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ON SUPERSINGULAR PERTURBATIONS OF NON-SEMIBOUNDED SELF-ADJOINT OPERATORS

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ABSTRACT. In this paper self-adjoint realizations of the formal expression $A_\alpha := A + \alpha\langle\phi,\cdot\rangle\phi$ are described, where $\alpha \in \mathbb{R} \cup \{\infty\}$, the operator A is self-adjoint in a Hilbert space $\mathcal{H}$ and ϕ is a supersingular element from the scale space $\mathcal{H}_{-n-2}(A)\backslash\mathcal{H}_{-n-1}(A)$ for $n \geqslant 1$. The crucial point is that the spectrum of A may consist of the whole real line.

We construct two models to describe the family (A_α). It can be interpreted in a Hilbert space with a twisted version of Krein's formula, or with a more classical version of Krein's formula but in a Pontryagin space. Finally, we compare the two approaches in terms of the respective Q-functions.

KEYWORDS: *Unbounded self-adjoint operator, supersingular perturbation, generalized Nevanlinna function.*

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1. INTRODUCTION

Classical extension theory of symmetric operators answers the question if a given symmetric operator possesses self-adjoint extensions (in the same space) and if so, how many there are. In the work of von Neumann these extensions are parametrized in terms of certain classes of unitary operators [12]. An equivalent description in terms of Hermitian operators is due to Birman, Krein and Vishik; for an exposition cf. [2]. Another parametrization of the family of such self-adjoint extensions is also achieved via the classical Krein formula which additionally describes their resolvents.

Another classical problem is the investigation of finite rank perturbations of self-adjoint operators. In particular, given a self-adjoint operator $A = A^*$ in a Hilbert space $(\mathcal{H}, \langle\cdot,\cdot\rangle)$, one can consider rank one perturbations A_α formally given by

$$A_\alpha := A + \alpha\langle\phi,\cdot\rangle\phi,$$

where the coupling parameter α is usually taken to be a real number or formally ∞ (the latter case is made more precise below (1.2)). The construction of A_α depends on the singularity of the element ϕ: if ϕ is an element from the Hilbert space then the perturbation is called regular and the perturbed operator is defined on the same domain as the original operator. If ϕ lies outside the original Hilbert space then the perturbation is called singular or supersingular, depending on whether the perturbed operator can be defined in the original Hilbert space or not. To charaterize such perturbations it is natural to assume that ϕ belongs to a certain space $\mathcal{H}_{-m}(A)$ for $m \in \mathbb{N}$ from the scale associated with the given operator A. (We briefly recall the definition of the spaces $(\mathcal{H}_m(A))_{m\in\mathbb{Z}}$ in the Appendix.) The case of singular perturbations corresponds to $\phi \in \mathcal{H}_{-2}(A)\backslash\mathcal{H}$ and is generally well-understood [1], [13]. We give a very brief recollection of this below.

The cases $\phi \in \mathcal{H}_{-n-2}(A)\backslash\mathcal{H}_{-2}(A)$ for $n \geqslant 1$ are fundamentally different. The technique that works for $\mathcal{H}_{-1}(A)$ and $\mathcal{H}_{-2}(A)$ — namely, restricting A to a certain subspace of $\mathcal{H}$, treating the resulting symmetric operator and then employing extension theory to define the family of self-adjoint perturbations inside the original Hilbert space — fails. The reason for this is that the symmetric operator one receives from the above procedure is already essentially self-adjoint and thus has the unique self-adjoint extension A. Therefore such perturbations have been called supersingular.

Nevertheless, one can find several approaches in order to interpret the formal perturbations A_α. One such possibility is to move from the Hilbert space $\mathcal{H}$ to a Pontryagin space setting [5]. Another possibility, albeit under the *extra assumption that A is semibounded*, has been developed in a series of papers [8], [9], [10]: here, the perturbations are modeled in a new Hilbert space $\mathbb{H}$ which essentially contains the original space $\mathcal{H}$. Additionally, (a certain finite number of) elements of the form $\phi_z := (A-z)^{-1}\phi$ — which lie outside $\mathcal{H}$ — are added into $\mathbb{H}$ so that Krein's formula really does again involve ϕ_z, i.e., an expression closely related to the perturbation ϕ. This formula then gives a parametrization of the family of perturbed operators A_α. The semiboundedness of A enters in such a way that real points z from the resolvent set of A can be used to define the (necessary number of) elements ϕ_z. A comparison of the two models constructed — Pontryagin and Hilbert space — can be found in [4].

The aim of this paper is to investigate how the assumption of A being semibounded can be removed while still staying close to the spirit of the model for semibounded operators. We give a short review of the results mentioned so far in the following two Subsections 1.1 and 1.2, whereas in the last Subsection 1.3 we formulate in detail the question we investigate in this paper.

1.1. CLASSICAL AND SINGULAR PERTURBATIONS OF OPERATORS. We begin by briefly recalling the cases of $\phi \in \mathcal{H}$ (classical, regular) as well as $\phi \in \mathcal{H}_{-2}(A)\backslash\mathcal{H}$ (singular), cf. for example [1], [13]. In the first instance, where ϕ belongs to the

Hilbert space, the definition of

$$A_\alpha := A + \alpha\langle\phi,\cdot\rangle\phi, \quad \alpha \in \mathbb{R}, \tag{1.1}$$

gives no difficulties and in terms of resolvents a straightforward calculation yields

$$(A_\alpha - z)^{-1} = (A - z)^{-1} - \frac{\langle\phi_{\bar z},\cdot\rangle}{q(z) + 1/\alpha}\phi_z \tag{1.2}$$

for $z \notin \sigma(A) \cup \sigma(A_\alpha)$ with $\phi_z := (A - z)^{-1}\phi$ and $q(z) := \langle\phi,(A - z)^{-1}\phi\rangle$. For the parameter value $\alpha = \infty$, i.e. the case of so-called infinite coupling, formula (1.2) serves as a definition for A_∞. Here and in the following we adopt the common convention $1/\infty = 0$ and $1/0 = \infty$.

For a singular ϕ, that is $\phi \in \mathcal{H}_{-2}(A)\backslash\mathcal{H}$ the formal sum (1.1) needs to be interpreted as an operator in $\mathcal{H}$ since the perturbation does not immediately make sense. This can be achieved by looking at a symmetric restriction S of A, namely the restriction to all $u \in \operatorname{dom} A$ such that $\langle u,\phi\rangle = 0$. It turns out that S has deficiency indices $(1,1)$ so that the well-known extension theory for symmetric operators can be applied: the self-adjoint extensions of S in $\mathcal{H}$ are parametrized by Krein's formula

$$(A^\tau - z)^{-1} = (A - z)^{-1} - \frac{\langle\phi_{\bar z},\cdot\rangle}{q(z) + 1/\tau}\phi_z \tag{1.3}$$

with ϕ_z as above and $q(z)$ defined by the relation $\frac{q(z)-\overline{q(z_0)}}{z-\bar z_0} = \langle\phi_{\bar z_0},\phi_z\rangle$. This family of self-adjoint operators $(A^\tau)_{\tau\in\mathbb{R}\cup\{\infty\}}$ can be used to give meaning to (1.1). If $\phi \in \mathcal{H}_{-1}(A)$ and given a certain α, it is possible to pick out one particular A^τ to define A_α. For $\phi \in \mathcal{H}_{-2}\backslash\mathcal{H}_{-1}$ such a direct definition is not possible — at least not without additional assumptions — but the whole family of self-adjoint operators $(A_\alpha)_{\alpha\in\mathbb{R}\cup\{\infty\}}$ in (1.1) is identified with the family $(A^\tau)_{\tau\in\mathbb{R}\cup\{\infty\}}$.

1.2. SUPERSINGULAR PERTURBATIONS FOR SEMIBOUNDED OPERATORS. When one tries the above procedure for elements $\phi \in \mathcal{H}_{-n-2}(A)\backslash\mathcal{H}_{-2}(A)$ for $n \geqslant 1$ one finds that restricting A in $\mathcal{H}$ gives an essentially self-adjoint operator. Hence, there is no family (A^τ) to define (1.1). One could of course then consider A as an operator in $\mathcal{H}_n(A)$ where a symmetric restriction as above will again have defect indices $(1,1)$. However, it then remains unclear how ϕ and (1.1) are connected to the self-adjoint extensions inside $\mathcal{H}_n(A)$. Thus, some different approach is needed at this point.

In this section we shall briefly recall the operator model in the case of semibounded operators. Detailed arguments and proofs can be found in [10].

In the following let $A \geqslant 0$ and $\phi \in \mathcal{H}_{-n-2}(A)\backslash\mathcal{H}_{-n-1}$ for a fixed $n \geqslant 1$. The main idea is to still consider A in the smaller space $\mathcal{H}_n(A)$, where a symmetric restriction to $u \in \operatorname{dom} A$ with $\langle u,\phi\rangle = 0$ has the properties we need. At the same time, elements $\phi_z := (A - z)^{-1}\phi$ are added to the space so that they will naturally appear in Krein's formula. Due to the resolvent identity, it is enough to add n such elements. Thus, choose distinct points $\mu_1,\dots,\mu_n < 0$ and define:

the polynomial

$$b(z) := \prod_{k=1}^{n}(z-\mu_k), \tag{1.4}$$

the diagonal matrix

$$M := \operatorname{diag}(\mu_1, \dots, \mu_n), \tag{1.5}$$

the set of coefficients from the partial fraction decompostion of $b(z)^{-1}$

$$a_j := \prod_{k=1, k\neq j}^{n} \frac{1}{\mu_j - \mu_k}, \quad \vec{a} := (a_1, \dots, a_n), \tag{1.6}$$

the n elements

$$g(\mu_i) := \frac{1}{A-\mu_i}\phi \in \mathcal{H}_{-n}. \tag{1.7}$$

Formally, these then solve $(A-\mu_i)g(\mu_i) = \phi$. Finally, for some number $\mu < 0$ distinct from the μ_i above, we define also the element

$$G(\mu) := \frac{1}{A-\mu}\prod_{k=1}^{n}\frac{1}{A-\mu_k}\phi \in \mathcal{H}_n. \tag{1.8}$$

Note that the μ_i are chosen “to the left of the spectrum” of A such that the polynomial $b(z)$ is positive on $\sigma(A)$. Hence, instead of the standard scalar product $\langle f, g\rangle_{\mathcal{H}_n} = \langle f, (A+1)^n g\rangle_{\mathcal{H}}$ in $\mathcal{H}_n$ the equivalent one $\langle f, b(A)g\rangle_{\mathcal{H}}$ can be used. Furthermore, a positive definite Gram matrix Γ can be chosen such that $\Gamma M = M\Gamma$, e.g., by taking a diagonal matrix with positive entries.

A Hilbert space is then given as

$$\mathbb{H} := \mathcal{H}_n \oplus \mathbb{C}^n \tag{1.9}$$

with elements $\mathbb{H} \ni \mathbb{U} = (U, \vec{u})$ and scalar product

$$\langle \mathbb{U}, \mathbb{V}\rangle_{\mathbb{H}} := \langle U, b(A)V\rangle_{\mathcal{H}} + \langle \vec{u}, \Gamma\vec{v}\rangle_{\mathbb{C}^n}. \tag{1.10}$$

It is clear that $\mathbb{H}$ can be embedded in $\mathcal{H}_{-n}$ via $\mathfrak{i}(U, \vec{u}) := U + \sum_{i=1}^{n} u_i g(\mu_i)$. In this new space, A gives rise to two operators.

First, the operator $A_{\max}$ is defined via the following procedure: consider the operator $A|_{\{u\in\mathcal{H}_{n+2}:\langle u,\phi\rangle=0\}}$, then one can calculate its triplet adjoint operator $A^{\dagger}$ with respect to the Gelfand triplet $\mathcal{H}_n \subseteq \mathcal{H} \subseteq \mathcal{H}_{-n}$, and finally restrict $A^{\dagger}$ to $\mathbb{H}$. The operator $A_{\min}$ is then defined as the adjoint of $A_{\max}$ in $\mathbb{H}$. It turns out that these two operators act in the following way:

(i) on $\operatorname{dom} A_{\max} = \{\mathbb{U} \in \mathbb{H} : U = U_r + uG(\mu),\ U_r \in \mathcal{H}_{n+2},\ u \in \mathbb{C}\}$

$$A_{\max}\begin{pmatrix} U_r + uG(\mu) \\ \vec{u}\end{pmatrix} = \begin{pmatrix} AU_r + \mu u G(\mu) \\ M\vec{u} + u\vec{a}\end{pmatrix}; \tag{1.11}$$

(ii) on $\operatorname{dom} A_{\min} = \{\mathbb{U} \in \operatorname{dom} A_{\max} : u = 0, \langle \Gamma\vec{a}, \vec{u}\rangle = \langle \phi, U_r\rangle\}$

$$A_{\min}\begin{pmatrix} U_r \\ \vec{u}\end{pmatrix} = \begin{pmatrix} AU_r \\ \Gamma^{-1}M\Gamma\vec{u}\end{pmatrix} = \begin{pmatrix} AU_r \\ M\vec{u}\end{pmatrix}. \tag{1.12}$$

Due to Γ and M commuting $A_{\min}$ is symmetric with deficiency indices $(1,1)$ and the defect element can be calculated to be

$$\Phi(z) := \begin{pmatrix} G(z) \\ -\frac{1}{M-z}\vec{a}\end{pmatrix}$$

for nonreal z. Embedded in $\mathcal{H}_{-n}$ this is the element $\mathrm{i}\Phi(z) = b(z)^{-1}(A-z)^{-1}\phi$. From this point on, classical extension theory can be employed to find all self-adjoint extensions of $A_{\min}$ in $\mathbb{H}$. In [10] this is achieved via restricting $A_{\max}$ by certain conditions. This gives the operator family A^{θ}, $\theta \in [0,\pi)$, defined on the sets

$$\operatorname{dom} A^{\theta} := \{\mathbb{U} \in \operatorname{dom} A_{\max} : \sin\theta\langle\phi, U_r\rangle + \cos\theta u - \sin\theta\langle\Gamma\vec{a},\vec{u}\rangle = 0\}$$

and acting like $A_{\max}$ there. If $A^0 = A \oplus M$ is fixed then the resolvents of all other selfadjoint operators can be related to it via Krein's formula in $\mathbb{H}$. The beauty of this model is that by restricting this formula to $\mathcal{H}_n$ and then embedding it into $\mathcal{H}_{-n}$ one arrives at

$$\mathrm{i}\frac{1}{A^{\theta}-z}|_{\mathcal{H}_n} = \frac{1}{A-z} - \frac{1}{b(z)\big(Q(z)+\cot\theta\big)}\Big\langle \frac{1}{A-\bar{z}}\phi, \cdot\Big\rangle \frac{1}{A-z}\phi \tag{1.13}$$

with $Q(z) := \langle \phi, (z-\mu)(A-\mu)^{-1}G(z)\rangle + \langle \vec{a}, \Gamma(M-z)^{-1}\vec{a}\rangle$ the Q-function from Krein's formula and the factor $b(z)$ in the denominator arising from the embedding of the defect element. The model for supersingular perturbations of semibounded operators has thus two key features that we want to preserve in generalizations, namely:

(F1) the perturbation is modeled in a Hilbert space, and
(F2) the description of the perturbation is achieved by a Krein type formula.

REMARK 1.1. Another nice feature of the model is that spectral properties of the perturbation operators are described by a certain generalized Nevanlinna function. This function can also be obtained by regularizing the bordered resolvent $\langle \phi, (A-z)^{-1}\phi\rangle$, cf. Section 8 of [10].

1.3. SUPERSINGULAR PERTURBATIONS. THE NON-SEMIBOUNDED CASE. From now on we assume that A is a self-adjoint but not necessarily semibounded operator in a given Hilbert space $\mathcal{H}$. In particular, it might occur that $\sigma(A) = \mathbb{R}$. Furthermore, let $\phi \in \mathcal{H}_{-n-2}(A)\backslash\mathcal{H}_{-n-1}(A)$ for $n \geqslant 1$ be given. The requirement that $\phi \notin \mathcal{H}_{-n-1}(A)$ is a minimality condition so that the constructed model is not unnecessarily big but it does not play any role otherwise.

As before, our aim is to interpret (1.1), namely $A + \alpha\langle\phi,\cdot\rangle\phi$ for $\alpha \in \mathbb{R}\cup\{\infty\}$, as self-adjoint operators in a suitable model space.

REMARK 1.2. If the spectrum of A has gaps, it is possible to employ the model for semibounded operators because an appropriate number of regularization points μ_i can then be chosen in the gaps such that the function $b(z)$ is positive on $\sigma(A)$. If there are parts of the spectrum to the left of the μ_i, this requires choosing an even number of points. Thus, the model space might turn out to be slightly bigger compared to the case of semibounded operators.

In the following sections we will look at two very natural ways to generalize the existing Hilbert space model for semibounded operators to the non-semibounded case. In order to really be able to talk about a generalization we want to keep both features (F1) and (F2) in our more general case. The Hilbert space property (F1) can be of particular interest as this is often a more natural setting for many situations motivated by physics. Compare for example with formulations of quantum mechanics in a Pontryagin space where models involving self-adjoint operators there sometimes are restricted to certain positive subspaces that reduce a given operator in order to make it "physical" whereas formulations in a Hilbert space do not require such a step.

More to the point, we pose the question: *Is the assumption that A is semibounded only a technical property necessary for the construction of a Hilbert space model? Or is it intrinsic in that without it a generalized model will fail?*

The problem we face lies in the fact that we cannot use real regularization points μ_i since all of the real line might be part of the spectrum of A. Thus, we present two approaches:

(i) Split the Hilbert space $\mathcal{H}$ and the operator A into a direct sum with respect to the positive and negative parts of the spectrum. This way, the spectrum of the respective operators is contained in a half-line and this allows us to still choose real regularization points so that in each component we can use the semibounded model. This idea is described in the following Section 2.

(ii) We move the regularization points into the complex plane. In order to define an inner product we need conjugate pairs but this is the only immediate restriction. Otherwise the general ideas for the semibounded operators is still applicable to define a suitable space and a symmetric operator acting in it so that extension theory comes into play. This is done in Section 3.

In the last Section 4 we also compare the two approaches in terms of their Q-functions.

2. HILBERT SPACE MODELS

We decompose the operator A in the following way: $A = A^+ \oplus (-A^-)$, where $\sigma(A^\pm) \subseteq [0, \infty)$, i.e., we split A according to the two spectral subspaces $\mathcal{H}^+$ and $\mathcal{H}^-$ corresponding to the two parts of the spectrum contained in $[0, \infty)$ and $(-\infty, 0]$, respectively. If $\lambda = 0$ is an eigenvalue of A, we choose to add this spectral point to A^+ but this convention is not essential for what follows. Hence, $A^\pm \geqslant 0$ and we can in each subspace employ the existing model for supersingular perturbations.

REMARK 2.1. Choosing the splitting point at $\lambda = 0$ is completely arbitrary. Any other point would lead to a model exhibiting similar features.

This splitting of the Hilbert space $\mathcal{H}$ also continues through the scale of Hilbert spaces, $\mathcal{H}_k(A) = \mathcal{H}_k(A^+) \oplus \mathcal{H}_k(A^-)$ for $k \in \mathbb{Z}$. In the following, we just write $\mathcal{H}_k^\pm := \mathcal{H}_k(A^\pm)$ and suppress the operators that are used to define the spaces. Finally, we also decompose $\phi = \phi^+ + \phi^-$, with $\phi^\pm \in \mathcal{H}_{-n-2}^\pm$ and for the sake of simplicity both $\phi^+ \notin \mathcal{H}_{-n-1}^+$ and $\phi^- \notin \mathcal{H}_{-n-1}^-$. We comment on this below in Remark 2.2.

2.1. THE HILBERT SPACE $\mathbb{H}$.

We choose distinct numbers $\mu_1, \ldots, \mu_n < 0$ and define $b(z)$, M and $\vec{a}$ as in (1.4), (1.5) and (1.6), respectively. Furthermore, let as in (1.7)

$$g^\pm(\mu_i) := \frac{1}{A^\pm - \mu_i}\phi^\pm \in \mathcal{H}_{-n}^\pm \quad 1 \leqslant i \leqslant n.$$

We also choose two positive definite Hermitian matrices $\Gamma^\pm \in \mathbb{C}^{n\times n}$. So we can build $\mathbb{H}^\pm$ as in (1.9), i.e.,

$$\mathbb{H}^\pm := \mathcal{H}_n^\pm \oplus \mathbb{C}^n$$

and equip each of the spaces with scalar products as in (1.10). Consequently, we put

$$\mathbb{H} := \mathbb{H}^+ \oplus \mathbb{H}^- \tag{2.1}$$

as the Hilbert space we shall work in. Clearly, $\mathbb{H}$ is a $2n$-dimensional extension of $\mathcal{H}_n$ and can be embedded into $\mathcal{H}_{-n}$ by

$$\mathrm{i}_{\mathbb{H}}(U^+, \vec{u}^+, U^-, \vec{u}^-) := U^+ + \sum_{k=1}^n u_k^+ \frac{1}{A^+ - \mu_k}\phi^+ + U^- + \sum_{k=1}^n u_k^- \frac{1}{A^- - \mu_k}\phi^-.$$

REMARK 2.2. In case that either of the two conditions for $\phi^\pm$ is not met, i.e, $\phi^+ \in \mathcal{H}_{-n^+-2}^+ \backslash \mathcal{H}_{-n^+-1}^+$ and $\phi^- \in \mathcal{H}_{-n^--2}^- \backslash \mathcal{H}_{-n^--1}^-$ with $n^+ \neq n^-$, which in general will happen, then the space $\mathbb{H}$ and the formulas that follow need to be adapted. Let with loss of generality $n_+ > n_-$. Then we still will need $\mathcal{H}_{n^+}$ to model the extension problem. However, while we extend $\mathcal{H}_{n^+}^+$ by $\mathbb{C}^{n^+}$, for $\mathcal{H}_{n^+}^-$ it will be enough to add $\mathbb{C}^s$ with $s = n^- + \lfloor (n^+ - n^-)/2 \rfloor$. In this case, $\iota_{\mathbb{H}}$ will still be an injective map into $\mathcal{H}_{-n^+}$. The changes that need to be made for the scalar products and in the following formulas should be obvious from that.

2.2. ACTION OF THE OPERATOR. We start by defining a maximal operator $A_{\max}$ induced by A. It is clear that for any $f^{\pm} \in \mathcal{H}^{\pm}_{n+2}$ we have that $A^{\pm} f \in \mathcal{H}^{\pm}_{n}$. Additionally, we choose an additional parameter $\mu \in (-\infty, 0)\setminus\{\mu_1, \dots, \mu_n\}$ and define

$$\begin{aligned} G^{+}(\mu) &:= \frac{1}{(A^{+}-\mu)b(A^{+})}\phi^{+} \in \mathcal{H}^{+}_{n}, \\ G^{-}(\mu) &:= \frac{1}{(A^{-}-\mu)b(A^{-})}\phi^{-} \in \mathcal{H}^{-}_{n}. \end{aligned} \tag{2.2}$$

Now we can set

$$A_{\max} := A^{+}_{\max} \oplus (-A^{-}_{\max}), \tag{2.3}$$

where $A^{\pm}_{\max}$ are the maximal operators obtained from $A^{\pm}$ in $\mathbb{H}^{\pm}$, respectively, by the procedure used for semibounded self-adjoint operators in [10], see also (1.11). As a direct consequence of this definition of $A_{\max}$ we obtain the following result.

PROPOSITION 2.3. *The maximal operator $A_{\max}$ has domain*

$$\operatorname{dom} A_{\max} = \left\{ \mathbb{U} \in \mathbb{H} : \quad \begin{array}{c} U^{\pm} = U^{\pm}_{r} + u^{\pm} G^{\pm}(\mu), \\ U^{\pm}_{r} \in \mathcal{H}^{\pm}_{n+2},\ u^{\pm} \in \mathbb{C},\ \vec{u}^{\pm} \in \mathbb{C}^{n} \end{array} \right\} \tag{2.4}$$

and acts as

$$A_{\max} \begin{pmatrix} U^{+}_{r} + u^{+} G^{+}(\mu) \\ \vec{u}^{+} \\ U^{-}_{r} + u^{-} G^{-}(\mu) \\ \vec{u}^{-} \end{pmatrix} = \begin{pmatrix} A^{+} U^{+}_{r} + \mu u^{+} G^{+}(\mu) \\ M\vec{u}^{+} + u^{+}\vec{a} \\ -A^{-} U^{-}_{r} - \mu u^{-} G^{-}(\mu) \\ -M\vec{u}^{-} - u^{-}\vec{a} \end{pmatrix}.$$

As in the semibounded case, taking the adjoint of $A_{\max}$ will give us a symmetric operator to apply extension theory, compare also (1.12).

PROPOSITION 2.4. *The minimal operator $A_{\min} := A^{*}_{\max}$ has domain*

$$\operatorname{dom} A_{\min} = \{ \mathbb{U} \in \mathbb{H} : U^{\pm} \in \mathcal{H}^{\pm}_{n+2},\ \vec{u}^{\pm} \in \mathbb{C}^{n},\ \langle \phi^{\pm}, U^{\pm} \rangle = \langle \Gamma^{\pm}\vec{a}, \vec{u}^{\pm} \rangle \}$$

and its action is given by

$$A_{\min} \begin{pmatrix} U^{+} \\ \vec{u}^{+} \\ U^{-} \\ \vec{u}^{-} \end{pmatrix} = \begin{pmatrix} A^{+} U^{+} \\ (\Gamma^{+})^{-1} M \Gamma^{+} \vec{u}^{+} \\ -A^{-} U^{-} \\ -(\Gamma^{-})^{-1} M \Gamma^{-} \vec{u}^{-} \end{pmatrix}.$$

It is symmetric with deficiency indices $(2,2)$ if and only if $(\Gamma^{\pm})^{-1} M \Gamma^{\pm} = M$ and in this case it is the restriction of $A_{\max}$ by four conditions

$$A_{\min} = A_{\max}\big|_{\{\mathbb{U} \in \operatorname{dom} A_{\max}:\ u^{\pm}=0,\ \langle \phi^{\pm}, U^{\pm}_{r} \rangle = \langle \Gamma^{\pm}\vec{a}, \vec{u}^{\pm} \rangle\}}. \tag{2.5}$$

The proof is similar to the one in [10] but we include it for the sake of completeness.

Proof. Let $\mathbb{F} \in \mathbb{H}$, then $\mathbb{F} \in \operatorname{dom} A_{\min}$ if and only if there exists $\mathbb{W} \in \mathbb{H}$ such that $\langle \mathbb{F}, A_{\max}\mathbb{U}\rangle - \langle \mathbb{W}, \mathbb{U}\rangle = 0$ for all $\mathbb{U} \in \operatorname{dom} A_{\max}$. This $\mathbb{W}$ will be unique since $A_{\max}$ is densely defined. Expanding the scalar product we get

$$
\begin{aligned}
0 &= \left\langle \begin{pmatrix} F^+ \\ \vec{f}^+ \\ F^- \\ \vec{f}^- \end{pmatrix}, \begin{pmatrix} A^+U_r^+ + \mu u^+ G^+(\mu) \\ M\vec{u}^+ + u^+\vec{a} \\ -A^-U_r^- - \mu u^- G^-(\mu) \\ -M\vec{u}^- - u^-\vec{a} \end{pmatrix} \right\rangle - \left\langle \begin{pmatrix} W^+ \\ \vec{w}^+ \\ W^- \\ \vec{w}^- \end{pmatrix}, \begin{pmatrix} U_r^+ + u^+G^+(\mu) \\ \vec{u}^+ \\ U_r^- + u^-G^-(\mu) \\ \vec{u}^- \end{pmatrix} \right\rangle \\
&= \left\langle F^+, b(A^+)A^+U_r^+ + \mu u^+ \frac{1}{A^+ - \mu}\phi^+ \right\rangle + \langle \vec{f}^+, \Gamma^+(M\vec{u}^+ + u^+\vec{a})\rangle \\
&\quad + \left\langle F^-, b(A^-)(-A^-)U_r^- - \mu u^- \frac{1}{A^- - \mu}\phi^- \right\rangle + \langle \vec{f}^-, \Gamma^-(-M\vec{u}^- - u^-\vec{a})\rangle \\
&\quad - \left\langle W^+, b(A^+)U_r^+ + u^+ \frac{1}{A^+ - \mu}\phi^+ \right\rangle - \langle \vec{w}^+, \Gamma^+\vec{u}^+\rangle \\
&\quad - \left\langle W^-, b(A^-)U_r^- + u^- \frac{1}{A^- - \mu}\phi^- \right\rangle - \langle \vec{w}^-, \Gamma^-\vec{u}^-\rangle \\
&= \langle A^+F^+ - W^+, b(A^+)U_r^+\rangle + \langle -A^-F^- - W^-, b(A^-)U_r^-\rangle \\
&\quad + \langle M\Gamma^+\vec{f}^+ - \Gamma^+\vec{w}^+, \vec{u}^+\rangle + \langle -M\Gamma^-\vec{f}^- - \Gamma^-\vec{w}^-, \vec{u}^-\rangle \\
&\quad + u^+\Big(\Big\langle \mu F^+ - W^+, \frac{1}{A^+ - \mu}\phi^+ \Big\rangle + \langle \vec{f}^+, \Gamma^+\vec{a}\rangle\Big) \\
&\quad + u^-\Big(\Big\langle -\mu F^- - W^-, \frac{1}{A^- - \mu}\phi^- \Big\rangle - \langle \vec{f}^-, \Gamma^-\vec{a}\rangle\Big).
\end{aligned}
$$

If $U_r^- = 0, u^\pm = 0, \vec{u}^\pm = 0$, then we must have

$$
0 = \langle A^+F^+ - W^+, b(A^+)U_r^+\rangle \quad \forall U_r^+ \in \mathcal{H}_{n+2}^+
$$

and, thus, $F^+ \in \mathcal{H}_{n+2}^+$ as well as $A^+F^+ = W^+$ must hold. Similarly, one concludes $F^- \in \mathcal{H}_{n+2}^-$ and $-A^-F^- = W^-$ as well as the rest of the claim.

The condition for symmetry and the particular description as a restriction of $A_{\max}$ is now easily seen from the description of $\mathbb{A}_{\min}$.

As $A^\pm$ have defect indices $(1,1)$ in $\mathbb{H}^\pm$, summing them gives the defect indices of $A_{\min}$ as claimed. ∎

In the following we assume that the matrices $\Gamma^\pm$ both commute with M so that we have a symmetric operator $A_{\min} \subseteq A_{\max}$.

Let $\mathfrak{N}_z$ be the defect space for $z \in \mathbb{C}\backslash\mathbb{R}$. To find the deficiency elements, we solve $(A_{\max} - z)\mathbb{U} = 0$. Solving this system in the positive and negative component of $\mathbb{H}$ separately leads to the two linearly independent solutions

$$\Phi^+(z) := \begin{pmatrix} \frac{1}{(A^+-z)b(A^+)}\phi^+ \\ -\frac{1}{M-z}\vec{a} \\ 0 \\ \vec{0} \end{pmatrix}, \quad \Phi^-(z) := \begin{pmatrix} 0 \\ \vec{0} \\ \frac{1}{(-A^- -z)b(A^-)}\phi^- \\ -\frac{1}{-M-z}\vec{a} \end{pmatrix}.$$

Hence, $\mathfrak{N}_z$ for $z \in \mathbb{C}\backslash\mathbb{R}$ is spanned by $\Phi^+(z)$ and $\Phi^-(z)$. Note that they satisfy $\Phi^\pm(w) = \frac{A-z}{A-w}\Phi^\pm(z)$ and that embedding them into $\mathcal{H}_{-n}$ gives

$$\mathrm{i}_{\mathbb{H}}\Phi^\pm(z) = \frac{1}{b(\pm z)}\frac{1}{\pm A^\pm - z}\phi^\pm.$$

REMARK 2.5. As expected from the model for semibounded operators, Φ^+ has $G^+(z)$ in its first component:

$$\Phi^+(z) = (G^+(z), -(M-z)^{-1}\vec{a}, 0, \vec{0})^\top.$$

In comparison to this, the second deficiency element Φ^- is:

$$\Phi^-(z) = (0, \vec{0}, -G^-(-z), (M-(-z))^{-1}\vec{a})^\top.$$

Standard extension theory now enables us to find all self-adjoint operators A^Θ such that

$$A_{\min} \subseteq A^\Theta = (A^\Theta)^* \subseteq A_{\max} = A^*_{\min}.$$

However, this family is parametrized by 2×2 matrices or linear relations and corresponds rather to defining formal sums

$$A + \sum_{i,j\in\{+,-\}} \alpha^{ij}\langle\phi^i, \cdot\rangle\phi^j \tag{2.6}$$

with Hermitian matrices

$$\begin{pmatrix} \alpha^{++} & \alpha^{+-} \\ \alpha^{-+} & \alpha^{--} \end{pmatrix}$$

instead of (1.1). It is, so to say, too large to interpret the family $(A_\alpha)_{\alpha\in\mathbb{R}\cup\{\infty\}}$ since, motivated by the semibounded model, we would expect a one-parameter family instead. There are two immediate possibilities to select a suitable one-parameter family from all of the A^Θ.

(i) On the one hand, we could think of selecting the sub-family where all α^{ij}, with $i, j \in \{+,-\}$, are equal as in this case (2.6) and (1.1) coincide. This corresponds formally to a restriction of the parameter Θ and the resulting operator is an extension of $A|_{\{u\in\mathcal{H}_{n+2}:\langle\phi,u\rangle=0\}}$.

(ii) On the other hand, we can restrict the domain of $A_{\max}$ by certain conditions that ensure the appearance of $\langle\phi, U_r\rangle = \langle\phi^+, U_r^+\rangle + \langle\phi^-, U_r^-\rangle$. Motivated by the semibounded case this boundary value, directly involving the original perturbation element ϕ instead of ϕ^+ and ϕ^- separately, should explicitly appear in our model.

Both choices are motivated by what happens in the semibounded case and are thus not as arbitrary as it might appear. In the following, we will continue along both paths and show that the families we select coincide.

In order to describe all self-adjoint extensions of $A_{\min}$ we fix a certain extension as a reference operator. A somewhat obvious choice for this is the diagonal operator

$$\begin{aligned} \operatorname{dom} A^0 &:= \{\mathbb{U} \in \operatorname{dom} A_{\max} :\ u^{\pm} = 0\} \cong \mathcal{H}^+_{n+2} \oplus \mathbb{C}^n \oplus \mathcal{H}^-_{n+2} \oplus \mathbb{C}^n, \\ A^0 &:= A^+ \oplus M \oplus (-A^-) \oplus (-M). \end{aligned}$$

More naturally, when instead considering as a domain $\mathcal{H}_{n+2} \oplus \mathbb{C}^{2n}$ the operator takes the form $A^0 \cong A \oplus \operatorname{diag}(M, -M)$.

REMARK 2.6. Note that $A_{\min}$ is the restriction of A^0 by the two conditions $\langle (A^0 - \overline{z}_0)\mathbb{U}, \Phi^{\pm}(z_0)\rangle = 0$ for arbitrary $z_0 \in \mathbb{C}\backslash\mathbb{R}$, since

$$\begin{aligned} \langle U^{\pm}, \phi^{\pm}\rangle &= \Big\langle (\pm A^{\pm} - \overline{z}_0)U^{\pm}, \frac{1}{\pm A^{\pm} - z_0}\phi^{\pm}\Big\rangle, \\ -\langle \vec{u}^{\pm}, \Gamma^{\pm}\vec{a}\rangle &= \Big\langle (\pm M - \overline{z}_0)\vec{u}^{\pm}, \Gamma^{\pm}\Big(-\frac{1}{\pm M - z_0}\Big)\vec{a}\Big\rangle \end{aligned}$$

and summing the terms from $\mathbb{H}^+$ and $\mathbb{H}^-$ separately gives the restriction.

2.3. SELF-ADJOINT FAMILY OF OPERATORS VIA KREIN'S FORMULA. Let us calculate the Q-function for the symmetric operator $A_{\min}$. In our case this will be a 2×2-matrix function $\mathfrak{Q}(z)$. We choose an arbitrary $z_0 \in \mathbb{C}^+$ as a base point. Then the Q-function is defined by $\frac{\mathfrak{Q}(z)-\overline{\mathfrak{Q}(z_0)}}{z-\overline{z}_0} = \langle \Phi(z_0), \Phi(z)\rangle$, i.e.

$$\frac{\mathfrak{Q}(z) - \overline{\mathfrak{Q}(z_0)}}{z - \overline{z}_0} = \begin{pmatrix} \langle \Phi^+(z_0), \Phi^+(z)\rangle & \langle \Phi^+(z_0), \Phi^-(z)\rangle \\ \langle \Phi^-(z_0), \Phi^+(z)\rangle & \langle \Phi^-(z_0), \Phi^-(z)\rangle \end{pmatrix}.$$

The matrix on the right side is diagonal since $\langle \Phi^{\pm}(z_0), \Phi^{\mp}(z)\rangle = 0$. Rearranging yields

$$\mathfrak{Q}(z) = (z - \overline{z}_0)\begin{pmatrix} \langle \Phi^+(z_0), \Phi^+(z)\rangle & 0 \\ 0 & \langle \Phi^-(z_0), \Phi^-(z)\rangle \end{pmatrix} + \Re\mathfrak{Q}(z_0) - \mathrm{i}\Im\mathfrak{Q}(z_0)$$

where

$$-\mathrm{i}\Im\mathfrak{Q}(z_0) = -\mathrm{i}\frac{\mathfrak{Q}(z_0) - \overline{\mathfrak{Q}(z_0)}}{2\mathrm{i}} = -\frac{z_0 - \overline{z}_0}{2}\begin{pmatrix} \|\Phi^+(z_0)\|_{\mathbb{H}^+} & 0 \\ 0 & \|\Phi^-(z_0)\|_{\mathbb{H}^-} \end{pmatrix}$$

is diagonal as well. Regarding $\Re\mathfrak{Q}(z_0)$ we can assume this to be the zero matrix. Let

$$Q^{\pm}_A(z) := \Big\langle \phi^{\pm}, \Big[\frac{z - z_0}{\pm A^{\pm} - z_0} + \frac{z - \overline{z}_0}{\pm A^{\pm} - \overline{z}_0}\Big]\frac{1}{2(\pm A^{\pm} - z)b(A^{\pm})}\phi^{\pm}\Big\rangle, \tag{2.7}$$

$$Q^{\pm}_M(z) := \Big\langle \vec{a}, \Gamma^{\pm}\Big[\frac{z - z_0}{\pm M - z_0} + \frac{z - \overline{z}_0}{\pm M - \overline{z}_0}\Big]\frac{1}{2(\pm M - z)}\vec{a}\Big\rangle. \tag{2.8}$$

With the help of the resolvent identity one easily calculates

$$(z-\overline{z}_0)\langle \Phi^+(z_0),\Phi^+(z)\rangle - \frac{z_0-\overline{z}_0}{2}\|\Phi^+(z_0)\| = Q_A^+(z)+Q_M^+(z)$$

and similarly one concludes that the negative parts sum to $Q_A^-(z)+Q_M^-(z)$. So

$$\mathfrak{Q}(z)=\begin{pmatrix} Q^+(z) & 0 \\ 0 & Q^-(z)\end{pmatrix} := \begin{pmatrix} Q_A^+(z)+Q_M^+(z) & 0 \\ 0 & Q_A^-(z)+Q_M^-(z)\end{pmatrix}. \tag{2.9}$$

Let furthermore

$$\gamma_{z_0}:\mathbb{C}^2\to\mathfrak{N}_{z_0}:(\lambda_1,\lambda_2)\mapsto \lambda_1\Phi^+(z_0)+\lambda_2\Phi^-(z_0),$$

whence its adjoint is given by

$$\gamma_{\overline{z}_0}^*:\mathbb{H}\to\mathbb{C}^2:\mathbb{U}\mapsto(\langle\Phi^+(z_0),\mathbb{U}\rangle,\langle\Phi^-(z_0),\mathbb{U}\rangle)^\top.$$

We have now collected all ingredients for Krein's formula:

$$A_{\min}\subseteq A_{\max},\ A^0,\ z_0,\ \mathfrak{N}_z,\ \gamma_z,\ \gamma_{\overline{z}}^*,\ \mathfrak{Q}(z).$$

Krein's formula parametrises the whole family of self-adjoint extensions of $A_{\min}$ by

$$\frac{1}{A^\Theta-z}=\frac{1}{A^0-z}-\gamma_z\Theta(I+\mathfrak{Q}(z)\Theta)^{-1}\gamma_{\overline{z}}^* \tag{2.10}$$

when Θ runs through the set of all self-adjoint linear relations of $\mathbb{C}^2\times\mathbb{C}^2$.

The entire family "describes" in particular self-adjoint perturbations of A by all possible linear combinations of ϕ^+ and ϕ^-. In order to see only the relevant combination $\phi^++\phi^-=\phi$ we only have to consider those self-adjoint linear relations τ_β — that is, we restrict ourselves to a certain subset of all the possible parameter values of Θ — that are of the form

$$\tau_\beta=\beta\begin{pmatrix}1&1\\1&1\end{pmatrix}\quad \beta\in\mathbb{R}\cup\{\infty\}.$$

One then easily finds

$$\tau_\beta(I+\mathfrak{Q}(z)\tau_\beta)^{-1}=\frac{1}{1/\beta+Q^+(z)+Q^-(z)}\begin{pmatrix}1&1\\1&1\end{pmatrix},$$

$$\gamma_z\begin{pmatrix}1&1\\1&1\end{pmatrix}\gamma_{\overline{z}}^*=\langle\Phi(\overline{z}),\cdot\rangle\Phi(z),$$

where

$$\Phi(z):=\Phi^+(z)+\Phi^-(z). \tag{2.11}$$

Let $Q(z):=Q^+(z)+Q^-(z)$. Thus, we arrive at

$$\frac{1}{A^{\tau_\beta}-z}:=\frac{1}{A^0-z}-\frac{1}{1/\beta+Q(z)}\langle\Phi(\overline{z}),\cdot\rangle\Phi(z), \tag{2.12}$$

which gives a parametrization of the family of self-adjoint operators (A^{τ_β}) describing the perturbations $A+\alpha\langle\phi,\cdot\rangle\phi$.

REMARK 2.7. Clearly, $Q^{\pm}(z)$ — and thus also their sum $Q(z)$ — are Nevanlinna functions as they are the Q-functions of self-adjoint extensions of symmetric operators in Hilbert spaces. Alternatively, one can also easily check directly that they are analytic in $\mathbb{C}\backslash\mathbb{R}$, symmetric with respect to the real axis, i.e., $Q^{\pm}(z) = \overline{Q^{\pm}(\overline{z})}$, and that

$$\frac{\Im Q^{\pm}(z)}{\Im z} = \left\| \frac{1}{(\pm A^{\pm} - z)b(A^{\pm})}\phi^{\pm} \right\|^2_{\mathcal{H}_{n+2}} + \left\| \frac{1}{M-z}\vec{a} \right\|^2_{\mathbb{C}^n} = \|\Phi^{\pm}(z)\|^2_{\mathbb{H}} > 0.$$

2.4. DIRECT DESCRIPTION VIA BOUNDARY CONDITIONS. In this section we investigate how a one-parameter family of self-adjoint operators describing (1.1) can be chosen by restricting the maximal operator $A_{\max}$. We start by calculating the boundary form for $A_{\min} \subseteq A_{\max}$.

LEMMA 2.8. *The boundary form* $\langle A_{\max}\mathbb{U}, \mathbb{V}\rangle - \langle \mathbb{U}, A_{\max}\mathbb{V}\rangle$ *is given by*

$$\left\langle \begin{pmatrix} u^+ \\ -u^- \end{pmatrix}, \begin{pmatrix} \langle \vec{a}, \Gamma^+ \vec{v}^+\rangle - \langle \phi^+, V_r^+\rangle \\ \langle \vec{a}, \Gamma^- \vec{v}^-\rangle - \langle \phi^-, V_r^-\rangle \end{pmatrix} \right\rangle - \left\langle \begin{pmatrix} \langle \vec{a}, \Gamma^+ \vec{u}^+\rangle - \langle \phi^+, U_r^+\rangle \\ \langle \vec{a}, \Gamma^- \vec{u}^-\rangle - \langle \phi^-, U_r^-\rangle \end{pmatrix}, \begin{pmatrix} v^+ \\ -v^- \end{pmatrix} \right\rangle.$$

Proof. This follows immediately using

$$A_{\max} = A^+_{\max} \oplus -A^-_{\max}$$

with $A^{\pm}_{\max} := P_{\mathbb{H}^{\pm}} A_{\max}|_{\mathbb{H}^{\pm}}$ where we have orthogonal projections $P_{\pm} : \mathbb{H} \to \mathbb{H}^{\pm}$. This way we can use the model for semibounded operators in each component $\mathbb{H}^+$ and $\mathbb{H}^-$ and find that the boundary form $\langle A_{\max}\mathbb{U}, \mathbb{V}\rangle - \langle \mathbb{U}, A_{\max}\mathbb{V}\rangle$ is equal to

$$\langle A^+_{\max}\mathbb{U}^+, \mathbb{V}^+\rangle - \langle \mathbb{U}^+, A^+_{\max}\mathbb{V}^+\rangle - \langle A^-_{\max}\mathbb{U}^-, \mathbb{V}^-\rangle + \langle \mathbb{U}^-, A^-_{\max}\mathbb{V}^-\rangle. \qquad \blacksquare$$

Given the boundary form, a parametrization of all self-adjoint extensions of $A_{\min}$ can be given via suitable matrices B, C ensuring

$$B \begin{pmatrix} \langle \vec{a}, \Gamma^+ \vec{u}^+\rangle - \langle \phi^+, U_r^+\rangle \\ \langle \vec{a}, \Gamma^- \vec{u}^-\rangle - \langle \phi^-, U_r^-\rangle \end{pmatrix} = C \begin{pmatrix} u^+ \\ -u^- \end{pmatrix}. \tag{2.13}$$

Suitable in this context means that B^*C is Hermitian and that $(B|_C)$ has maximal rank, i.e., rank two. When we interpret $A + \alpha\langle\phi, \cdot\rangle\phi$ as an operator then elements that satisfy $\langle U_r, \phi\rangle = 0$ should always belong to the respective domain. These elements can be thought of as invisible to the perturbation term so they should not be affected by introducing A_α. To ensure the appearance of this term, it seems then natural to choose matrices of the form

$$\gamma \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

in the place of B because in this case we calculate $\langle \phi^+, U_r^+\rangle + \langle \phi^-, U_r^-\rangle = \langle \phi, U_r\rangle$. Furthermore, we make the choice that C is the identity matrix and in this case all requirements on B and C are satisfied. In the light of this the following definition is then straightforward.

DEFINITION 2.9. The domains of the operators A^γ for $\gamma \in \mathbb{R} \cup \{\infty\}$ are given by

$$\operatorname{dom} A^\gamma := \{\mathbb{U} \in \operatorname{dom} A_{\max} : u^+ = -u^- = \gamma(\langle \vec{a}, \Gamma^+ \vec{u}^+ + \Gamma^- \vec{u}^- \rangle - \langle \phi, U_r \rangle)\}.$$

In the next theorem we shall relate the two families (A^{τ_β}) and (A^γ) to each other by looking at the resolvents of A^γ.

THEOREM 2.10. *The family* $(A^\gamma)_{\gamma \in \mathbb{R} \cup \{\infty\}}$ *coincides with the family of self-adjoint operators* $(A^{\tau_\beta})_{\beta \in \mathbb{R} \cup \{\infty\}}$.

Proof. We proceed in two steps. First, we calculate the resolvent of A^γ and relate it to the resolvent of A^0. Second, we show that this parametrizes the same family as in (2.12).

Step 1. We invert $(A^\gamma - z)\mathbb{U} = \mathbb{F}$, i.e. for given $\mathbb{F} \in \mathbb{H}$ we need to find $\mathbb{U} \in \operatorname{dom} A^\gamma$. We thus have to solve, for $z \notin \mathbb{R} \supseteq \sigma(A^\gamma)$, the system

$$\begin{aligned} (A^+ - z)U_r^+ + (\mu - z)G^+(\mu)u^+ &= F^+ \\ (M - z)\vec{u}^+ + u^+\vec{a} &= \vec{f}^+ \\ (-A^- - z)U_r^- + (-\mu - z)G^+(\mu)u^- &= F^- \\ (-M - z)\vec{u}^- - u^-\vec{a} &= \vec{f}^-. \end{aligned}$$

Applying the respective resolvents and entering the definition of $G^\pm(\mu)$ from (2.2) gives

$$U_r^+ = \frac{1}{A^+ - z}F^+ + \frac{z - \mu}{(A^+ - z)(A^+ - \mu)b(A^+)}\phi^+ u^+ \tag{2.14}$$

$$\vec{u}^+ = \frac{1}{M - z}\vec{f}^+ - \frac{1}{M - z}\vec{a}u^+ \tag{2.15}$$

$$U_r^- = \frac{1}{-A^- - z}F^- + \frac{z + \mu}{(-A^- - z)(A^- - \mu)b(A^-)}\phi^- u^- \tag{2.16}$$

$$\vec{u}^- = \frac{1}{-M - z}\vec{f}^- + \frac{1}{-M - z}\vec{a}u^-. \tag{2.17}$$

So we have found $\mathbb{U} = (U_r^+ + u^+G^+(\mu), \vec{u}^+, U_r^- + u^-G^-(\mu), \vec{u}^-)$ expressed in terms of $\mathbb{F}$ and the two parameters $u^\pm$. Note that the first summands on the right sides in (2.14)–(2.17) are the respective terms of the resolvent of A^0 applied to $\mathbb{F}$.

In order for $\mathbb{U}$ to belong to $\operatorname{dom} A^\gamma$ we require that $u^+ = -u^-$. Let us call their common value $\mathfrak{u}$. To calculate $\mathfrak{u}$ define first

$$\begin{aligned} q_A^\pm(z) &:= \left\langle \phi^\pm, \frac{\pm z - \mu}{(\pm A^\pm - z)(A^\pm - \mu)b(A^\pm)}\phi^\pm \right\rangle \\ q_M^\pm(z) &:= \left\langle \vec{a}, \Gamma^\pm \frac{1}{\pm M - z}\vec{a} \right\rangle \end{aligned}$$

and for the sum of these four terms set

$$q(z) := q_A^+(z) + q_M^+(z) + q_A^-(z) + q_M^-(z). \tag{2.18}$$

Then projecting (2.14) and (2.16) onto $-\phi^{\pm}$ and (2.15) and (2.17) onto $\Gamma^{\pm}\vec{a}$, respectively, gives

$$\begin{aligned}
-\langle \phi^+, U_r^+\rangle &= -\left\langle \phi^+, \frac{1}{A^+ - z}F^+\right\rangle - q_A^+(z)\mathfrak{u} \\
\langle \vec{a}, \Gamma^+\vec{u}^+\rangle &= \quad \left\langle \vec{a}, \Gamma^+\frac{1}{M-z}\vec{f}^+\right\rangle - q_M^+(z)\mathfrak{u} \\
-\langle \phi^-, U_r^-\rangle &= -\left\langle \phi^-, \frac{1}{-A^- - z}F^-\right\rangle - q_A^-(z)\mathfrak{u} \\
\langle \vec{a}, \Gamma^-\vec{u}^-\rangle &= \quad \langle \vec{a}, \Gamma^-\frac{1}{-M-z}\vec{f}^-\rangle - q_M^-(z)\mathfrak{u}.
\end{aligned}$$

Note that summing the first summands on the right sides gives just $-\langle \Phi(\bar{z}), \mathbb{F}\rangle_{\mathbb{H}}$ with $\Phi(z)$ defined as in (2.11). Hence, when we sum the above system of four equations we get

$$\langle \vec{a}, \Gamma^+\vec{u}^+ + \Gamma^-\vec{u}^-\rangle - \langle \phi, U_r\rangle = -\langle \Phi(\bar{z}), \mathbb{F}\rangle - q(z)\mathfrak{u}$$

and due to the requirement of $\mathbb{U} \in \operatorname{dom} A^{\gamma}$ the left side must be equal to $\gamma^{-1}\mathfrak{u}$. Hence,

$$\mathfrak{u} = -\frac{1}{1/\gamma + q(z)}\langle \Phi(\bar{z}), \mathbb{F}\rangle.$$

Thus, (2.15) and (2.17) give the vectors $\vec{u}^{\pm}$ and for the remaining two coordinates $U^{\pm} = U_r^{\pm} + u^{\pm}G^{\pm}(\mu)$ of $\mathbb{U}$ we calculate

$$\begin{aligned}
U^+ &= \frac{1}{A^+ - z}F^+ + \Big(\frac{z-\mu}{A^+ - z} + I\Big)G^+(\mu)\mathfrak{u} = \frac{1}{A^+ - z}F^+ + \mathfrak{u}\frac{1}{(A^+ - z)b(A^+)}\phi^+, \\
U^- &= \frac{1}{-A^- - z}F^- - \Big(\frac{z+\mu}{-A^- - z} + I\Big)G^-(\mu)\mathfrak{u} = \frac{1}{-A^- - z}F^- + \mathfrak{u}\frac{1}{(-A^- - z)b(A^-)}\phi^-.
\end{aligned}$$

Hence, $\mathbb{U} = (A^0 - z)^{-1}\mathbb{F} + \mathfrak{u}\Phi(z)$ and comparing the resolvents shows

$$\frac{1}{A^{\gamma} - z} = \frac{1}{A^0 - z} - \frac{1}{1/\gamma + q(z)}\langle \Phi(\bar{z}), \cdot\rangle \Phi(z). \tag{2.19}$$

Step 2. The only point of difference between (2.12) and (2.19) is the appearance of $q(z) + \gamma^{-1}$ instead of $Q(z) + \beta^{-1}$. We claim that

$$q(z) - Q(z) = \Re q(z_0), \tag{2.20}$$

i.e., the two functions differ only by a real constant. In this case, the appearance of β^{-1} and γ^{-1} is irrelevant when parametrizing the resolvents of the families A^{τ_β} and A^{γ} as this only amounts to a reparametrization. We begin by collecting all terms from the definitions:

$$q(z) - Q(z) = \sum_{s\in\{+,-\},\, J\in\{A,M\}} q_J^s(z) - Q_J^s(z).$$

In each of the four possible combinations of s and J we can apply the resolvent identity to simplify the relevant difference; for example, in the case $s = +$ and $J = A$ we have

$$
\begin{aligned}
&q_A^+(z) - Q_A^+(z)\\
&\quad = \Big\langle \phi^+, \Big[\frac{z-\mu}{(A^+ - z)(A^+ - \mu)} - \frac{z - z_0}{2(A^+ - z)(A^+ - z_0)} - \frac{z - \overline{z}_0}{2(A^+ - z)(A^+ - \overline{z}_0)}\Big]\phi^+\Big\rangle\\
&\quad = \Big\langle \phi^+, \frac{1}{2}\Big[\frac{z_0 - \mu}{(A^+ - \mu)(A^+ - z_0)} + \frac{\overline{z}_0 - \mu}{(A^+ - \mu)(A^+ - \overline{z}_0)}\Big]\phi^+\Big\rangle = \Re q_A^+(z_0).
\end{aligned}
$$

Hence, we find that each difference sums to a term of the form $\Re q_J^s(z_0)$. Collecting all terms gives the claim.

So (2.19) parametrizes the same family of self-adjoint extensions of $A_{\min}$ as (2.12) and, thus, we also have a description of (A^{τ_β}) via boundary values. ∎

Note also that the function $q(z)$, as defined in (2.18), is a Nevanlinna function since $Q(z)$ certainly is a Nevanlinna function and thus $q(z)$ shares this property by (2.20).

COROLLARY 2.11. *The restricted-embedded resolvents for the family A^{τ_β} satisfy*

$$
i_{\mathbb{H}} \frac{1}{A^{\tau_\beta} - z}\Big|_{\mathcal{H}_n} = \frac{1}{A - z} - \frac{\langle (1/(A-\overline{z}))\phi, \cdot\rangle}{1/\beta + Q(z)}\Big(\frac{1}{b(z)}\frac{1}{A^+ - z}\phi^+ + \frac{1}{b(-z)}\frac{1}{-A^- - z}\phi^-\Big).
$$

REMARK 2.12. In the case of a semibounded operator, one could take out the factor $b(z)^{-1}$ and consider the generalized Nevanlinna function $b(z)(\frac{1}{\beta} + Q(z))$, cf. [7], compare also (1.13). In the case of not necessarily semibounded operators, one gets an extra twist due to the minus sign in $b(\pm z)$. Thus, even though we could preserve the Hilbert space property (F1), the property (F2) has been distorted.

3. PONTRYAGIN SPACE MODELS

In the present section we want to investigate how (F2) can be saved. However, it turns out that this comes at the cost of losing the Hilbert space property of our model space.

From now on we work directly with the given A and ϕ, so the scale of Hilbert spaces $\mathcal{H}_n$ is taken with respect to A. We modify our assumption on ϕ by requiring that $\phi \in \mathcal{H}_{-2k-2} \backslash \mathcal{H}_{-2k}$ for $k \geqslant 1$. The model we will build is again closely related to the one for semibounded operators. However, since the spectrum of A might occupy the whole real line, some modifications relating to the regularization points are necessary.

3.1. MODEL SPACE $\mathbb{K}$. We choose k regularization points $\nu_1, \dots, \nu_k \in \mathbb{C}^+$ and add $\nu_{k+j} := \overline{\nu}_j$ for $1 \leqslant j \leqslant k$. Let us define

$$d(z) := \prod_{j=1}^{2k}(z-\nu_j) = d_0(z)\overline{d_0(\overline{z})} \quad \text{where } d_0(z) := \prod_{j=1}^{k}(z-\nu_j) \quad \text{and} \tag{3.1}$$

$$N := \operatorname{diag}(\nu_1, \nu_2, \dots, \nu_{2k}). \tag{3.2}$$

Furthermore, set $g(\nu_j) := (A-\nu_j)^{-1}\phi$ and let

$$c_j := \prod_{\ell=1,\,\ell\neq j}^{2k} \frac{1}{\nu_j - \nu_\ell}, \quad \vec{c} := (c_1, \dots, c_{2k})$$

be the coefficients appearing in the partial fraction decomposition of $d(z)^{-1}$.

It is important to take conjugate pairs of complex numbers as regularization points in order to define a scalar product. We formulate this in a lemma to draw attention to it.

LEMMA 3.1. *The standard scalar product $\langle U, V\rangle_{\mathcal{H}_{2k}} = \langle U, (|A|+1)^{2k}V\rangle_{\mathcal{H}}$ is equivalent to $\langle U, d(A)V\rangle_{\mathcal{H}}$.*

Proof. First we note that $\langle U, (|A|+1)^{2k}V\rangle$ is equivalent to $\langle U, (A^{2k}+1)V\rangle$ and using positivity of $d(z)$ on $\mathbb{R}$ this in turn is equivalent to $\langle U, d(A)V\rangle$. ∎

Furthermore, choose an invertible self-adjoint matrix $\Gamma \in \mathbb{C}^{2k\times 2k}$. In order to build a model space, we add again a finite dimensional space to $\mathcal{H}_{2k}$ and define

$$\mathbb{K} := \mathcal{H}_{2k} \oplus \mathbb{C}^{2k}$$

with scalar product

$$\langle \mathbb{U}, \mathbb{V}\rangle_{\mathbb{K}} := \langle U, d(A)V\rangle_{\mathcal{H}} + \langle \vec{u}, \Gamma\vec{v}\rangle_{\mathbb{C}^{2k}}. \tag{3.3}$$

We can embed $\mathbb{K}$ into $\mathcal{H}_{-2k}$ by way of

$$\mathrm{i}_{\mathbb{K}}(U, \vec{u}) := U + \sum_{j=1}^{2k} u_j \frac{1}{A-\nu_j}\phi.$$

Thus, $\mathbb{K}$ can be thought of as a $2k$-dimensional extension of $\mathcal{H}_{2k}$ inside $\mathcal{H}_{-2k}$.

REMARK 3.2. The Hilbert space $\mathbb{H}$ was a $2n$-dimensional extension of $\mathcal{H}_n$. Since $n = 2k$, the extension $\mathbb{H}$ of $\mathcal{H}_n = \mathcal{H}_{2k}$ had twice as many dimensions as the present one $\mathbb{K}$.

We note that the scalar product in the first component is surely positive definite due to Lemma 3.1. The question is thus whether the matrix Γ can be chosen positive definite as well, which we will answer in the negative after recovering the operator induced by A in $\mathbb{K}$.

3.2. ACTION OF THE OPERATOR. First, take some $\nu \in \mathbb{C}^+ \setminus \{\nu_1, \dots, \nu_{2k}\}$ and define

$$G(\nu) := \frac{1}{(A-\nu)d(A)}\phi \in \mathcal{H}_{2k}.$$

Define the maximal operator $\mathbb{A}_{\max}$ through the procedure as laid out in [10]: Restrict A such that

$$S := A|_{\{u \in \mathcal{H}_{2k+2} : \langle u, \phi \rangle = 0\}}$$

and calculate its triplet adjoint operator $S^\dagger$ with respect to $\mathcal{H}_{2k} \subseteq \mathcal{H} \subseteq \mathcal{H}_{-2k}$. This construction does not depend on A being semibounded, so it carries over to our situation without any big changes in the arguments. Finally we can take $\mathbb{A}_{\max}$ to be the restriction of $S^\dagger$ to $\mathbb{K}$. The operator $\mathbb{A}_{\max}$ can also be described in the following explicit way.

PROPOSITION 3.3. *The maximal operator $\mathbb{A}_{\max}$ has domain*

$$\operatorname{dom} \mathbb{A}_{\max} = \{\mathbb{U} \in \mathbb{K} : U = U_r + uG(\nu),\ U_r \in \mathcal{H}_{2k+2},\ u \in \mathbb{C}\}$$

and acts as

$$\mathbb{A}_{\max} \begin{pmatrix} U_r + uG(\nu) \\ \vec{u} \end{pmatrix} = \begin{pmatrix} AU_r + \nu u G(\nu) \\ N\vec{u} + u\vec{c} \end{pmatrix}.$$

Proof. This follows as in [10] in the proofs of Lemmata 5.1 and 5.2. The obvious modifications of the argument come from using the complex numbers $\nu_1, \dots, \nu_{2k}, \nu$ instead of negative real regularization points. ∎

PROPOSITION 3.4. *The minimal operator $\mathbb{A}_{\min} := \mathbb{A}_{\max}^*$ has domain*

$$\operatorname{dom} \mathbb{A}_{\min} = \{\mathbb{U} \in \mathbb{K} : U = U_r \in \mathcal{H}_{2k+2}, \vec{u} \in \mathbb{C}^{2k}, \langle U, \phi \rangle = \langle \vec{u}, \Gamma \vec{c} \rangle\}$$

and acts as

$$\mathbb{A}_{\min} \begin{pmatrix} U \\ \vec{u} \end{pmatrix} = \begin{pmatrix} AU \\ \Gamma^{-1} N^* \Gamma \vec{u} \end{pmatrix}.$$

It is symmetric if and only if $N^*\Gamma = \Gamma N$. In this case, $\mathbb{A}_{\min}$ has deficiency indices $(1,1)$ and it is a restriction of $\mathbb{A}_{\max}$ by two conditions:

$$\mathbb{A}_{\min} = \mathbb{A}_{\max}|_{\{\mathbb{U} \in \operatorname{dom} \mathbb{A}_{\max} : u = 0,\ \langle U_r, \phi \rangle = \langle \vec{u}, \Gamma \vec{c} \rangle\}}. \tag{3.4}$$

Proof. The proof runs along the lines of the proof of Lemma 5.3 in [10]. The statement on symmetry and on $\mathbb{A}_{\min}$ being a restriction of $\mathbb{A}_{\max}$ follows once we have shown the formulas for $\operatorname{dom} \mathbb{A}_{\min}$ and the action of the operator.

An element $\mathbb{F} \in \mathbb{H}$ belongs to $\operatorname{dom} \mathbb{A}_{\min}$ if and only if there is a (unique, since $\mathbb{A}_{\max}$ is densely defined) $\mathbb{L} \in \mathbb{H}$ such that $\langle \mathbb{F}, \mathbb{A}_{\max}\mathbb{U} \rangle - \langle \mathbb{L}, \mathbb{U} \rangle = 0$ for all $\mathbb{U} \in \operatorname{dom} \mathbb{A}_{\max}$. In this case that means that

$$\begin{aligned} 0 &= \left\langle \begin{pmatrix} F \\ \vec{f} \end{pmatrix}, \begin{pmatrix} AU_r + \nu u G(\nu) \\ N\vec{u} + u\vec{c} \end{pmatrix} \right\rangle - \left\langle \begin{pmatrix} L \\ \vec{\ell} \end{pmatrix}, \begin{pmatrix} U_r + uG(\nu) \\ \vec{u} \end{pmatrix} \right\rangle \\ &= \langle AF - L, d(A)U_r \rangle + u\Big(\Big\langle \overline{\nu} F - L, \frac{1}{A-\nu}\phi \Big\rangle + \langle \vec{f}, \Gamma \vec{c} \rangle \Big) + \langle N^* \vec{f} - \vec{\ell}, \Gamma \vec{u} \rangle. \end{aligned}$$

For $u = 0, \vec{u} = \vec{0}$ one concludes that $AF - L$ must belong to $\mathcal{H}_{2k-2}$ for the scalar product to be well-defined, so that $F \in \mathcal{H}_{2k}$ and $AF = L$.

Using the latter relation in the product with u, we get $\langle F, \phi \rangle - \langle \vec{f}, \Gamma \vec{c} \rangle = 0$ and for that to be well-defined F must even belong to $\mathcal{H}_{2k+2}$. ∎

In the case that $N^* \Gamma = \Gamma N$, the deficiency element of $\mathbb{A}_{\min}$ is

$$\Psi(z) = \begin{pmatrix} \frac{1}{(A-z)d(A)} \phi \\ -\frac{1}{N-z} \vec{c} \end{pmatrix} = \begin{pmatrix} G(z) \\ -\frac{1}{N-z} \vec{c} \end{pmatrix} \tag{3.5}$$

and embedded in $\mathcal{H}_{-2k}$ we have

$$\mathrm{i}_{\mathbb{K}} \Psi(z) = \frac{1}{d(z)} \frac{1}{A-z} \phi.$$

We conclude that the defect space $\mathfrak{N}_z$ for nonreal z is generated by $\Psi(z)$. Furthermore, it also holds that $\Psi(w) = \frac{A-z}{A-w} \Psi(z)$.

For the following sections, we shall again fix one self-adjoint extension of $\mathbb{A}_{\min}$, namely the diagonal operator

$$\begin{aligned} \operatorname{dom} \mathbb{A}^0 &:= \{ \mathbb{U} \in \operatorname{dom} \mathbb{A}_{\max} : u = 0 \} \cong \mathcal{H}_{2k+2} \oplus \mathbb{C}^{2k}, \\ \mathbb{A}^0 &:= A \oplus N. \end{aligned}$$

REMARK 3.5. It holds that $\mathbb{A}_{\min}$ is $\mathbb{A}^0$ restricted by $\langle (\mathbb{A}^0 - \bar{z}_0) \mathbb{U}, \Psi(z_0) \rangle = 0$ for any nonreal z_0.

We finish this section with a closer look at Γ, which will imply that $\mathbb{K}$ cannot be a Hilbert space.

LEMMA 3.6. *Let N be the diagonal matrix in* (3.2) *and $\Gamma = \Gamma^* \in \mathbb{C}^{2k \times 2k}$, then $N^* \Gamma = \Gamma N$ holds if and only if*

$$\Gamma = \begin{pmatrix} 0 & \Xi \\ \Xi^* & 0 \end{pmatrix}$$

with $\Xi = \operatorname{diag}(\xi_1, \ldots, \xi_k) \in \mathbb{C}^{k \times k}$. Moreover, Γ is non-degenerate if and only if none of the ξ_j are equal to zero.

Proof. Write $\Gamma = (\gamma_{ij})_{i,j=1}^{2k}$ and note that $N^* = \operatorname{diag}(\nu_{k+1}, \ldots, \nu_{2k}, \nu_1, \ldots, \nu_k)$ since $\bar{\nu}_i = \nu_{i+k}$ for $i \leqslant k$. Let $N^* \Gamma - \Gamma N =: (m_{ij})_{i,j=1}^{2k}$ and we want to know when this is the zero matrix. Clearly, $N^* \Gamma$ is the matrix where the i-th row of Γ is multiplied by ν_{i+k} if $i \leqslant k$ and by ν_{i-k} if $i > k$. Furthermore, ΓN is the matrix where the j-th column of Γ is multiplied by ν_j. Then

$$m_{ij} = \begin{cases} \gamma_{ij}(\nu_{i+k} - \nu_j) & i \leqslant k, \\ \gamma_{ij}(\nu_{i-k} - \nu_j) & i > k. \end{cases}$$

We see that when $\nu_{i+k} \neq \nu_j$ or $\nu_{i-k} \neq \nu_j$ hold, the corresponding γ_{ij} must vanish. Only in the cases $j = i + k$ and $j = i - k$, for $i \leqslant k$ and $i > k$ respectively, can the entries of Γ be different from zero. Since as a Gram matrix Γ should be self-adjoint, choosing $\gamma_{i,i+k} =: \xi_i \in \mathbb{C}$ for $1 \leqslant i \leqslant k$ already determines the rest of the entries and Γ is indeed of the block off-diagonal form as claimed. ∎

This leads us immediately to conclude the following corollary.

COROLLARY 3.7. *The matrix Γ has exactly k negative eigenvalues and thus $\mathbb{K}$ is a Pontryagin space with negative index k.*

Proof. Let I_{2k} and I_k be the identities on $\mathbb{C}^{2k}$ and $\mathbb{C}^k$, respectively. Then since $-\lambda I_k$ and Ξ commute it follows that

$$\det(\Gamma - \lambda I_{2k}) = \det\begin{pmatrix} -\lambda I_k & \Xi \\ \Xi^* & -\lambda I_k \end{pmatrix} = \det((-\lambda I_k)(-\lambda I_k) - \Xi\Xi^*)$$

and thus the determinant equals $\prod_{j=1}^{k}(\lambda^2 - |\xi_j|^2)$ so that the eigenvalues of Γ are exactly $\pm|\xi_j|$ for $1 \leqslant j \leqslant k$. Since $\langle\cdot,\cdot\rangle_{\mathcal{H}_{2k}} = \langle\cdot, d(A)\cdot\rangle_{\mathcal{H}}$ is positive definite, $\mathbb{K}$ gets its k negative squares exactly from Γ. ∎

REMARK 3.8. With a similar argument one can show that the matrices $\Gamma^{\pm}$ in the previous section both have to be diagonal. All entries are real numbers and it is in particular possible to choose all of them strictly positive. So even though we could possibly also turn $\mathbb{H}$ into a Pontryagin space, a clever choice of Γ avoids this. In contrast to this we see that in the case of $\mathbb{K}$ this Hilbert space possibility no longer exists.

3.3. SELF-ADJOINT FAMILY OF OPERATORS VIA KREIN'S FORMULA. Let us calculate the Q-function for the symmetry $\mathbb{A}_{\min}$. We first fix an arbitrary nonreal point z_0. In the present situation we will of course get a scalar Q-function, which is again defined by $\frac{Q^{\mathbb{K}}(z)-\overline{Q^{\mathbb{K}}(z_0)}}{z-\overline{z}_0} = \langle\Psi(z_0),\Psi(z)\rangle$, where the defect elements $\Psi(z)$ have been calculated in (3.5). In the constant $\overline{Q^{\mathbb{K}}(z_0)} = \Re Q^{\mathbb{K}}(z_0) - \mathrm{i}\Im Q^{\mathbb{K}}(z_0)$ we can assume the first summand to be zero. For the second summand, we have that

$$-\mathrm{i}\Im Q^{\mathbb{K}}(z_0) = -\mathrm{i}\frac{Q^{\mathbb{K}}(z_0) - \overline{Q^{\mathbb{K}}(z_0)}}{2\mathrm{i}} = -\frac{z_0 - \overline{z}_0}{2}\|\Psi(z_0)\|^2_{\mathbb{K}}.$$

If we define

$$Q^{\mathbb{K}}_A(z) := \Big\langle \phi, \Big[\frac{z - z_0}{A - z_0} + \frac{z - \overline{z}_0}{A - \overline{z}_0}\Big]\frac{1}{2(A - z)d(A)}\phi\Big\rangle, \tag{3.6}$$

$$Q^{\mathbb{K}}_N(z) := \Big\langle \vec{c}, \Gamma\Big[\frac{z - z_0}{N - z_0} + \frac{z - \overline{z}_0}{N - \overline{z}_0}\Big]\frac{1}{2(N - z)}\vec{c}\Big\rangle, \tag{3.7}$$

then we immediately get

$$Q^{\mathbb{K}}(z) = (z - \overline{z}_0)\langle\Psi(z_0),\Psi(z)\rangle - \frac{z_0 - \overline{z}_0}{2}\|\Psi(z_0)\|^2_{\mathbb{K}} = Q^{\mathbb{K}}_A(z) + Q^{\mathbb{K}}_N(z). \tag{3.8}$$

Next, define

$$\gamma_{z_0} : \mathbb{C} \to \mathfrak{N}_{z_0} : \lambda \mapsto \lambda \Psi(z_0),$$

which has the adjoint

$$\gamma^*_{\overline{z}_0} : \mathbb{K} \to \mathbb{C} : \mathbb{U} \mapsto \langle \Psi(z_0), \mathbb{U} \rangle.$$

With this, we can apply Krein's formula for

$$\mathbb{A}_{\min} \subseteq \mathbb{A}_{\max},\ \mathbb{A}^0,\ z_0,\ \mathfrak{N}_{z_0},\ \gamma_z,\ \gamma^*_{\overline{z}},\ Q^{\mathbb{K}}(z)$$

and parametrise all self-adjoint extensions of $\mathbb{A}_{\min}$, as t runs through $\mathbb{R} \cup \{\infty\}$, by

$$\frac{1}{\mathbb{A}^t - z} := \frac{1}{\mathbb{A}^0 - z} - \frac{1}{1/t + Q^{\mathbb{K}}(z)} \langle \Psi(\overline{z}), \cdot \rangle \Psi(z), \tag{3.9}$$

where the second term on the right is just $\gamma_z t(1 + Q^{\mathbb{K}}(z)t)^{-1} \gamma^*_{\overline{z}}$. As before, we use the family $(\mathbb{A}^t)_{t \in \mathbb{R} \cup \{\infty\}}$ to define the perturbated operators $A + \alpha\langle \phi, \cdot \rangle \phi$.

Regarding the goal of keeping the property (F2) intact, we can already conclude from this that

$$\mathrm{i}_{\mathbb{K}} \frac{1}{\mathbb{A}^t - z}\Big|_{\mathcal{H}_{2k}} = \frac{1}{A - z} - \frac{1}{1/t + Q^{\mathbb{K}}(z)} \left\langle \frac{1}{A - \overline{z}} \phi, \cdot \right\rangle \frac{1}{d(z)} \frac{1}{A - z} \phi. \tag{3.10}$$

REMARK 3.9. As the Q-function of an operator in a Pontryagin space with negative index k we clearly have that $Q^{\mathbb{K}}(z)$ belongs to the class of generalized Nevanlinna functions with negative index k, denoted by $\mathcal{N}_k$.

3.4. DIRECT DESCRIPTION VIA BOUNDARY CONDITIONS.

As in the previous section we want to complete the picture by giving a more concrete description of $(\mathbb{A}^t)_{t \in \mathbb{R} \cup \{\infty\}}$ through boundary conditions that make $\operatorname{dom} \mathbb{A}^t$ more palpable.

In the following, we need the positive constant

$$C := \|G(\nu)\|^2_{\mathcal{H}_{2k}} = \left\| \frac{1}{(A - \nu) d_0(A)} \phi \right\|^2_{\mathcal{H}}. \tag{3.11}$$

Note that $(A - \nu)^{-1} d_0(A)^{-1} \phi$ involves the least amount of resolvents needed to push ϕ into the Hilbert space $\mathcal{H}$.

LEMMA 3.10. *The boundary form $\langle \mathbb{A}_{\max} \mathbb{U}, \mathbb{V} \rangle - \langle \mathbb{U}, \mathbb{A}_{\max} \mathbb{V} \rangle$ is equal to*

$$(\langle \Gamma \vec{c}, \vec{v} \rangle - \langle \phi, V_r \rangle)\overline{u} - v\overline{(\langle \Gamma \vec{c}, \vec{u} \rangle - \langle \phi, U_r \rangle)} - 2\mathrm{i}\Im \nu \overline{u} v C,$$

and it vanishes if and only if

$$\langle \Gamma \vec{c}, \vec{u} \rangle - \langle \phi, U_r \rangle = \Big(\frac{1}{h} + \mathrm{i}\Im(\nu) C \Big) u$$

for arbitrary $h \in \mathbb{R} \cup \{\infty\}$.

REMARK 3.11. We point out that in comparison to the parameter μ in the Hilbert space model the parameter ν had to be chosen nonreal in the Pontryagin space case in order to avoid the spectrum of A. This leads to an additional term in the boundary form now.

Proof of Lemma 3.10. For $\mathbb{U}, \mathbb{V} \in \operatorname{dom} \mathbb{A}_{\max}$ we have to calculate

$$\left\langle \begin{pmatrix} AU_r + \nu u G(\nu) \\ N\vec{u} + u\vec{c} \end{pmatrix}, \begin{pmatrix} V_r + vG(\nu) \\ \vec{v} \end{pmatrix} \right\rangle - \left\langle \begin{pmatrix} U_r + uG(\nu) \\ \vec{u} \end{pmatrix}, \begin{pmatrix} AV_r + \nu v G(\nu) \\ N\vec{v} + v\vec{c} \end{pmatrix} \right\rangle.$$

Using that $\Gamma N = N^*\Gamma$, one can simplify most of the resulting terms to the first two summands in the lemma. In contrast to the semibounded (or Hilbert space from the previous section) case, $\langle \nu u G(\nu), d(A) v G(\nu) \rangle_{\mathcal{H}} - \langle uG(\nu), d(A) \nu v G(\nu) \rangle_{\mathcal{H}}$ does not cancel owing to $\Im \nu \neq 0$ and instead just sums up to $\overline{u} v(\overline{\nu} - \nu)C$. The claim about the form vanishing is then obvious. ∎

REMARK 3.12. For $h = \infty$ we set $\frac{1}{h} = 0$. The case $h = 0$ should be interpreted as $u = 0$, so we see that this is in agreement with the definition of the operator $\mathbb{A}^0$.

With this we can now give a description of the family $(\mathbb{A}^t)_{t \in \mathbb{R} \cup \{\infty\}}$ in terms of boundary conditions. For $h \in \mathbb{R} \cup \{\infty\}$ define $\mathbb{A}^h$ as the restriction of $\mathbb{A}_{\max}$ to the domain

$$\operatorname{dom} \mathbb{A}^h = \Big\{ \mathbb{U} \in \operatorname{dom} \mathbb{A}_{\max} : \langle \Gamma \vec{c}, \vec{u} \rangle - \langle \phi, U_r \rangle = \Big(\frac{1}{h} + \mathrm{i} \Im \nu C \Big) u \Big\}.$$

THEOREM 3.13. *The family* $(\mathbb{A}^h)_{h \in \mathbb{R} \cup \{\infty\}}$ *coincides with* $(\mathbb{A}^t)_{t \in \mathbb{R} \cup \{\infty\}}$.

Proof. We follow the technique used in the proof of Theorem 2.10. In a first step we relate the resolvent of $\mathbb{A}^h$ to the one of $\mathbb{A}^0$. In a second step we show that the formula giving this relation is (3.9) up to a change in a real constant.

Step 1. For nonreal z and given $\mathbb{F} \in \mathbb{K}$, we solve $(\mathbb{A}^h - z)\mathbb{U} = \mathbb{F}$, i.e., we consider the system

$$(A - z)U_r + (\nu - z)G(\nu)u = F \tag{3.12}$$

$$(N - z)\vec{u} + \vec{c}u = \vec{f}. \tag{3.13}$$

A general formula for $\mathbb{U} = (U, \vec{u})$ can be expressed in terms of u since

$$U = U_r + uG(\nu) = \frac{1}{A - z} F + \frac{z - \nu}{A - z} G(\nu) u + uG(\nu) = \frac{1}{A - z} F + uG(z)$$

and a formula for $\vec{u}$ is obvious. In order for $\mathbb{U}$ to belong to $\operatorname{dom} A^h$ we thus need to specify the parameter u. So to do this, apply $(A - z)^{-1}$ to (3.12) and project the result on $-\phi$, and apply $(N - z)^{-1}$ to (3.13) and project on $\Gamma \vec{c}$. With the notation

$$q_A^{\mathbb{K}}(z) := \Big\langle \phi, \frac{z - \nu}{(A - z)(A - \nu) d(A)} \phi \Big\rangle, \quad q_N^{\mathbb{K}}(z) := \Big\langle \Gamma \vec{c}, \frac{1}{N - z} \vec{c} \Big\rangle,$$

the above procedure yields

$$-\langle \phi, U_r \rangle = -\Big\langle \phi, \frac{1}{A - z} F \Big\rangle - q_A^{\mathbb{K}}(z) u, \quad \langle \Gamma \vec{c}, \vec{u} \rangle = \Big\langle \Gamma \vec{c}, \frac{1}{N - z} \vec{f} \Big\rangle - q_N^{\mathbb{K}}(z) u.$$

The first terms on the right from each equation together give $-\langle \Psi(\overline{z}), \mathbb{F} \rangle$ where $\Psi(z)$ is the defect element calculated in (3.5). Summing the above equations yields $\langle \Gamma\vec{c},\vec{u}\rangle - \langle \phi, U_r\rangle = -\langle \Psi(\bar{z}),\mathbb{F}\rangle - (q_A^{\mathbb{K}}(z)+q_N^{\mathbb{K}}(z))u$. Requiring $\mathbb{U} \in \operatorname{dom} \mathbb{A}^h$ allows us to express the left side in terms of u, whence

$$u = -\frac{1}{1/h + \mathrm{i}\Im\nu C + q_A^{\mathbb{K}}(z) + q_N^{\mathbb{K}}(z)}\langle \Psi(\bar{z}),\mathbb{F}\rangle.$$

Hence, $\mathbb{U} = (\mathbb{A}^0 - z)^{-1}\mathbb{F} + u\Psi(z)$. If we set

$$q^{\mathbb{K}}(z) := q_A^{\mathbb{K}}(z) + q_N^{\mathbb{K}}(z) + \mathrm{i}\Im\nu C \tag{3.14}$$

we can finally relate the resolvents of $\mathbb{A}^h$ and $\mathbb{A}^0$ via

$$\frac{1}{\mathbb{A}^h - z} = \frac{1}{\mathbb{A}^0 - z} - \frac{1}{1/h + q^{\mathbb{K}}(z)}\langle \Psi(\bar{z}),\cdot\rangle\Psi(z). \tag{3.15}$$

Step 2. Comparing (3.15) with (3.9) shows that we are done once we show the following claim:

$$q^{\mathbb{K}}(z) - Q^{\mathbb{K}}(z) = \Re q^{\mathbb{K}}(z_0). \tag{3.16}$$

Note first that

$$\mathrm{i}\Im\nu C = \frac{1}{2}\Big\langle \phi, \frac{\nu-\bar{\nu}}{(A-\nu)(A-\bar{\nu})d(A)}\phi\Big\rangle.$$

Hence, from

$$\begin{aligned}\frac{z-\nu}{(A-z)(A-\nu)} + \frac{\nu-\bar{\nu}}{2(A-\nu)(A-\bar{\nu})} - \frac{z-z_0}{2(A-z)(A-z_0)} - \frac{z-\bar{z}_0}{2(A-z)(A-\bar{z}_0)}&\\ = \frac{1}{2}\Big(\frac{z_0-\nu}{(A-z_0)(A-\nu)} + \frac{\bar{z}_0-\bar{\nu}}{(A-\bar{z}_0)(A-\bar{\nu})}\Big)&\end{aligned}$$

it readily follows that $q_A^{\mathbb{K}}(z) + \mathrm{i}\Im\nu C - Q_A^{\mathbb{K}}(z) = \Re q_A^{\mathbb{K}}(z_0)$. Secondly, also $q_N^{\mathbb{K}}(z) - Q_N^{\mathbb{K}}(z) = \Re q_N^{\mathbb{K}}(z_0)$ becomes clear via a similar calculation. The claim is shown.

Hence, the families of self-adjoint operators $\mathbb{A}^h$ and $\mathbb{A}^t$ do coincide. ∎

COROLLARY 3.14. *The function $q^{\mathbb{K}}(z)$ belongs to the generalized Nevanlinna class with negative index k.*

Proof. Since $Q^{\mathbb{K}}(z) \in \mathcal{N}_k$ and $q^{\mathbb{K}}(z)$ only differs from it by a real constant, the claim follows immediately. ∎

4. COMPARISON OF THE $\mathbb{H}$- AND $\mathbb{K}$-MODELS

The two models obtained in the previous sections preserve different aspects of the original model for semibounded operators. They are still rather closely related to each other when considering the Q-functions that appear. In the following we make the assumption that

$$n = 2k,$$

i.e., to build the Hilbert space model we consider $\phi \in \mathcal{H}_{-n+2}\backslash\mathcal{H}_{-n}$ for even $n \geqslant 1$.

We have already pointed out in Remark 3.9 that $Q^{\mathbb{K}}(z)$ is a generalized Nevanlinna function. From its definition as the sum of (3.6) and (3.7) it is then clear that it has generalized poles not of positive type exactly in $\nu_1, \dots, \nu_k$ and they all arise from the term $Q_N^{\mathbb{K}}(z)$ associated with the indefinite component $\mathbb{C}^{2k}$ in $\mathbb{K}$. The degree of non-positivity ρ_{ν_j} in ν_j is just the order of the pole in each of these nonreal points and it is thus clearly equal to one for $1 \leqslant j \leqslant k$, with of course $\sum_{j=1}^{k} \rho_{\nu_j} = k$, cf. [11]. We also recall that for a generalized Nevanlinna function $\widetilde{q}(z)$ with a generalized pole at ∞, the degree of non-positivity ρ_∞ is given by the number that satisfies

$$\lim_{z \widehat{\rightarrow} \infty} z^{2\rho_\infty - 1} \widetilde{q}\Big(-\frac{1}{z} \Big) \in (0, \infty], \quad \lim_{z \widehat{\rightarrow} \infty} z^{2\rho_\infty + 1} \widetilde{q}\Big(-\frac{1}{z} \Big) \in (-\infty, 0].$$

LEMMA 4.1. *Let $d(z)$ be the regularizing polynomial given with respect to the regularization points $\nu_1, \dots, \nu_k$. Then the function $d(z)Q^{\mathbb{K}}(z)$ belongs to $\mathcal{N}_k$ with a generalized pole not of positive type only in ∞ and with degree of non-positivity $\rho_\infty = k$.*

Proof. As was discussed, $Q^{\mathbb{K}}(z)$ belongs to $\mathcal{N}_k$ with generalized poles not of positive type exactly in $\nu_1, \dots, \nu_k$. Furthermore, d is symmetric, i.e., it is of the form $d(z) = d_0(z)\overline{d_0(\overline{z})}$ and so $d(z)Q^{\mathbb{K}}(z)$ is a generalized Nevanlinna function as well, with negative index k'. The zeros of $d_0(z)$ are exactly the generalized poles not of positive type of $Q^{\mathbb{K}}$. Thus, the negative index cannot grow and so $k' \leqslant k$. The strict inequality $k' < k$ holds if and only if ∞ is a zero not of positive type of the function $Q^{\mathbb{K}}$, cf. for example equation (3.2) of [3] and consequences.

We need the following two well-known facts:

(i) A generalized Nevanlinna function q has a generalized zero at ∞ if and only if (cf. [6])

$$\lim_{y \uparrow \infty} y |q(\mathrm{i}y)| < \infty.$$

(ii) For a generalized Nevanlinna function of the form

$$q(z) = \overline{q(z_0)} + (z - \overline{z}_0)[v, (I + (z - z_0)(\mathcal{A} - z)^{-1})v]$$

with $\mathcal{A}$ an operator it holds that

$$v \in \operatorname{dom} \mathcal{A} \quad \Leftrightarrow \quad \lim_{y \uparrow \infty} y |\Im q(\mathrm{i}y)| < \infty.$$

So let us now assume that the above inequality is strict, so that $k' < k$. In this case $\lim_{y \uparrow \infty} y |Q^{\mathbb{K}}(\mathrm{i}y)|$ has to be finite. In particular, the same must be true for $\lim_{y \uparrow \infty} y |\Im Q^{\mathbb{K}}(\mathrm{i}y)|$.

Look at $Q^{\mathbb{K}}(z) = Q_A^{\mathbb{K}}(z) + Q_N^{\mathbb{K}}(z)$ as defined in (3.8). It is straight-forward to conclude $\overline{Q^{\mathbb{K}}(z_0)} = -Q^{\mathbb{K}}(z_0)$ and from there to calculate

$$Q_A^{\mathbb{K}}(z) - \overline{Q_A^{\mathbb{K}}(z_0)} = (z - \overline{z}_0) \Big\langle \frac{1}{(A - z_0)d_0(A)} \phi, \frac{A - z_0}{A - z} \frac{1}{(A - z_0)d_0(A)} \phi \Big\rangle,$$

$$Q_N^{\mathbb{K}}(z) - \overline{Q_N^{\mathbb{K}}(z_0)} = (z-\overline{z}_0)\Big\langle \frac{1}{N-z_0}\vec{c}, \Gamma\frac{N-z_0}{N-z}\frac{1}{N-z_0}\vec{c}\Big\rangle.$$

Hence,

$$Q^{\mathbb{K}}(z) = \overline{Q^{\mathbb{K}}(z_0)} + (z-\overline{z}_0)\left[\mathbb{V}, \left(\begin{pmatrix} I_{\mathcal{H}} & 0 \\ 0 & I_{\mathbb{C}^{2k}}\end{pmatrix} + (z-z_0)\begin{pmatrix}\frac{1}{A-z} & 0 \\ 0 & \frac{1}{N-z}\end{pmatrix}\right)\mathbb{V}\right]$$

with the vector $\mathbb{V} := ((A-z_0)^{-1}d_0(A)^{-1}\phi, (N-z_0)^{-1}\vec{c}) \in \mathbb{K}$ and the inner product $[\mathbb{F},\mathbb{G}] = \langle F, G\rangle_{\mathcal{H}} + \langle \vec{f}, \Gamma\vec{g}\rangle_{\mathbb{C}^{2k}}$. We consider the domain of the operator $A\oplus N$. Of course, $(N-z_0)^{-1}\vec{c} \in \operatorname{dom} N = \mathbb{C}^{2k}$. However, since $\phi \in \mathcal{H}_{-2k-2}\setminus\mathcal{H}_{-2k}$ we get

$$\frac{1}{(N-z_0)d_0(A)}\phi \in \mathcal{H}_0\setminus\mathcal{H}_2 = \mathcal{H}\setminus \operatorname{dom} A.$$

Put together, this means $\mathbb{V} \notin \operatorname{dom}(A\oplus N)$ and thus $\lim\limits_{y\uparrow\infty} y|\Im Q^{\mathbb{K}}(\mathrm{i}y)|$ cannot be finite. We have arrived at a contradiction and thus $k = k'$. ∎

In the Pontryagin space $\mathbb{K}$ we have not split the operator A into a positive or negative part related to spectral subspaces $\mathcal{H}^+\oplus\mathcal{H}^-$ but nothing prevents us from doing this: we can split $A = A^+\oplus(-A^-)$ and $\phi = \phi^+ + \phi^-$ in the Hilbert space component $\mathcal{H}_{2k}$ of $\mathbb{K}$, i.e.,

$$\mathbb{K} = \mathcal{H}_{2k}\oplus\mathbb{C}^{2k} = \mathcal{H}_{2k}^+\oplus\mathcal{H}_{2k}^-\oplus\mathbb{C}^{2k},$$

so that we can compare the positive and negative parts of the models individually. The function $Q_A^{\mathbb{K}}(z)$ consequently splits into the summands

$$Q_A^{\mathbb{K},\pm}(z) := \Big\langle \phi^{\pm}, \Big[\frac{z-z_0}{\pm A^{\pm}-z_0} + \frac{z-\overline{z}_0}{\pm A^{\pm}-\overline{z}_0}\Big]\frac{1}{2(\pm A^{\pm}-z)d(\pm A^{\pm})}\phi^{\pm}\Big\rangle. \tag{4.1}$$

Considering the Krein-type formulas in Corollary 2.11 and in (3.10) it seems natural to compare the models when restricted to $\mathcal{H}_n^{\pm}$, respectively. In this case, the Q-functions $b(z)Q^+(z)$ and $b(-z)Q^-(z)$ appear in the Hilbert space model and they should then have a connection to $d(z)Q^{\mathbb{K}}(z)$.

THEOREM 4.2. *Let $Q^{\mathbb{K}}(z)$ be given as in* (3.8) *and $Q_A^{\mathbb{K},\pm}(z)$ by* (4.1). *Let $Q^{\pm}(z)$ be defined as in* (2.9). *Let $b(z)$ be the regularizing polynomial given in terms of the regularization points $\mu_1,\ldots,\mu_n$. Then there exist polynomials $p^{\pm}(z)$ of degree at most n satisfying $p^{\pm}(z) = \overline{p^{\pm}(\overline{z})}$ such that*

$$b(z)Q_A^+(z) = d(z)Q_A^{\mathbb{K},+}(z) + p^+(z), \tag{4.2}$$

$$b(-z)Q_A^-(z) = d(z)Q_A^{\mathbb{K},-}(z) + p^-(z). \tag{4.3}$$

Consequently, we also have

$$(b(z)Q^+(z) + b(-z)Q^-(z)) = d(z)Q^{\mathbb{K}}(z) + p(z) \tag{4.4}$$

for some polynomial $p(z)$ of degree at most n and satisfying the same kind of symmetry about the real axis.

Proof. We can assume without loss of generality that all Q-functions involved are defined with respect to the same nonreal number z_0. Furthermore, when regarding (4.4) we see that each of the three Q-functions are the sum of an inner product in a scale space involving (parts of) the operator A and an inner product in $\mathbb{C}^n$ involving the matrices M and N, respectively.

For the inner products in $\mathbb{C}^n$ we have to study the expression

$$\sum_{s\in\{+,-\}}\left\langle \vec{a},\Gamma^s\left[\frac{z-z_0}{sM-z_0}+\frac{z-\overline{z}_0}{sM-\overline{z}_0}\right]\frac{b(sz)}{2(sM-z)}\vec{a}\right\rangle-\left\langle \vec{c},\Gamma\left[\frac{z-z_0}{N-z_0}+\frac{z-\overline{z}_0}{N-\overline{z}_0}\right]\frac{d(z)}{2(N-z)}\vec{c}\right\rangle.$$

Since of course

$$(\pm M-z)^{-1}=\operatorname{diag}((\pm\mu_1-z)^{-1},\dots,(\pm\mu_n-z)^{-1}),$$
$$(N-z)^{-1}=\operatorname{diag}((\nu_1-z)^{-1},\dots,(\nu_{2k}-z)^{-1})$$

we see that

$$\frac{b(z)(z-\overline{z}_0)}{M-z},\quad \frac{b(-z)(z-\overline{z}_0)}{-M-z},\quad \frac{d(z)(z-\overline{z}_0)}{N-z}$$

give diagonal matrices with polynomials of degree n as entries and thus the complete sum is a polynomial of degree at most n as well. Furthermore, it is clear that this polynomial also has the stated symmetry property.

Regarding (4.2), i.e., the Q-functions in $\mathcal{H}^+_{2k}$, we have to consider the difference $b(z)Q^+_A(z)-d(z)Q^{\mathbb{K},+}_A(z)$, which amounts to

$$\left\langle \phi^+,\left[\frac{z-z_0}{A^+-z_0}+\frac{z-\overline{z}_0}{A^+-\overline{z}_0}\right]\frac{1}{2(A^+-z)}\left[\frac{b(z)}{b(A^+)}-\frac{d(z)}{d(A^+)}\right]\phi^+\right\rangle \tag{4.5}$$

and we want to show that $b(z)d(A^+)-d(z)b(A^+)$ has a factor A^+-z. As a function of ζ we have in any case that $d(z)b(\zeta)-b(z)d(\zeta)=(\zeta-z)p(\zeta,z)$ with $p(\zeta,z)\in\mathbb{C}[z][\zeta]$ being a polynomial in ζ of degree at most $n-1$ with coefficients that are polynomials in z of degree also at most $n-1$. Thus, (4.5) is formally the same as

$$\left\langle \phi^+,\left[\frac{z-z_0}{A^+-z_0}+\frac{z-\overline{z}_0}{A^+-\overline{z}_0}\right]\frac{p(A^+,z)}{2b(A^+)d(A^+)}\phi^+\right\rangle. \tag{4.6}$$

Since $p(A^+,z)$ gives at most a contribution of $(A^+)^{n-1}$, the element on the right in the scalar product above always belongs to $\mathcal{H}^+_{n+2}$. Hence, we see that (4.6) is well-defined. Thus (4.5) and (4.6) are indeed equal. The resulting expression (4.5) can be rearranged with respect to z and gives a polynomial of degree at most n with the stated symmetry property.

For (4.3), i.e., in $\mathcal{H}^-_n$, we have $b(-z)Q^-_A(z)-d(z)Q^{\mathbb{K},-}_A(z)$ to consider, which is

$$\left\langle \phi^-,\left[\frac{z-z_0}{-A^--z_0}+\frac{z-\overline{z}_0}{-A^--\overline{z}_0}\right]\frac{1}{2(-A^--z)}\left[\frac{b(-z)}{b(A^-)}-\frac{d(z)}{d(-A^-)}\right]\phi^-\right\rangle$$

and just as above we cancel a factor $(-A^- - z)$ from the difference in the square brackets to end up with a polynomial of degree at most n in the variable z and symmetric with respect to the real axis.

Thus, the claim is proven. ∎

COROLLARY 4.3. *The function $b(z)Q^+(z) + b(-z)Q^-(z)$ is from the class $\mathcal{N}_k$ with its pole not of positive type at ∞ and with corresponding degree of non-positivity $\widetilde{\rho}_\infty = k$.*

Proof. We know already that $d(z)Q^{\mathbb{K}}(z) \in \mathcal{N}_k$. Furthermore, polynomials that are symmetric with respect to the real axis always belong to some class $\mathcal{N}_\kappa$. By Theorem 4.2 the function $b(z)Q^+(z) + b(-z)Q^-(z)$ is the sum of two generalized Nevanlinna functions. Thus, it belongs to some class $\mathcal{N}_{k'}$ as well.

In order to show $k = k'$ we study the generalized poles not of positive type of the right side in (4.4). For the case of $d(z)Q^{\mathbb{K}}(z)$ we already know that the only such pole is ∞ and its degree of non-positivity is $\rho_\infty = k$.

Let $p(z)$ be the polynomial on the right side of (4.4). We know that its degree is at most $n = 2k$ and that $p(z) = \overline{p(\overline{z})}$ with only generalized pole located at ∞.

Then, k' arises as the degree of non-positivity of the generalized pole ∞ of $d(z)Q^{\mathbb{K}}(z) + p(z)$, i.e., it is equal to the number $\widetilde{\rho}_\infty$ satisfying

$$\lim_{z \widehat{\to} 0} d\Big(-\frac{1}{z}\Big)Q^{\mathbb{K}}\Big(-\frac{1}{z}\Big)z^{2\widetilde{\rho}_\infty - 1} + p\Big(-\frac{1}{z}\Big)z^{2\widetilde{\rho}_\infty - 1} \in (0, \infty],$$
$$\lim_{z \widehat{\to} 0} d\Big(-\frac{1}{z}\Big)Q^{\mathbb{K}}\Big(-\frac{1}{z}\Big)z^{2\widetilde{\rho}_\infty + 1} + p\Big(-\frac{1}{z}\Big)z^{2\widetilde{\rho}_\infty + 1} \in (-\infty, 0].$$

Since $\deg p \leqslant n = 2k$ it follows that the limit of the second summand either behaves in the same way as the first one, which happens if $\deg p = n$, or is equal to zero in both cases, which happens if $\deg p < n$, and thus does not even give a contribution when determining ρ. We conclude that $k' = \rho = \rho_\infty = k$ and are done. ∎

5. CONCLUSION

In the beginning we formulated as a goal to generalize an existing operator model to describe supersingular perturbations of semibounded operators to also include not necessarily semibounded operators. The two properties exhibited by the model in the semibounded case were

(F1) the perturbation is modeled in a Hilbert space, and
(F2) the description of the perturbation is achieved by a Krein type formula.

Throughout our investigation it has become clear that we cannot achieve to keep both properties intact in the case where our operators might have a spectrum covering all of the real line.

By keeping (F1) as a requirement, we showed in Corollary 2.11 that the Krein type formula we wanted to find does not appear in the expected “natural” form. Conversely, when (F2) is used as a starting point, Corollary 3.7 demonstrates why negative squares will have to appear in our model space.

The conclusion we draw from this is the following: the operator model for the semibounded case is intrinsically linked to and subtly built around the fact that the spectrum does not occupy all of the real line. If one thus wants to have both (F1) and (F2) in a perturbation model for the more general operators we considered in this paper then this model needs to be built up in a different way instead.

6. APPENDIX

We use the standard scale of Hilbert spaces $(\mathcal{H}_n(A))_{n\in\mathbb{Z}}$ associated to a self-adjoint operator A in $\mathcal{H}$, that is the scale

$$\cdots \supseteq \mathcal{H}_{-2}(A) \supseteq \mathcal{H}_{-1}(A) \supseteq \mathcal{H}_0(A) \supseteq \mathcal{H}_1(A) \supseteq \mathcal{H}_2(A) \supseteq \cdots$$

where the space $\mathcal{H}_n(A)$ for $n \geqslant 1$ is the domain of $(|A|+1)^{n/2}$ equipped with the norm $\|\cdot\|_n = \|(|A|+1)^{n/2}\cdot\|$ and $\mathcal{H}_0(A)$ is the original Hilbert space $\mathcal{H}$. The spaces with negative indices $\mathcal{H}_{-n}(A)$ are the completions of $\mathcal{H}$ with respect to the similarly defined norms $\|\cdot\|_{-n} := \|(|A|+1)^{-n/2}\cdot\|_{\mathcal{H}}$ and are dual spaces in the sense that $\mathcal{H}_n(A)^* = \mathcal{H}_{-n}(A)$. For every positive integer, we thus have a Gelfand triplet $\mathcal{H}_n(A) \subseteq \mathcal{H} \subseteq \mathcal{H}_{-n}(A)$.

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