Proposition 6.2 and the construction above. Define the closed symmetric relation H in $\mathcal{K}\times\mathcal{H}$ by (7.7) and let $\{\mathbb{C},\widehat{\Gamma}_0,\widehat{\Gamma}_1\}$ be the boundary triplet for H^+ in (7.8). We set $\widetilde{A}:=\ker\,\widehat{\Gamma}_0$. As A and T have finitely many negative squares the same holds for $\widetilde{A}$. One verifies that all points in $\rho(A_0\times T_0)\cap\mathfrak{h}((m+\tau)^{-1})$ belong to $\rho(\widetilde{A})$ and hence the γ-field $\widehat{\gamma}$ and Weyl function $\widehat{M}$ corresponding to $\{\mathbb{C},\widehat{\Gamma}_0,\widehat{\Gamma}_1\}$ are defined on $\rho(\widetilde{A})$. Therefore (7.11), (7.12), (7.13) and (7.14) hold and hence the compressed resolvent of $\widetilde{A}$ onto $\mathcal{K}$ satisfies (7.3). Furthermore, it follows from (7.13) and (7.14) that

$$\operatorname{ran}\big(P_{\mathcal{H}}(\widetilde{A}-\lambda)^{-1}\restriction_{\mathcal{K}}\big)=\operatorname{ran}\big(\gamma'(\lambda)(m(\lambda)+\tau(\lambda))^{-1}\gamma(\overline{\lambda})^{+}\big)=\mathcal{N}_{\lambda,T^+}$$

holds and therefore (7.15) implies that $\widetilde{A}$ is a minimal self-adjoint exit space extension of A.

It remains to show that $\widetilde{A}$ is determined uniquely up to a weak isomorphism by (7.3). Suppose that besides the minimal self-adjoint extension $\widetilde{A}$ of A with finitely many negative squares in $\mathcal{K}\times\mathcal{H}$ also the minimal self-adjoint extension $\widetilde{B}$ of A with finitely many negative squares in the Krein space $\mathcal{K}\times\mathcal{H}'$ satisfies (7.3). Then it follows that the linear relation

$$V:=\left\{\left\{\begin{pmatrix}k_0\\0\end{pmatrix}+\sum_{i=1}^{n}(\widetilde{A}-\lambda_i)^{-1}\begin{pmatrix}k_i\\0\end{pmatrix},\begin{pmatrix}k_0\\0\end{pmatrix}+\sum_{i=1}^{n}(\widetilde{B}-\lambda_i)^{-1}\begin{pmatrix}k_i\\0\end{pmatrix}\right\}:\begin{matrix}k_0,\dots,k_n\in\mathcal{K}\\ \lambda_i\in\rho(\widetilde{A})\cap\rho(\widetilde{B})\end{matrix}\right\}$$

is isometric with dense domain in $\mathcal{K} \times \mathcal{H}$ and dense range in $\mathcal{K} \times \mathcal{H}'$. Therefore V is the graph of an isometric operator and it is not difficult to verify that

$$V(\widetilde{A} - \lambda)^{-1}x = (\widetilde{B} - \lambda)^{-1}Vx$$

is fulfilled for all $x \in \operatorname{dom} V$ and all $\lambda \in \rho(\widetilde{A}) \cap \rho(\widetilde{B})$. Observe also that

$$\big[(1 + \lambda(\widetilde{B} - \lambda)^{-1})Vx, (\widetilde{B} - \lambda)^{-1}Vx\big]_{\mathcal{K}\times\mathcal{H}'} = \big[(1 + \lambda(\widetilde{A} - \lambda)^{-1})x, (\widetilde{A} - \lambda)^{-1}x\big]_{\mathcal{K}\times\mathcal{H}}$$

holds for all $x \in \operatorname{dom} V$ and hence the number of negative squares of $\widetilde{A}$ and $\widetilde{B}$ coincide. □

In the next theorem the number of negative squares of the self-adjoint relation $\widetilde{A}$ in Theorem 7.5 is expressed in terms of the behavior of the $\mathcal{D}_\kappa$-functions m and τ at the points 0 and ∞. We leave it to the reader to formulate the corollary for nonnegative selfadjoint extensions $\widetilde{A}$. The case that $\widetilde{A}$ in (7.3) is a canonical self-adjoint extension (i.e., there is no exit space and, hence, $\widetilde{A}$ is a self-adjoint extension in $\mathcal{K}$) of the symmetry A was already treated in [11, 18].

Theorem 7.6 *Let A be a closed symmetric operator of defect one in the Krein space $\mathcal{K}$ and let $\{\mathbb{C}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^+ with corresponding γ-field γ and Weyl function m. Assume that $A_0 = \ker \Gamma_0$ has κ_m negative squares, $\rho(A_0) \neq \emptyset$, and that $\mathcal{K} = \operatorname{clsp}\{\mathcal{N}_\lambda : \lambda \in \rho(A_0)\}$ holds. If $\widetilde{A}$ is a minimal self-adjoint extension of A in a Krein space $\mathcal{K} \times \mathcal{H}$, $\mathcal{H} \neq \{0\}$, and $\tau \in \mathcal{D}_{\kappa_\tau}$ is such that (7.3) holds, then $\widetilde{A}$ has*

$$\kappa = \kappa_m + \kappa_\tau + \Delta_0 + \Delta_\infty$$

negative squares, where

$$\Delta_0 = \begin{cases} -1 & \text{if } \lim\limits_{\lambda \hat{\to} 0} m(\lambda) \text{ and } \lim\limits_{\lambda \hat{\to} 0} \tau(\lambda) \text{ exist and } \lim\limits_{\lambda \hat{\to} 0}(m(\lambda) + \tau(\lambda)) \leq 0, \\ 0 & \text{otherwise,} \end{cases}$$

and

$$\Delta_\infty = \begin{cases} 0 & \text{if } \lim\limits_{\lambda \hat{\to} \infty} m(\lambda) \text{ and } \lim\limits_{\lambda \hat{\to} \infty} \tau(\lambda) \text{ exist and } \lim\limits_{\lambda \hat{\to} \infty}(m(\lambda) + \tau(\lambda)) \geq 0, \\ 1 & \text{otherwise.} \end{cases}$$

Proof. Assume that $\widetilde{A}$ and $\tau \in \widetilde{\mathcal{D}}$ are such that the correspondence (7.3) holds. According to the proof of Theorem 7.5 τ is the Weyl function of the operator $T = \widetilde{A} \cap \mathcal{H}^2$ and the boundary triplet $\{\mathbb{C}, \Gamma_0', \Gamma_1'\}$ defined in (7.5); cf. [22]. In particular, τ is not equal to a constant. Furthermore, the minimality of $\widetilde{A}$ implies that T has finitely many negative squares and that

$$\mathcal{H} = \operatorname{clsp}\big\{\mathcal{N}_{\lambda,T^+} : \lambda \in \rho(\widetilde{A})\big\} \tag{7.16}$$

holds. Hence it follows from Lemma 7.3 that the self-adjoint extensions $T_0 = \ker \Gamma_0'$ and $T_1 = \ker \Gamma_1'$ in $\mathcal{H}$ have nonempty resolvent sets.

Let $\{\mathbb{C}^2, \widetilde{\Gamma}_0, \widetilde{\Gamma}_1\}$,

$$\widetilde{\Gamma}_0\{\hat{f}, \hat{g}\} = \begin{pmatrix} -\Gamma_1\hat{f} + \Gamma_1'\hat{g} \\ \Gamma_0\hat{f} + \Gamma_0'\hat{g} \end{pmatrix}, \quad \widetilde{\Gamma}_1\{\hat{f}, \hat{g}\} = \begin{pmatrix} \Gamma_0\hat{f} \\ \Gamma_1'\hat{g} \end{pmatrix}, \quad \hat{f} \in A^+,\ \hat{g} \in T^+,$$

be the boundary triplet for $A^+ \times T^+$ from Proposition 6.1. Then by (7.10) the self-adjoint relation $\widetilde{A}$ in $\mathcal{K} \times \mathcal{H}$ coincides with $\ker \widetilde{\Gamma}_0$. Moreover it follows $\rho(\ker \widetilde{\Gamma}_1) = \rho(A_0) \cap \mathfrak{h}(\tau^{-1})$; cf. (5.8). By assumption $m \neq -\tau$ and (7.4) and Proposition 6.1 (ii) show that the Weyl function $\widetilde{M}$ of $\{\mathbb{C}^2, \widetilde{\Gamma}_0, \widetilde{\Gamma}_1\}$ has the form

$$\widetilde{M}(\lambda) = -\begin{pmatrix} m(\lambda) & -1 \\ -1 & -\tau(\lambda)^{-1} \end{pmatrix}^{-1}$$

for all λ belonging to

$$\rho(\widetilde{A}) \cap \rho(A_0) \cap \rho(T_1) \cap \rho(T_0) = \mathfrak{h}\big((m+\tau)^{-1}\big) \cap \rho(A_0) \cap \mathfrak{h}(\tau^{-1}) \cap \mathfrak{h}(\tau).$$

Now the relations $\mathcal{K} = \operatorname{clsp}\{\mathcal{N}_\lambda : \lambda \in \rho(A_0)\}$ and (7.16) imply that the γ-field $\widetilde{\gamma}$ of $\{\mathbb{C}^2, \widetilde{\Gamma}_0, \widetilde{\Gamma}_1\}$ satisfies $\mathcal{K} \times \mathcal{H} = \{\widetilde{\gamma}(\lambda)x : \lambda \in \rho(\widetilde{A}),\ x \in \mathbb{C}^2\}$. The assertion on the number of negative squares of $\widetilde{A}$ is now an immediate consequence of Theorem 4.5 and Lemma 7.1. □

Remark 7.7 We note that the number of negative squares $\kappa = \kappa_m + \kappa_\tau + \Delta_0 + \Delta_\infty$ of the self-adjoint extension $\widetilde{A}$ in $\mathcal{K} \times \mathcal{H}$ in Theorem 7.6 is larger or equal to the number κ_A of negative squares of the underlying closed symmetric operator A in $\mathcal{K}$ and that $\kappa_m = \kappa_A$ or $\kappa_m = \kappa_A + 1$ by Lemma 7.3. In the special case $\kappa_\tau = 0$ it is not difficult to construct examples with $\kappa = \kappa_A$.

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