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Integral Equations and Operator Theory

High Order Singular Rank One Perturbations of a Positive Operator

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Abstract. In this paper self-adjoint realizations in Hilbert and Pontryagin spaces of the formal expression

$$L_\alpha = L + \alpha\langle\,\cdot\,,\varphi\rangle\,\varphi$$

are discussed and compared. Here L is a positive self-adjoint operator in a Hilbert space $\mathcal{H}$ with inner product $\langle\,\cdot\,,\,\cdot\,\rangle$, α is a real parameter, and φ in the rank one perturbation is a singular element belonging to $\mathcal{H}_{-n}\setminus\mathcal{H}_{-n+1}$ with $n \geq 3$, where $\{\mathcal{H}_s\}_{s=-\infty}^{\infty}$ is the scale of Hilbert spaces associated with L in $\mathcal{H}$.

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1. Introduction

1.1. The singular perturbation problem

Let $\mathcal{H}$ be a Hilbert space with inner product $\langle\,\cdot\,,\,\cdot\,\rangle$ and let L be a positive self-adjoint operator in $\mathcal{H}$. Denote by $(\mathcal{H}_n)_{n=-\infty}^{\infty}$ the scale of Hilbert spaces associated with L and $\mathcal{H}$: $\mathcal{H}_0 = \mathcal{H}$, for $n > 0$, $\mathcal{H}_n$ is the Hilbert space $\operatorname{dom} L^{n/2}$ equipped with norm

$$\|f\|_n = \|(L+1)^{n/2} f\|, \tag{1.1}$$

and for $n < 0$, $\mathcal{H}_n$ is the completion of $\mathcal{H}$ with respect to the norm (1.1). In a natural way $\mathcal{H}_n$ and $\mathcal{H}_{-n}$ are duals and the inner product can be generalized to a pairing $\langle f, g\rangle$ between the spaces $\mathcal{H}_n$ and $\mathcal{H}_{-n}$:

$$|\langle f, g\rangle| \leq \|f\|_n \|g\|_{-n}, \quad f \in \mathcal{H}_n,\ g \in \mathcal{H}_{-n},$$

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and $\langle g, f\rangle = \langle f, g\rangle^*$. For $\pm n, m = 1, 2, \ldots$, the operator $(L+1)^{-m/2}$ is an isometry from $\mathcal{H}_n$ to $\mathcal{H}_{n+m}$. Finally, $\mathcal{H}_n \hookrightarrow \mathcal{H}_m$, $n > m$, $n, m \in \mathbb{Z}$, and the inclusion map is contractive and has a dense range. For more details, see, for example, [33, 2]. Later we redefine the inner product on one of the scale spaces, see (2.1).
In this paper we consider the expression

$$L_\alpha = L + \alpha\langle\,\cdot\,,\varphi\rangle\,\varphi. \tag{1.2}$$

It is called a *rank one perturbation* of L with *coupling parameter* α, which is a real number, and *generalized element* φ, which is an element of the space $\mathcal{H}_{-n}\setminus\mathcal{H}_{-n+1}$, $n = 0, 1, 2, \ldots$; the perturbation $\alpha\langle\,\cdot\,,\varphi\rangle\,\varphi$ is also called an *interaction*. If $n = 0$, or more generally, if $\varphi \in \mathcal{H}_0$, the perturbation (1.2) is called *regular*, otherwise it is called *singular*. The cases $n = 0, 1$, and 2 are well known; we give a short overview below. In this paper we focus on *high order singular* perturbations, that is, on perturbations with $n \geq 3$. Then L_α is just a formal expression on $\mathcal{H}_0$ and the aim of this paper is to present for this expression (one-parameter families of) self-adjoint realizations, that is, operators or relations, in a Hilbert or Pontryagin space. For the theory of operators on spaces with an indefinite, we refer to [4, 8, 18].
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1.2. The extension method

Self-adjoint realizations of L_α for $n \geq 3$ can be obtained by a procedure as used in, for example, spectral theory of formally symmetric differential expressions; see, for instance, [11]. If ℓ is such an expression, one associates with ℓ a minimal and a maximal realization in a suitable inner product space of functions. The minimal realization is a closed symmetric operator whose adjoint is the maximal realization. The self-adjoint realizations of ℓ in the space (assuming they exist) are self-adjoint extensions of the minimal realization and hence restrictions of the maximal one: these restrictions are the self-adjoint boundary conditions. To get good eigenfunction expansion results for the self-adjoint realizations, the inner product space and the maximal realization should be chosen such that the domain of the latter contains sufficiently many eigenfunctions, that is, solutions of the equation $\ell y = zy$, and such that these eigenfunctions form a dense set. The description of all self-adjoint extensions is part of extension theory which concerns defect functions, Q-functions, Krein's resolvent parametrization formula, etc. We shall use these notions also in the setting of Pontryagin spaces; see [21] and also [12].

1.3. The A- and B-models

In this paper we associate with the singular perturbation (1.2), in a similar way, two suitable inner product spaces and two maximal operators whose domains contain the solutions of $(L_\alpha - z)f = 0$, that is, the elements

$$\frac{1}{L-z}\,\varphi, \quad z \in \rho(L).$$

This gives rise to two kinds of self-adjoint realizations and we explain what they have in common and where they differ. Roughly speaking, what they have in

common is that they are constructed starting from the same space $\mathbf{H}$ and the same closed maximal operator $\mathbf{L}_{\max}$ in this space, and where they differ is that subsequently in each case the space $\mathbf{H}$ is provided with a different new inner product. In the historically first approach to the singular perturbation problem the inner product is indefinite and leads to a one-parameter family of self-adjoint realizations of L_α in a Pontryagin space. We call this family the B-model after F. Berezin [6] who first introduced such models. The B-models were used and further developed in [31, 32, 17, 30, 19, 20, 10, 13, 14, 15]. The other one-parameter family of self-adjoint realizations, which we call the A-model, was proposed recently in [27, 28, 24, 25]. In the case $n = 3$ it was shown in [27] that a nontrivial realization of (1.2) exists in a Hilbert space. In this paper we show that this is also true for higher singular perturbations.
The relation between the operators in the A- and B-models can be described by the following commutative diagram:

$$\begin{array}{ccccc} \mathcal{H}_A & \xrightarrow{\mathbf{i}} & \mathbf{H} & \xrightarrow{\mathbf{j}} & \mathcal{H}_B \\ A_{\max}\downarrow & & \downarrow \mathbf{L}_{\max} & & \downarrow B_{\max} \\ \mathcal{H}_A & \xrightarrow{\mathbf{i}} & \mathbf{H} & \xrightarrow{\mathbf{j}} & \mathcal{H}_B \end{array} \tag{1.3}$$

In the middle are the space and the maximal operator we start with. Using the embeddings $\mathbf{i}$ and $\mathbf{j}$ the operator $\mathbf{L}_{\max}$ can be pulled backward and pushed forward to the operator $A_{\max}$ in the space $\mathcal{H}_A$ in the A-model on the lefthand side and to the operator $B_{\max}$ in the space $\mathcal{H}_B$ in the B-model on the righthand side, respectively. The space $\mathcal{H}_A$ can be a Hilbert space or a Pontryagin space, depending on other parameters that come into play. The embedding $\mathbf{i}$ is an isomorphism and hence the operator $A_{\max}$ is a closed operator in $\mathcal{H}_A$. The inner product space $\mathcal{H}_B$ is a pre-Pontryagin space. The embedding $\mathbf{j}$ is continuous but not boundedly invertible, and the operator $B_{\max}$ is not closed. It turns out that its closure in the completion of the space $\mathcal{H}_B$ is a linear relation. In this paper we focus on the operators in the space $\mathcal{H}_B$ rather than on the closures of these operators in its completion. This makes the comparison between the two models more transparent. To make sure that the adjoints of the maximal operators are symmetric, additional restrictions on the parameters in the inner products have to be imposed. The self-adjoint restrictions of the maximal operators are the self-adjoint realizations of the singular perturbation.

1.4. The regularization method

Another way to generate the same self-adjoint realizations for L_α is to apply a regularization method to the formal expression $\langle \frac{1}{L-z}\varphi, \varphi\rangle$ when $\varphi \in \mathcal{H}_{-n}\backslash\mathcal{H}_{-n+1}$, $n \geq 3$. This procedure is analogous to the regularization of dispersion integrals in quantum field theory, see, for example, [9, 26]: Let $a_1, a_2, \ldots, a_{n-1}$ be $n-1$ positive real numbers, and set $b_0(z) = 1$ and

$$b_j(z) = (z + a_1)(z + a_2)\cdots(z + a_j), \quad j = 1, 2, \ldots, n-1.$$

By the resolvent identity for L we have

$$\frac{1}{L-z} = \frac{1}{b_1(L)} + \frac{b_1(z)}{b_2(L)} + \cdots + \frac{b_{n-2}(z)}{b_{n-1}(L)} + \frac{b_{n-1}(z)}{b_{n-1}(L)}\,\frac{1}{L-z}, \tag{1.4}$$

which leads to the formal identity

$$\left\langle \frac{1}{L-z}\,\varphi,\varphi\right\rangle \overset{\text{formal}}{=} \left\langle \frac{1}{b_1(L)}\,\varphi,\varphi\right\rangle + b_1(z)\left\langle \frac{1}{b_2(L)}\,\varphi,\varphi\right\rangle$$
$$+\cdots + b_{n-2}(z)\left\langle \frac{1}{b_{n-1}(L)}\,\varphi,\varphi\right\rangle + b_{n-1}(z)\left\langle \frac{1}{b_{n-1}(L)}\,\frac{1}{L-z}\,\varphi,\varphi\right\rangle$$

If we substitute real numbers c_{j-1} for the formal pairings

$$\left\langle \frac{1}{b_j(L)}\,\varphi,\varphi\right\rangle, \quad j = 1, 2, \ldots, n-1,$$

the righthand side becomes a well defined function which we denote by $Q(z)$:

$$Q(z) = b_{n-1}(z)\left\langle \frac{1}{L-z}\,\varphi, \frac{1}{b_{n-1}(L)}\,\varphi\right\rangle + p_{n-2}(z)$$

with

$$p_{n-2}(z) = c_0 + c_1 b_1(z) + \cdots + c_{n-2} b_{n-2}(z).$$

The function $Q(z)$ is called a *regularization* of $\langle \frac{1}{L-z}\varphi,\varphi\rangle$ for $\varphi \in \mathcal{H}_{-n} \setminus \mathcal{H}_{-n+1}$. Clearly, it is not unique. The family of regularizations $Q(z)$ with fixed positive real numbers $a_1, a_2, \ldots, a_{n-1}$ can be parametrized by the polynomials $p_{n-2}(z)$ with real coefficients and of degree at most $n-2$. It can be shown that a change in the numbers $a_1, a_2, \ldots, a_{n-1}$ corresponds to a change in the polynomial $p_{n-2}(z)$. For this reason these numbers are called the *normalization points*. The functions $Q(z)$ are generalized Nevanlinna functions with $[(n-1)/2]$ negative squares. The class N_κ of generalized Nevanlinna functions with κ negative squares was introduced by M.G. Krein and H. Langer in [21]. Each function from N_κ is the Q-function of a symmetric operator with defect indices $(1,1)$ and a self-adjoint extension in a Pontryagin space with negative index κ. The one-parameter family of self-adjoint extensions of this symmetric operator is interpreted as the family of realizations of L_α. This approach leads to the B-model. In a similar way a family of self-adjoint realizations of L_α is obtained in the A-model. The Hilbert space structure from the A-model can be explained in part by writing $Q(z)$ as

$$Q(z) = b_{n-2}(z)(Q_0(z) + r(z)),$$

where $r(z) = (p_{n-2}(z) - c_{n-2}b_{n-2}(z))/b_{n-2}(z)$ is a generalized Nevanlinna function, but

$$Q_0(z) = (z + a_{n-1})\left\langle \frac{1}{L-z}\,\varphi, \frac{1}{b_{n-1}(L)}\,\varphi\right\rangle + c_{n-2}$$

is a Nevanlinna function and hence the Q-function of a symmetric operator with defect indices $(1,1)$ and a self-adjoint extension in a Hilbert space.

1.5. The contents of the paper

Besides this introduction, there are 5 sections. In Section 2 we define the space $\mathbf{H}$ and the operator $\mathbf{L}_{\max}$ from which the models are constructed. The A-model and B-model are defined in Sections 3 and 4 respectively. The one-parameter families A_θ and B_θ of self-adjoint operators are the realizations of the singular perturbation L_α (1.2). The two models are compared in Section 5, and in Section 6 we provide some examples.

1.6. The cases $n = 0, 1, 2$

We show the differences between the perturbations for $0 \leq n \leq 2$ and $n \geq 3$ and their analogies by briefly recalling some of the results for the smaller values of n; see [2].

(i) If $n = 0$ or, more generally, $\varphi \in \mathcal{H}_0$, the interaction

$$\alpha\langle\,\cdot\,,\varphi\rangle\,\varphi \tag{1.5}$$

defines a bounded self-adjoint operator on $\mathcal{H}$ and L_α is a self-adjoint operator in $\mathcal{H}$ with $\operatorname{dom} L_\alpha = \operatorname{dom} L$. The resolvent of L_α is given by

$$\frac{1}{L_\alpha - z} = \frac{1}{L - z} - \frac{1}{Q_1(z) + \frac{1}{\alpha}}\left\langle\,\cdot\,,\frac{1}{L - z^*}\,\varphi\right\rangle\frac{1}{L - z}\,\varphi, \tag{1.6}$$

where

$$Q_1(z) = \left\langle\frac{1}{L - z}\,\varphi,\varphi\right\rangle.$$

For $\alpha = 0$ the second term on the righthand side of (1.6) should be deleted: $L_0 = L$.

(ii) If $n = 1$, the perturbation (1.5) is relatively form bounded with respect to the sesquilinear form of the operator L and the perturbed operator can be determined using the form perturbation technique. Its resolvent is also given by (1.6). The main difference with the case $n = 0$ is that the domain of the perturbed operator does not coincide with the domain of the original operator in general, but the perturbed operator is uniquely defined as a self-adjoint operator in the original Hilbert space $\mathcal{H}$; see [33, 2]. Another way to obtain this operator is by considering the restriction

$$L_{\min} = L|_{\{u\in\mathcal{H}_n\cap\operatorname{dom} L\,|\,\langle u,\varphi\rangle=0\}} \tag{1.7}$$

with $n = 1$ which is a symmetric operator in $\mathcal{H}$ with defect indices $(1, 1)$. A theorem of Krein states that the resolvent formula

$$\frac{1}{H_\tau - z} = \frac{1}{L - z} - \frac{1}{Q_1(z) + \tau}\left\langle\,\cdot\,,\frac{1}{L - z^*}\,\varphi\right\rangle\frac{1}{L - z}\,\varphi \tag{1.8}$$

gives a one-to-one correspondence between all self-adjoint extensions H_τ of $L_{\min}$ in $\mathcal{H}$ and all $\tau \in \mathbb{R} \cup \{\infty\}$. In this case we have $H_\tau = L_\alpha$ for $\tau = 1/\alpha$. Note that $Q_1(z)$ is a Nevanlinna function.

(iii) In the case $n = 2$ the perturbation (1.5) is not relatively form bounded and only extension theory can be applied. The operator $L_{\min}$ in (1.7) with $n = 2$ is still symmetric with defect indices $(1,1)$. But the perturbed operator is no longer uniquely defined. It is now interpreted as one of the self-adjoint extensions of $L_{\min}$. These extensions can be parametrized by one real parameter $\gamma \in \mathbb{R} \cup \{\infty\}$ as follows:

$$\frac{1}{L^\gamma - z} = \frac{1}{L-z} - \frac{1}{Q_2(z)+\gamma} \left\langle \cdot\,, \frac{1}{L-z^*}\,\varphi \right\rangle \frac{1}{L-z}\,\varphi,$$

$$Q_2(z) = \left\langle \frac{z+a_1}{(L-z)(L+a_1)}\,\varphi, \varphi \right\rangle.$$

Here $a_1 > 0$ is a fixed real number, which plays no essential role: changing a_1 corresponds to changing the parameter γ. The relation between the parameter γ in L^γ and the coupling parameter α in L_α cannot be established without additional assumptions like homogeneity of the original operator L and the interaction determined by φ. Note that $Q_2(z)$ is a Nevanlina function and a regularization of the expression $\langle \frac{1}{L-z)}\varphi, \varphi\rangle$.

(iv) If $n \geq 3$ the perturbation L_α in (1.5) cannot be treated as in the cases $n = 0, 1$, and 2, because then $L_{\min}$ in (1.7) is essentially self-adjoint in $\mathcal{H}$, that is, $L_{\min}$ is not closed and its closure is a self-adjoint operator in $\mathcal{H}$. One needs to resort to other methods such as the ones introduced above.

2. An intermediate space and a maximal operator.

From now on, unless specified otherwise, we assume that the interaction φ belongs to $\mathcal{H}_{-n} \setminus \mathcal{H}_{-n+1}$ with $n \geq 3$. We choose $n-1$ positive real normalization points $a_1, a_2, \ldots, a_{n-1}$ and associate with them the polynomials $b_0(z) = 1$ and

$$b_j(z) = (z+a_1)(z+a_2)\cdots(z+a_j), \quad j = 1, 2, \ldots n-1,$$

and the singular elements

$$\varphi_j = \frac{1}{b_j(L)}\,\varphi \in \mathcal{H}_{-n+2j} \setminus \mathcal{H}_{-n+2j+1}, \quad j = 0, 1, \ldots, n-1.$$

In the sequel we assume that the space $\mathcal{H}_{n-2}$ is endowed with the new inner product

$$\langle u, v\rangle_{n-2} = \langle b_{n-2}(L)u, v\rangle, \quad u, v \in \mathcal{H}_{n-2}. \tag{2.1}$$

2.1. The space H and the operator $\mathbf{L}_{\max}$

Our first choice for a minimal operator associated with the singular perturbation (1.2) is the operator $L_{\min}$ in the space $\mathcal{H}_{n-2}$:

$$L_{\min} = \{\{f, Lf\} \mid f \in \mathcal{H}_n, \langle f, \varphi\rangle = 0\}.$$

We frequently identify an operator with its graph to expedite the presentation. For graph notation and linear relations see for example [1, Section 51], [4, Section 2.1], and [16]. A natural candidate for the maximal operator is the adjoint $L_{\max} = L_{\min}^\dagger$ of $L_{\min}$ relative to the Gelfand triple $\mathcal{H}_{n-2} \hookrightarrow H \hookrightarrow \mathcal{H}_{-n+2}$. Recall from, for example, [5] that if $\mathcal{K} \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{K}'$ is a Gelfand triple and B is a densely defined operator in $\mathcal{K}$ then the *adjoint of B relative to the Gelfand triple* is the operator in $\mathcal{K}'$ defined by

$$B^\dagger = \{\{f,g\} \mid \langle f, Bu\rangle = \langle g,u\rangle, u \in \operatorname{dom} B\}.$$

Here the scalar product in the definition should be understood as the pairing between $\mathcal{K}$ and $\mathcal{K}'$ induced by the inner product $\langle\,\cdot\,,\,\cdot\,\rangle$ of $\mathcal{H}$. The adjoint operator just defined coincides with the standard adjoint operator in the case $\mathcal{K} = \mathcal{H} = \mathcal{K}'$.

Theorem 2.1. *The adjoint of $L_{\min}$ in $\mathcal{H}_{n-2}$ relative to the Gelfand triple $\mathcal{H}_{n-2} \hookrightarrow H \hookrightarrow \mathcal{H}_{-n+2}$ is the operator in $\mathcal{H}_{-n+2}$ given by*

$$L_{\max} = \{f + f_1\varphi_1, Lf - a_1 f_1 \varphi_1\} \mid f \in \mathcal{H}_{-n+4}, f_1 \in \mathbb{C}\}.$$

Proof. The operator $L_{\min}$ in $\mathcal{H}_{n-2}$ is densely defined, so the operator $L_{\max} = L_{\min}^\dagger$ is well defined. If $\widetilde{f}, \widetilde{g} \in \mathcal{H}_{-n+2}$, then $\{\widetilde{f}, \widetilde{g}\} \in L_{\max}$ if and only if

$$0 = \langle \widetilde{f}, Lu\rangle - \langle \widetilde{g}, u\rangle = \langle L\widetilde{f} - \widetilde{g}, u\rangle, \quad u \in \operatorname{dom} L_{\min},$$

and hence if and only if $L\widetilde{f} - \widetilde{g} = f_1\varphi$ for some $f_1 \in \mathbb{C}$. It follows that

$$\widetilde{f} = (L + a_1)^{-1}(\widetilde{g} + a_1\widetilde{f}) + f_1\varphi_1 = f + f_1\varphi_1,$$

where $f = (L + a_1)^{-1}(\widetilde{g} + a_1\widetilde{f}) \in \mathcal{H}_{-n+4}$, and

$$\widetilde{g} = L\widetilde{f} - f_1\varphi = Lf + f_1(L\varphi_1 - \varphi) = Lf - a_1 f_1\varphi_1. \qquad \square$$

The space $\mathcal{H}_{-n+2}$ in which the maximal operator is defined is too large for our considerations. It is sufficient that it contains the functions $\frac{1}{L-z}\,\varphi$, $z \in \rho(L)$, and the space $\mathcal{H}_{n-2}$ in which the minimal operator acts. In view of the resolvent formula (1.4) we consider the linear space

$$\mathbf{H} = \mathcal{H}_{n-2} \dotplus \operatorname{span}\{\varphi_1, \varphi_2, \ldots, \varphi_{n-2}\}$$

equipped with the inner product

$$\left\langle u + \sum_{j=1}^{n-2} \varphi_j u_j, v + \sum_{j=1}^{n-2} \varphi_j v_j \right\rangle_{\mathbf{H}} = \langle u, v\rangle_{n-2} + \sum_{j=1}^{n-2} v_j^* u_j, \tag{2.2}$$

where $u, v \in \mathcal{H}_{n-2}$ and $u_j, v_j \in \mathbb{C}$.It is contained in $\mathcal{H}_{-n+2}$ and only a finite dimensional extension of $\mathcal{H}_{n-2}$. By the resolvent formula (1.4) the space $\mathbf{H}$ does not depend on the choice of the normalization points a_j. The space is large enough to contain the ranges of the bounded operators

$$R(z) = \frac{1}{L-z} - \frac{1}{Q(z)} \left\langle \cdot, \frac{1}{L-z^*}\,\varphi \right\rangle \frac{1}{L-z}\,\varphi, \quad z \in \rho(L),\ Q(z) \neq 0,$$

mapping $\mathcal{H}_{n-2}$ to $\mathcal{H}_{-n+2}$. Indeed,

$$\operatorname{ran} R(z) \subset \mathcal{H}_n \dotplus \operatorname{span}\{\varphi_1, \varphi_2, \ldots, \varphi_{n-2}, \varphi_{n-1}\} =: \mathbf{D}$$

and $\mathbf{D} \subset \mathbf{H}$. Note that $R(z)$ is defined by a formula similar to the righthand side of Krein's formula (1.8) to which we shall refer again later.

Evidently, the domain of the operator $L_{\max}$ contains the space $\mathbf{H}$. But the range of the restriction of $L_{\max}$ to $\mathbf{H}$ is not contained in $\mathbf{H}$. A suitable restriction of $L_{\max}$ which has this property is the restriction to the space $\mathbf{D}$ just defined. We denote this operator in $\mathbf{H}$ by $\mathbf{L}_{\max}$: $\operatorname{dom}\mathbf{L}_{\max} = \mathbf{D}$ and for elements in $\mathbf{D}$ we have

$$\mathbf{L}_{\max}\left(u + u_{n-1}\varphi_{n-1} + \sum_{j=1}^{n-2} u_j\varphi_j\right) = Lu - a_{n-1}u_{n-1}\varphi_{n-1} + \sum_{j=1}^{n-2}(u_{j+1} - a_j u_j)\varphi_j. \tag{2.3}$$

Note that $\mathbf{L}_{\max}$ is closed in $\mathbf{H}$.

2.2. Vector notation

In the sequel we shall use the following notation. Elements in $\mathbb{C}^{n-2}$ are always considered as column vectors. If $\vec{u} \in \mathbb{C}^{n-2}$, its entries are denoted by u_j:

$$\vec{u} = \begin{pmatrix} u_1 & u_2 & \cdots & u_{n-2} \end{pmatrix}^\top$$

and we write $\vec{u}^*$ for the row vector

$$\vec{u}^* = \begin{pmatrix} u_1^* & u_2^* & \cdots & u_{n-2}^* \end{pmatrix}.$$

The inner product in $\mathbb{C}^{n-2}$ is given by $\langle \vec{u}, \vec{v} \rangle_{\mathbb{C}^{n-2}} = \vec{v}^*\,\vec{u}$. By $\vec{e}_1, \vec{e}_2, \ldots, \vec{e}_{n-2}$ we denote the standard basis in $\mathbb{C}^{n-2}$. Thus, for example, we have $\vec{e}_j^{\,*}\,\vec{u} = u_j$. The vector $\vec{\varphi}$ stands for the row vector

$$\vec{\varphi} = \begin{pmatrix} \varphi_1 & \varphi_2 & \cdots & \varphi_{n-2} \end{pmatrix}$$

so that

$$\vec{\varphi}\vec{u} = \sum_{j=1}^{n-2} \varphi_j\, u_j, \quad L\vec{\varphi} = \begin{pmatrix} L\varphi_1 & L\varphi_2 & \cdots & L\varphi_{n-2} \end{pmatrix},$$

and the inner product (2.2) can be shortened to

$$\langle u + \vec{\varphi}\vec{u}, v + \vec{\varphi}\vec{v} \rangle_{\mathbf{H}} = \langle u, v \rangle_{n-2} + \vec{v}^*\,\vec{u}.$$

We extend the vector notation to the pairing:

$$\langle \vec{\varphi}, x \rangle = \begin{pmatrix} \langle \varphi_1, x \rangle & \langle \varphi_2, x \rangle & \cdots & \langle \varphi_{n-2}, x \rangle \end{pmatrix},$$

whenever the pairings on the righthand side are defined, and $\langle x, \vec{\varphi} \rangle = \langle \vec{\varphi}, x \rangle^*$, so that, for example,

$$\langle \vec{\varphi}\vec{u}, x \rangle = \langle \vec{\varphi}, x \rangle \vec{u}, \quad \langle x, L\vec{\varphi}\vec{u} \rangle = \vec{u}^* \langle x, L\vec{\varphi} \rangle.$$

These formulas also make sense when $\vec{u} \in \mathbb{C}^{n-2}$ is replaced by a matrix of size $(n-2) \times k$ for some k.

Finally, we introduce the $(n-2)\times(n-2)$ matrix

$$\mathfrak{M} = \begin{pmatrix} -a_1 & 1 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & -a_2 & 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & -a_3 & 1 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & -a_4 & \dots & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & -a_{n-4} & 1 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & -a_{n-3} & 1 \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & -a_{n-2} \end{pmatrix}.$$

Then (2.3) can be written as

$$\mathbf{L}_{\max}(u + u_{n-1}\varphi_{n-1} + \vec{\varphi}\vec{u}) = Lu - a_{n-1}u_{n-1}\varphi_{n-1} + \vec{\varphi}(\mathfrak{M}\vec{u} + u_{n-1}\vec{e}_{n-2}).$$

This formula is the starting point for the maximal operators in the A- and B-models, which we introduce in the next two sections.

3. The A-model

This section concerns the lefthand side of the commutative diagram (1.3) in the Introduction:

$$\begin{array}{ccc} \mathcal{H}_A & \xrightarrow{\ \mathbf{i}\ } & \mathbf{H} \\ A_{\max}\downarrow & & \downarrow \mathbf{L}_{\max} \\ \mathcal{H}_A & \xrightarrow{\ \mathbf{i}\ } & \mathbf{H} \end{array}$$

Our aim is to construct a one-parameter family of self-adjoint operators A_θ acting in an inner product space $\mathcal{H}_A$ topologically isomorphic to $\mathbf{H}$ under the isomorphism $\mathbf{i}$. The self-adjoint operators are restrictions of the operator $A_{\max}$ which is the copy of $L_{\max}$ under $\mathbf{i}$. They are the self-adjoint realizations of the singular perturbation L_α in (1.2). In general the space $\mathcal{H}_A$ will be a Pontryagin space, but the interesting feature of this model is that when the normalization points a_j are mutually distinct the inner product can be chosen so that $\mathcal{H}_A$ is a Hilbert space.

3.1. The space $\mathcal{H}_A$ and the maximal operator

We consider the space $\mathcal{H}_A = \mathbb{C}^{n-2} \oplus \mathcal{H}_{n-2}$ of elements of the form

$$U = \begin{pmatrix} \vec{u} \\ u \end{pmatrix}, \quad \vec{u} \in \mathbb{C}^{n-2}, u \in \mathcal{H}_{n-2},$$

and endow it with the inner product determined by the Gram matrix

$$G_A = \Gamma_\alpha \oplus I_{\mathcal{H}_{n-2}},$$

that is, by the formula (see also (2.1))

$$\langle U, V\rangle_A = \vec{v}^*\Gamma_\alpha\vec{u} + \langle b_{n-2}(L)u, v\rangle,$$

where $\Gamma_\alpha = (\alpha_{j,k})_{j,k=1}^{n-2}$ is a non-degenerate Hermitian $(n-2)\times(n-2)$ matrix whose entries $\alpha_{j,k}$ will be specified later. Thus $\mathcal{H}_A$ is a Hilbert space if Γ_α is positive and a Pontryagin space otherwise. The mapping $\mathbf{i} : \mathcal{H}_A \to \mathbf{H}$ defined by

$$\mathbf{i}\begin{pmatrix}\vec{u}\\ u\end{pmatrix} = \vec{\varphi}\,\vec{u} + u$$

is a natural topological isomorphism and we define the maximal operator $A_{\max}$ in $\mathcal{H}_A$ as the isomorphic copy of $\mathbf{L}_{\max}$ in $\mathbf{H}$:

$$\begin{aligned} A_{\max} &= \mathbf{i}^{-1}\mathbf{L}_{\max}\mathbf{i} \\ &= \left\{\left\{\begin{pmatrix}\vec{u}\\ u_r + u_{n-1}\varphi_{n-1}\end{pmatrix}, \begin{pmatrix}\mathfrak{M}\vec{u} + u_{n-1}\vec{e}_{n-2}\\ Lu_r - a_{n-1}u_{n-1}\varphi_{n-1}\end{pmatrix}\right\} \mid \begin{matrix}\vec{u}\in\mathbb{C}^{n-2}, u_{n-1}\in\mathbb{C},\\ u_r\in\mathcal{H}_n\end{matrix}\right\}. \end{aligned}$$

The minimal operator is defined by $A_{\min} = A_{\max}^*$, the adjoint of $A_{\max}$ in $\mathcal{H}_A$. Since $\mathbf{L}_{\max}$ is closed, $A_{\max}$ is closed and hence $A_{\min}^* = A_{\max}$.

Theorem 3.1. *The operator $A_{\min}$ is given by*

$$A_{\min} = \left\{\left\{\begin{pmatrix}\vec{u}\\ u\end{pmatrix}, \begin{pmatrix}\Gamma_\alpha^{-1}\mathfrak{M}^*\Gamma_\alpha\vec{u}\\ Lu\end{pmatrix}\right\} \mid \begin{matrix}\vec{u}\in\mathbb{C}^{n-2}, u\in\mathcal{H}_n,\\ \langle u,\varphi\rangle - \vec{e}_{n-2}^{\,*}\Gamma_\alpha\vec{u} = 0\end{matrix}\right\} \tag{3.1}$$

and it is symmetric if and only if Γ_α satisfies the relation

$$\Gamma_\alpha\mathfrak{M} - \mathfrak{M}^*\Gamma_\alpha = 0. \tag{3.2}$$

In this case the symmetric operator $A_{\min}$ is the restriction of $A_{\max}$ by two conditions:

$$\begin{aligned} &\operatorname{dom} A_{\min} \\ &= \left\{\begin{pmatrix}\vec{u}\\ u_r + u_{n-1}\varphi_{n-1}\end{pmatrix} \in \operatorname{dom} A_{\max} \mid u_{n-1} = 0,\ \langle u_r,\varphi\rangle - \vec{e}_{n-2}^{\,*}\Gamma_\alpha\vec{u} = 0\right\}. \end{aligned}$$

Note that the operator $A_{\min}$ is not isomorphic under $\mathbf{i}$ with the operator $L_{\min}$ defined in (1.7).

Proof of Theorem 3.1. If $F, G \in \mathcal{H}_A$, then $\{F, G\} \in A_{\min}$ if and only if for all $\vec{u}\in\mathbb{C}^{n-2}$, $u_{n-2}\in\mathbb{C}$, and $u_r\in\mathcal{H}_n$ we have

$$\begin{aligned} 0 &= \left\langle F, A_{\max}\begin{pmatrix}\vec{u}\\ u_r + u_{n-1}\varphi_{n-1}\end{pmatrix}\right\rangle_A - \left\langle G, \begin{pmatrix}\vec{u}\\ u_r + u_{n-1}\varphi_{n-1}\end{pmatrix}\right\rangle_A \\ &= (\mathfrak{M}\vec{u} + u_{n-1}\vec{e}_{n-2})^*\Gamma_\alpha\vec{f} - \langle b_{n-2}(L)f, Lu_r - a_{n-1}u_{n-1}\varphi_{n-1}\rangle \\ &\quad -\vec{u}^*\Gamma_\alpha\vec{g} - \langle b_{n-2}(L)g, u_r + u_{n-1}\varphi_{n-1}\rangle. \end{aligned}$$

Choosing $\vec{u} = 0$ and $u_{n-1} = 0$ we find that for all $u_r\in\mathcal{H}_n$,

$$0 = \langle b_{n-2}(L)f, Lu_r\rangle - \langle b_{n-2}(L)g, u_r\rangle$$

and hence

$$f\in\mathcal{H}_n, \quad g = Lf.$$

It follows that for all $\vec{u} \in \mathbb{C}^{n-2}$ and $u_{n-1} \in \mathbb{C}$,

$$\begin{aligned} 0 &= (\mathfrak{M}\vec{u} + u_{n-1}\vec{e}_{n-2})^*\Gamma_\alpha \vec{f} + \langle f, a_{n-1}u_{n-1}\varphi_{n-1}\rangle - \vec{u}^*\Gamma_\alpha \vec{g} - \langle g, u_{n-1}\varphi_{n-1}\rangle \\ &= (\mathfrak{M}\vec{u} + u_{n-1}\vec{e}_{n-2})^*\Gamma_\alpha \vec{f} - \vec{u}^*\Gamma_\alpha \vec{g} + \langle f, u_{n-1}\varphi_{n-2}\rangle, \end{aligned}$$

where we used that $(L + a_{n-1})\varphi_{n-1} = \varphi_{n-2}$. Choosing $u_{n-1} = 0$ we find that

$$\vec{g} = \Gamma_\alpha^{-1}\mathfrak{M}^*\Gamma_\alpha \vec{f},$$

and choosing $\vec{u} = 0$ we obtain

$$\langle f, \varphi\rangle - \vec{e}^{\,*}_{n-2}\Gamma_\alpha \vec{f} = 0. \tag{3.3}$$

The calculations can be traced backwards to complete the proof of the representation of $A_{\min}$.
Evidently, $\operatorname{dom} A_{\min} \subset \operatorname{dom} A_{\max}$ and if Γ_α is a solution of (3.2) then $A_{\min} \subset A_{\max}$, that is, $A_{\min}$ is symmetric. To prove the converse, assume that $A_{\min}$ is symmetric. Choose an arbitrary vector $\vec{f} \in \mathbb{C}^{n-2}$ and then choose an $f \in \mathcal{H}_n$ such that (3.3) holds and set $F = \begin{pmatrix} \vec{f} \\ f \end{pmatrix}$. The symmetry implies that $A_{\min}F = A_{\max}F$ and hence

$$\Gamma_\alpha^{-1}\mathfrak{M}^*\Gamma_\alpha \vec{f} = \mathfrak{M}\vec{f}.$$

Since $\vec{f}$ is arbitrary, Γ_α satisfies (3.2).
The proof of the last statement is left to the reader. □

The following theorem shows that if the diagonal entries of the matrix $\mathfrak{M}$ are mutually distinct, then there are many positive Hermitian solutions Γ_α of the equation (3.2); otherwise the Hermitian solutions are necessarily non-positive.

Theorem 3.2. (i) *The equation* (3.2) *has a family of Hermitian solutions which can be parametrized with $n-2$ real parameters. This family contains infinitely many non-degenerate* (*and infinitely many degenerate*) *solutions.*
(ii) *If the normalization points a_j are mutually distinct, then* (3.2) *has a family of positive Hermitian solutions which can be parametrized with $n-2$ real parameters.*
(iii) *If at least two of the a_j's are equal then every non-degenerate Hermitian solution of* (3.2) *is indefinite.*

Proof. (i) Equation (3.2) implies that all entries $\alpha_{j,k}$ of the Hermitian matrix Γ_α are real

$$\alpha_{j,k} = \alpha_{k,j} \in \mathbb{R}$$

and satisfy the following recurrence relations

$$\begin{aligned} &\alpha_{j,k} = \alpha_{j-1,k+1} + (a_{k+1} - a_j)\alpha_{j,k+1}, \quad && 2 \le j \le k \le n-3, \\ &\alpha_{1,k} = (a_{k+1} - a_1)\alpha_{1,k+1}, && k = 1, ..., n-3. \end{aligned} \tag{3.4}$$

These equations show that the last column $\vec{\gamma}$ of the matrix Γ_α can be chosen arbitrarily among real vectors and that the entries of the first row are determined by the value of the last entry. They allow one to calculate all entries $\alpha_{j,k}, j \le k$.

All entries below the diagonal are determined taking into account that Γ_α is symmetric. The solution Γ_α depends continuously on $\vec{\gamma}$ and if we take $\vec{\gamma} = \vec{e}_1$ then Γ_α is non-degenerate; hence if we consider $\vec{\gamma}$ with nonzero first entry, then for sufficiently small values of the other entries the solution will be non-degenerate also. If we choose $\gamma_1 = 0$, then the second recurrence equality in (3.4) implies that the first row of the solution is the zero vector and hence the solution has a zero determinant.
(ii) Consider the following family of upper triangular matrices Y

$$Y = \text{diag}\,(\xi_1, \xi_2, \dots, \xi_{n-2})\; X$$

where $\xi_j,\ j = 1, ..., n-2$, are arbitrary nonzero complex numbers and X is the $(n-2) \times (n-2)$ matrix

$$X = \begin{pmatrix} (a_{n-2}-a_1)...(a_2-a_1) & (a_{n-2}-a_1)...(a_3-a_1) & ... & (a_{n-2}-a_1) & 1 \\ 0 & (a_{n-2}-a_2)...(a_3-a_2) & ... & (a_{n-2}-a_2) & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & (a_{n-2}-a_{n-3}) & 1 \\ 0 & 0 & \dots & 0 & 1 \end{pmatrix}.$$

Then the matrix $\Gamma_\alpha = Y^*\,Y$ satisfies equation (3.2). Indeed, we have that

$$Y\mathfrak{M} = -\text{diag}\,(a_1, a_2, \dots, a_{n-2})\,Y,$$

and this implies

$$\begin{aligned} Y^*Y\mathfrak{M} &= -Y^*\,\text{diag}\,(a_1, a_2, \dots, a_{n-2})\,Y = -\left(\text{diag}\,(a_1, a_2, \dots, a_{n-2})\,Y\right)^*\,Y \\ &= (Y\mathfrak{M})^*Y = \mathfrak{M}^*Y^*Y. \end{aligned}$$

The last column of the matrix $\Gamma_\alpha = Y^*Y$ is equal to

$$X^* \begin{pmatrix} |\xi_1|^2 \\ |\xi_2|^2 \\ \vdots \\ |\xi_{n-2}|^2 \end{pmatrix} X,$$

and this implies that the family of matrices just constructed is described by $n-2$ independent (positive) real parameters $|\xi_j|^2$.
(iii) Consider now the case when at least two of the parameters a_j, say a_1 and a_2, coincide. Then the second recurrence relation in (3.4) implies that $\alpha_{11} = 0$ and the matrix Γ_α has at least one negative eigenvalue. □

By way of example, suppose that all numbers a_j are equal, say $a_j = a$. Then the recurrence relations (3.4) imply that the matrix Γ_α is a Hankel matrix $\alpha_{j,k} = \alpha_{j+k}$

with $\alpha_l = 0, l = 2, ..., n-2$, that is, Γ_α is an anti-triangular matrix

$$\Gamma_\alpha = \begin{pmatrix} 0 & 0 & \dots & 0 & \alpha_{n-1} \\ 0 & 0 & \dots & \alpha_{n-1} & \alpha_n \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \alpha_{n-1} & \dots & \alpha_{2n-6} & \alpha_{2n-5} \\ \alpha_{n-1} & \alpha_n & \dots & \alpha_{2n-5} & \alpha_{2n-4} \end{pmatrix}.$$

The number of negative eigenvalues of this matrix is equal to

$$\begin{cases} \dfrac{n-2}{2}, & \text{if } n \text{ is even,} \\ \dfrac{n-1}{2}, & \text{if } n \text{ is odd and } \alpha_{n-1} > 0, \\ \dfrac{n+1}{2}, & \text{if } n \text{ is odd and } \alpha_{n-1} < 0. \end{cases}$$

3.2. The self-adjoint realizations A_θ

From now on we assume that Γ_α is an invertible Hermitian solution of (3.2). Then $A_{\min}$ is a symmetric operator. Its defect indices are $(1,1)$ and a defect element for $A_{\min}$ at $z \in \rho(L)$ is given by

$$\Phi_A(z) = \frac{1}{b_{n-2}(z)} \begin{pmatrix} \vec{b}(z) \\ \dfrac{1}{L-z} \frac{b_{n-2}(z)}{b_{n-2}(L)} \varphi \end{pmatrix}, \quad \vec{b}(z) = \begin{pmatrix} 1 \\ b_1(z) \\ \vdots \\ b_{n-3}(z) \end{pmatrix}, \tag{3.5}$$

Indeed, writing $\Phi_A(z)$ as

$$\Phi_A(z) = \begin{pmatrix} \dfrac{1}{b_{n-2}(z)} \vec{b}(z) \\ u + \varphi_{n-1} \end{pmatrix}, \quad u = \frac{z + a_{n-1}}{L-z} \varphi_{n-1} \in \mathcal{H}_n,$$

and using the identity

$$(\mathfrak{M} - z)\vec{b}(z) = -b_{n-2}(z)\vec{e}_{n-2}, \tag{3.6}$$

we find that $(A_{\max} - z)\Phi_A(z) = 0$. By (1.4) with n replaced by $n-1$, the element $\frac{1}{L-z}\varphi$ belongs to $\mathbf{H}$ and we have

$$\mathbf{i}\,\Phi_A(z) = \frac{1}{b_{n-2}(z)} \frac{1}{L-z} \varphi.$$

Among all self-adjoint extensions of $A_{\min}$ one resembles the original operator L, namely

$$A_0 = \mathfrak{M} \oplus L = \left\{ \left\{ \begin{pmatrix} \vec{u} \\ u \end{pmatrix}, \begin{pmatrix} \mathfrak{A}\vec{u} \\ Lu \end{pmatrix} \right\} \mid u \in \mathcal{H}_n, \vec{u} \in \mathbf{C}^{n-2} \right\},$$

where L is the self-adjoint operator on the space $\mathcal{H}_{n-2}$ with $\operatorname{dom} L = \mathcal{H}_n$. The operator $A_{\min}$ can be described as the restriction of the operator A_0 to the set of functions $U \in \operatorname{dom} A_0$ satisfying the condition

$$\langle (A_0 + a_{n-1})U, \Phi_A(-a_{n-1}) \rangle_A = 0. \tag{3.7}$$

To see this it suffices to show that this condition is equivalent to the condition

$$\langle u, \varphi \rangle - \vec{e}^{\,*}_{n-2}\Gamma_\alpha \vec{u} = 0$$

appearing in the formula (3.1) for $A_{\min}$. This follows from

$$\begin{aligned}
&\langle (\mathfrak{M} + a_{n-1})U, \Phi_A(-a_{n-1})\rangle_A \\
&= \left\langle \begin{pmatrix} (\mathfrak{M} + a_{n-1})\,\vec{u} \\ (L + a_{n-1})\,u \end{pmatrix}, \begin{pmatrix} \dfrac{1}{b_{n-2}(-a_{n-1})}\,\vec{b}\,(-a_{n-1}) \\ \varphi_{n-1} \end{pmatrix} \right\rangle_A \\
&= \frac{1}{b_{n-2}(-a_{n-1})}\,\vec{b}\,(-a_{n-1})^*\Gamma_\alpha(\mathfrak{M} + a_{n-1})\,\vec{u} + \langle b_{n-2}(L)(L + a_{n-1})\,u, \varphi_{n-1}\rangle \\
&= -\vec{e}^{\,*}_{n-2}\Gamma_\alpha \vec{u} + \langle u, \varphi \rangle,
\end{aligned}$$

where we used $\Gamma_\alpha \mathfrak{M} = \mathfrak{M}^*\Gamma_\alpha$ and (3.6) with $z = -a_{n-1}$.
The operator A_0 will be used to describe all self-adjoint extensions of $A_{\min}$ via Krein's resolvent formula. The defect elements $\Phi_A(z)$ in (3.5) at different points are related by the Hilbert identity

$$\Phi_A(z) - \Phi_A(\zeta) = (z - \zeta)\frac{1}{A_0 - z}\Phi_A(\zeta),$$

which means that $\Phi_A(z)$ is a defect function associated with A_0. The Q-function for the operators $A_{\min}$ and $\mathbf{A}_0$, by definition the solution of the equation

$$\frac{Q_A(z) - Q_A(\zeta)^*}{z - \zeta^*} = \langle \Phi_A(z), \Phi_A(\zeta)\rangle_A, \tag{3.8}$$

is given by

$$\begin{aligned}
Q_A(z) &= (z + a_{n-1})\,\langle \Phi_A(z), \Phi_A(-a_{n-1})\rangle_A + c \\
&= \left\langle \frac{z + a_{n-1}}{L - z}\,\varphi, d\frac{1}{b_{n-1}(L)}\,\varphi \right\rangle + r(z) - r(-a_{n-1}) + c,
\end{aligned}$$

where c is a real constant and $r(z)$ is the rational function

$$r(z) = \vec{e}^{\,*}_{n-2}\Gamma_\alpha \frac{1}{\mathfrak{M} - z}\,\vec{e}_{n-2} = -\sum_{k=1}^{n-2}\alpha_{k,n-2}\frac{b_{k-1}(z)}{b_{n-2}(z)}, \tag{3.9}$$

where to obtain the last equality we used (3.6). We normalize $Q_A(z)$ by the condition $Q_A(-a_{n-1}) = r(-a_{n-1})$ or, equivalently, $c = r(-a_{n-1})$, and shall use the fixed Q-function

$$Q_A(z) = \left\langle \frac{z + a_{n-1}}{L - z}\,\varphi, \frac{1}{b_{n-1}(L)}\,\varphi \right\rangle + r(z).$$

Formula (3.9) implies that $r(z) \in N_{\kappa_1}$, where κ_1 is the number of negative eigenvalues of Γ_α. Hence $\kappa_1 \leq n-2$. The poles of $r(z)$ lie at the points $-a_1, -a_2, \ldots, -a_{n-2}$ on the negative half axis and therefore outside of the spectrum of L. Then by [22, Satz 1.13] the function $Q_A(z)$ belongs to the class N_{κ_1} because $Q_A(z)$ is a sum

of a Nevanlinna function and a function from N_{κ_1} whose spectra are mutually disjoint.
Using the defect function and the Q-function all self-adjoint extensions of $A_{\min}$ in the space $\mathcal{H}_A$ can be described as a one-parameter family of operators by Krein's resolvent formula. This is formulated in the first part of the next theorem. Self-adjoint extensions of $A_{\min}$ are restrictions of $A_{\max}$ and these are described in the second part of the theorem.

Theorem 3.3. (i) *The resolvent relation*

$$\frac{1}{A_\theta - z} = \frac{1}{A_0 - z} - \frac{1}{Q_A(z) + \cot\theta}\langle\,\cdot\,, \Phi_A(z^*)\rangle_A \Phi_A(z). \tag{3.10}$$

defines a one-to-one correspondence between all self-adjoint extensions A_θ of $A_{\min}$ in $\mathcal{H}_A$ and the numbers $\theta \in [0, \pi)$.
(ii) *The self-adjoint operator A_θ is semi-bounded and the restriction of $A_{\max}$ by the condition*

$$U \in \operatorname{dom} A_{\max}, \quad \cos\theta\, u_{n-1} + \sin\theta(\langle u_r, \varphi\rangle - \vec{e}^{\,*}_{n-2}\Gamma_\alpha \vec{u}) = 0,\ \ \theta \in [0, \pi). \tag{3.11}$$

Proof. The proof of statement (i) is well known; see, for instance, [1]. We prove (ii). Consider $\theta \in (0, \pi)$ and fix a point $z \in \rho(L)$ such that $Q_A(z) + \cot\theta \neq 0$. Let $U \in \mathcal{H}_A$. Then $U \in \operatorname{dom} A_\theta$ if and only if for some $F \in \mathcal{H}_A$

$$U = \frac{1}{A_0 - z}\,F - \frac{1}{Q_A(z) + \cot\theta}\,\langle F, \Phi_A(z^*)\rangle_A \Phi_A(z).$$

Thus U can be written as

$$U = \begin{pmatrix} \vec{u} \\ u \end{pmatrix} = V + u_{n-1}\Phi(-a_{n-1}) = \begin{pmatrix} \vec{v} + \dfrac{u_{n-1}}{b_{n-2}(-a_{n-1})}\vec{b}\,(-a_{n-1}) \\ u_r + u_{n-1}\varphi_{n-1} \end{pmatrix} \tag{3.12}$$

with

$$\begin{aligned} u_{n-1} \quad &= \quad -\frac{1}{Q_A(z) + \cot\theta}\,\langle F, \Phi_A(z^*)\rangle_A \in \mathbb{C}, \\ V \quad &= \quad \begin{pmatrix} \vec{v} \\ u_r \end{pmatrix} = \frac{1}{A_0 - z}\,F + u_{n-1}\frac{z + a_{n-1}}{A_0 - z}\,\Phi_A(-a_{n-1}) \in \operatorname{dom} A_0; \end{aligned}$$

in particular, $u_r \in \mathcal{H}_n$. Using the defining relation (3.8) for $Q_A(z)$ and its normalization, we obtain

$$\langle (A_0 - z)V, \Phi_A(z^*)\rangle_A = -u_{n-1}(r(-a_{n-1}) + \cot\theta).$$

On the other hand using (3.6), the relation between the first components of U and V given by (3.12) and the formula (3.9) for the function $r(z)$ we find that the inner product on the lefthand side is equal to

$$\begin{aligned}
&\langle (A_0 - z)V, \Phi_A(z^*)\rangle_A = \\
&= \left\langle \begin{pmatrix} (\mathfrak{M} - z)\vec{v} \\ (L - z)u_r \end{pmatrix}, \begin{pmatrix} \frac{1}{b_{n-2}(z^*)}\vec{b}(z^*) \\ \frac{1}{L - z^*}\varphi_{n-2} \end{pmatrix} \right\rangle_A \\
&= \frac{1}{b_{n-2}(z)}\vec{b}(z^*)^*\Gamma_\alpha(\mathfrak{M} - z)\vec{v} + \langle u_r, b_{n-2}(L)\,\varphi_{n-2}\rangle \\
&= -\vec{e}^{\,*}_{n-2}\Gamma_\alpha\vec{v} + \langle v, \varphi\rangle \\
&= -\vec{e}^{\,*}_{n-2}\Gamma_\alpha\vec{u} + \frac{u_{n-1}}{b_{n-2}(-a_{n-1})}\vec{e}^{\,*}_{n-2}\Gamma_\alpha\vec{b}(-a_{n-1}) + \langle u_r, \varphi\rangle \\
&= -\vec{e}^{\,*}_{n-2}\Gamma_\alpha\vec{u} + \langle u_r, \varphi\rangle - u_{n-1}r(-a_{n-1}).
\end{aligned}$$

It follows that U satisfies the condition (3.11). It is easy to show that this condition determines a symmetric extension of $A_{\min}$. Therefore this extension necessarily coincides with the operator A_θ. It follows that A_θ is the restriction $A_{\max}$ to the set of elements in $\operatorname{dom} A_{\max}$ which satisfy (3.11).
In the case $\theta = 0$ the self-adjoint operator coincides with A_0. □

Note that in terms of A_0 and $\Phi_A(z)$ the maximal operator $A_{\max} = A^*_{\min}$ can be described as the relation

$$\begin{aligned}
A_{\max} &= \{\{U + u_{n-1}\Phi_A(-a_{n-1}), A_0U - a_{n-1}u_{n-1}\Phi_A(-a_{n-1})\} \mid \\
&\qquad U \in \operatorname{dom} A_0, u_{n-1} \in \mathbb{C}\}
\end{aligned}$$

and the self-adjoint operator A_θ as

$$\begin{aligned}
A_\theta = {}&\{\{U + u_{n-1}\Phi_A(-a_{n-1}), A_0U - a_{n-1}u_{n-1}\Phi_A(-a_{n-1})\} \mid U \in \operatorname{dom} A_0, \\
&u_{n-1} \in \mathbb{C},\ \langle (A_0 + a_{n-1})U, \Phi_A(-a_{n-1})\rangle_A = -(r(-a_{n-1}) + \cot\theta)u_{n-1}\}\,.
\end{aligned}$$

The first formula follows from (3.7); the second one from arguments in the foregoing proof.

3.3. Compressions of the resolvent of A_θ

The formula for the skew compression $\mathbf{i}\frac{1}{A_\theta - z}|_{\mathcal{H}_{n-2}}$ of the resolvent of A_θ follows immediately from (3.10):

$$\mathbf{i}\frac{1}{A_\theta - z}|_{\mathcal{H}_{n-2}} = \frac{1}{L - z} - \frac{1}{Q(z)}\left\langle \,\cdot\,, \frac{1}{L - z^*}\varphi \right\rangle \frac{1}{L - z}\varphi \tag{3.13}$$

where

$$Q(z) = b_{n-2}(z)(Q_A(z) + \cot\theta). \tag{3.14}$$

The function $Q(z)$ is always a generalized Nevanlinna function, even if the parameters of the model are chosen such that $\mathcal{H}_A$ is a Hilbert space.
The formula for the compression of the resolvent to $\mathcal{H}_{n-2}$ is given by:

$$P_{\mathcal{H}_{n-2}}\frac{1}{A_\theta - z}|_{\mathcal{H}_{n-2}} = \frac{1}{L - z} - \frac{1}{Q_A(z) + \cot\theta}\left\langle \,\cdot\,, \frac{1}{L - z^*}\varphi_{n-2} \right\rangle_{n-2} \frac{1}{L - z}\varphi_{n-2}.$$

This formula implies that the spectral problem for the operator A_θ is equivalent to the following explicit eigenvalue depending "boundary value" problem:

$$\begin{aligned}(L-z)u &= c\varphi_{n-1}, \quad u \in \mathcal{H}_n,\ c \in \mathbb{C},\\ (z+a_{n-1})\langle u,\varphi\rangle &= -c\,(r(z)+\cot\theta)\,.\end{aligned}$$

4. The B-model

In this section we discuss an extended form of the righthand side of the commutative diagram (1.3) in the Introduction:

$$\begin{array}{ccccc} \mathbf{H} & \xrightarrow{\mathbf{j}_1} & \mathcal{H}_B & \xrightarrow{\mathbf{j}_2} & \widehat{\mathcal{H}}_B \\ \mathbf{L}_{\max}\downarrow & & \downarrow B_{\max} & & \downarrow \widehat{B}_{\max} \\ \mathbf{H} & \xrightarrow{\mathbf{j}_1} & \mathcal{H}_B & \xrightarrow{\mathbf{j}_2} & \widehat{\mathcal{H}}_B \end{array}$$

which we use to construct a one-parameter family of self-adjoint realizations, called model B. The space $\mathcal{H}_B$ is a pre-Pontryagin space with negative index $\kappa = [(n-1)/2]$ obtained from $\mathbf{H}$ by equipping it with a new inner product. The mapping $\mathbf{j}_1$ is a bijection. The space $\widehat{\mathcal{H}}_B$ on the righthand side is the completion of $\mathcal{H}_B$ and $\mathbf{j}_2$ is the natural embedding. The operator $B_{\max}$ is the adjoint of a symmetric operator $B_{\min}$ and the self-adjoint extensions are considered as the self-adjoint realizations of the singular perturbation L_α in (1.2), but strictly speaking one should consider the closures of these operators in the space $\widehat{\mathcal{H}}_B$.

4.1. The space $\mathcal{H}_B$ and the operators $B_{\min}$ and B_θ

We define $\mathcal{H}_B$ as the inner product space $\mathcal{H}_B = \mathbb{C}^{n-2} \dot{+} \mathcal{H}_{n-2}$ with elements of the form

$$U = \begin{pmatrix}\vec{u}\\ u\end{pmatrix}, \quad \vec{u} \in \mathbb{C}^{n-2},\ u \in \mathcal{H}_{n-2},$$

and inner product

$$\langle U,V\rangle_B = \vec{v}^*\Gamma_\beta\vec{u} + \langle u,\vec{\varphi}\vec{v}\rangle + \langle\vec{\varphi}\vec{u},v\rangle + \langle u,v\rangle. \tag{4.1}$$

The matrix $\Gamma_\beta = (\beta_{j,k})_{j,k=1}^{n-2}$ is a non-degenerate Hermitian $(n-2)\times(n-2)$ matrix whose entries below the anti-diagonal are defined by

$$\beta_{j,k} := \langle\varphi_k,\varphi_j\rangle = \beta_{k,j}, \quad j,k = 2,3,\dots,n-2,\ j+k \ge n, \tag{4.2}$$

and the other entries will be specified later. We also set

$$\beta_{j,n-1} = \langle\varphi_{n-1},\varphi_j\rangle = \beta_{n-1,j}, j = 1,2,\dots,n-2,$$

so that by the resolvent identity we have

$$\beta_{j,k} = \beta_{j-1,k+1} + (a_{k+1}-a_j)\beta_{j,k+1}, \quad j,k = 2,3,\dots,n-2,\ j+k \ge n. \tag{4.3}$$

For later use we define the numbers

$$\beta_j := \beta_{1,j} + (a_1 - a_{j+1})\beta_{1,j+1}, \quad j = 1,2,\dots,n-2. \tag{4.4}$$

We restrict our considerations to the case where the entries of Γ_β are real. The inner product space $\mathcal{H}_B$ is not complete and therefore a pre-Pontryagin space and the identification mapping $\mathbf{j}_1 : \mathbf{H} \to \mathcal{H}_B$ defined by

$$\mathbf{j}_1(u + \vec{\varphi}\vec{u}) = \begin{pmatrix} \vec{u} \\ u \end{pmatrix}$$

is a continuous bijection but its inverse is not continuous. At a later stage we shall complete the space $\mathcal{H}_B$. The adjoint of a densely defined operator B in $\mathcal{H}_B$ relative to the inner product of $\mathcal{H}_B$ will be denoted by B^+:

$$B^+ = \{\{V, W\} \mid \langle V, BU\rangle_B - \langle W, U\rangle_B = 0, U \in \operatorname{dom} B\}.$$

The maximal operator $B_{\max}$ is defined by

$$\begin{aligned} B_{\max} &= \mathbf{j}_1 \mathbf{L}_{\max} \mathbf{j}_1^{-1} \\ &= \left\{ \left\{ \begin{pmatrix} \vec{u} \\ u_r + u_{n-1}\varphi_{n-1} \end{pmatrix}, \begin{pmatrix} \mathfrak{M}\vec{u} + u_{n-1}\vec{e}_{n-2} \\ Lu_r - a_{n-1}u_{n-1}\varphi_{n-1} \end{pmatrix} \right\} \mid \begin{matrix} \vec{u} \in \mathbb{C}^{n-2}, u_{n-1} \in \mathbb{C}, \\ u_r \in \mathcal{H}_n \end{matrix} \right\}. \end{aligned}$$

The operator $B_{\max}$ is densely defined. In fact, the set $\{0\} \oplus \mathcal{H}_n$ contained in its domain is already dense in $\mathcal{H}_B$: If $V \in \mathcal{H}_B$ is orthogonal to all elements $U \in \{0\} \oplus \mathcal{H}_n$, that is,

$$0 = \langle V, U\rangle_B = \langle \vec{\varphi}\vec{v} + v, u\rangle, \quad u \in \mathcal{H}_n,$$

then $\vec{\varphi}\vec{v} + v = 0$ and therefore, since the elements $\varphi_1, \dots, \varphi_{n-2}$ are linearly independent modulo $\mathcal{H}_{n-2}$, we have $\vec{v} = 0$ and $v = 0$, so $V = 0$.

Theorem 4.1. *The operator $B_{\max}^+$ is the restriction of $B_{\max}$ to all elements*

$$U = \begin{pmatrix} \vec{u} \\ u_r + u_{n-1}\varphi_{n-1} \end{pmatrix} \in \operatorname{dom} B_{\max}$$

which satisfy the three conditions

$$u_1 = 0, \quad P\left(\Gamma_\beta \mathfrak{M} - \mathfrak{M}^* \Gamma_\beta\right) P\vec{u} = 0, \quad F_\beta(U) = 0.$$

Here P is the orthogonal projection onto the subspace $\{\vec{e}_1\}^\perp$ of $\mathbb{C}^{n-2}$ and with β_j as in (4.4)

$$F_\beta(U) = \sum_{j=1}^{n-2} \beta_j u_{j+1} + \langle u_r, \varphi\rangle.$$

Moreover, $(B_{\max}^+)^+ = B_{\max}$ and $B_{\max}^+$ is a densely defined symmetric operator.

Proof. We have $\{X, Y\} \in B_{\max}^+$ if and only if for all $\vec{u} \in \mathbb{C}^{n-2}$, $u_{n-1} \in \mathbb{C}$ and $u_r \in \mathcal{H}_n$,

$$\left\langle \begin{pmatrix} \vec{x} \\ x \end{pmatrix}, \begin{pmatrix} \mathfrak{M}\vec{u} + u_{n-1}\vec{e}_{n-2} \\ Lu_r - a_{n-1}u_{n-1}\varphi_{n-1} \end{pmatrix} \right\rangle_B - \left\langle \begin{pmatrix} \vec{y} \\ y \end{pmatrix}, \begin{pmatrix} \vec{u} \\ u_r + u_{n-1}\varphi_{n-1} \end{pmatrix} \right\rangle_B = 0, \quad (4.5)$$

that is, if and only if

$$0 = Lx - y + L\vec{\varphi}\vec{x} - \varphi\vec{y}, \tag{4.6}$$

$$0 = \mathfrak{M}^*\Gamma_\beta\vec{x} + \langle x, \vec{\varphi}\mathfrak{M}\rangle - \Gamma_\beta\vec{y} - \langle y, \vec{\varphi}\rangle, \tag{4.7}$$

$$0 = \vec{e}^{\,*}_{n-2}\Gamma_\beta\vec{x} - \langle\vec{\varphi}\vec{x} + x, a_{n-1}\varphi_{n-1}\rangle + \langle x, \varphi_{n-2}\rangle - \langle\vec{\varphi}\vec{y} + y, \varphi_{n-1}\rangle. \tag{4.8}$$

These equalities were obtained from (4.5) by setting

$$\begin{array}{lll} \vec{u} = 0 & \text{and} & u_{n-1} = 0, \\ u_{n-1} = 0 & \text{and} & u_r = 0, \\ u_r = 0 & \text{and} & \vec{u} = 0, \end{array}$$

respectively. From (4.6) and

$$L\vec{\varphi} = \vec{\varphi}\mathfrak{M} + \varphi\vec{e}^{\,*}_1 \tag{4.9}$$

we obtain $0 = (Lx - y) + \vec{\varphi}(\mathfrak{M}\vec{x} - \vec{y}) + \varphi x_1$. If we write $x_{n-1} = -(\mathfrak{M}\vec{x} - \vec{y})_{n-2}$ and use that the elements $\varphi, \varphi_1, \ldots, \varphi_{n-3}$ are linearly independent modulo $\mathcal{H}_{n-4}$, we find that

$$x_1 = 0, \quad \vec{y} = \mathfrak{M}\vec{x} + x_{n-1}\vec{e}_{n-2}, \tag{4.10}$$

and $Lx - y = x_{n-1}\varphi_{n-2}$. This last equality can be written as

$$(L + a_{n-1})x = y + a_{n-1}x + x_{n-1}\varphi_{n-2},$$

which implies that

$$x = x_r + x_{n-1}\varphi_{n-1} \tag{4.11}$$

with

$$x_r = \frac{1}{L + a_{n-1}}\,(y + a_{n-1}x) \in \mathcal{H}_n$$

and

$$y = Lx_r - a_{n-1}x_{n-1}\varphi_{n-1}. \tag{4.12}$$

Hence $\{X, Y\} \in B_{\max}$. We substitute (4.10),(4.11), and (4.12) in (4.7) and use (4.9) and we obtain that

$$\begin{aligned} 0 &= (\mathfrak{M}^*\Gamma_\beta - \Gamma_\beta\mathfrak{M})\vec{x} + \langle x_r, \varphi\mathfrak{M} - L\vec{\varphi}\rangle \\ &\quad + x_{n-1}\{\langle\varphi_{n-1}, \vec{\varphi}(\mathfrak{M} + a_{n-1})\rangle - \Gamma_\beta\vec{e}_{n-2}\} \\ &= (\mathfrak{M}^*\Gamma_\beta - \Gamma_\beta\mathfrak{M})\vec{x} - \langle x_r, \varphi\rangle\vec{e}_1 + x_{n-1}(-\beta_{1,n-2} + (a_1 - a_{n-1})\beta_{1,n-1})\vec{e}_1. \end{aligned}$$

If we apply P to both sides and use that $x_1 = 0$ we get

$$P\left(\Gamma_\beta\mathfrak{M} - \mathfrak{M}^*\Gamma_\beta\right)P\vec{x} = 0$$

and if we take the inner product in $\mathbb{C}^{n-2}$ on both sides with $\vec{e}_1$ we see $F_\beta(X) = 0$. Finally, in the same way, if substitute (4.10), (4.11), and (4.12) in the righthand side of (4.8) and use (4.9) and (4.3) with $k = n-2$, we get after some calculations and cancellations that it is equal to

$$\langle\varphi_{n-1}, \vec{\varphi}(\mathfrak{M} + a_{n-1})\rangle - {\vec{e}_{n-2}}^{\,*}\Gamma_\beta\vec{x} = -\beta_{n-2}\,\vec{e}^{\,*}_1\vec{x}$$

and this equals 0 as $x_1 = 0$. In other words, (4.6) and (4.7) imply (4.8). The argument can easily be traced backwards to complete the proof that $B^+_{\max}$ is the restriction of $B_{\max}$ as stated in the theorem. That $(B^+_{\max})^+ = B_{\max}$ can be verified in a similar way and this is left to the reader. □

Recall that so far only the elements below the anti-diagonal of Γ_β have been specified, see (4.2). From now on we assume in addition that

$$P\left(\Gamma_\beta \mathfrak{M} - \mathfrak{M}^* \Gamma_\beta\right) P = 0. \tag{4.13}$$

Under this condition one of the three "boundary conditions" determining $B^+_{\max}$ as a restriction of $B_{\max}$ is always fulfilled. Together with the symmetry of the matrix Γ_β the matrix equality (4.13) is equivalent to the relations

$$\beta_{j,k-1} = \beta_{j-1,k} + (a_k - a_j)\beta_{j,k}, \quad j,k = 2,3,\ldots,n-2, j+k \leq n.$$

This implies that the not yet specified elements of Γ_β are completely determined by the elements of the first row, which we can choose arbitrarily. Since we want the matrix Γ_β to be real, we choose the entries $\beta_{1,1},\ldots,\beta_{1,n-1} \in \mathbb{R}$. Under these conditions on Γ_β we define the minimal operator

$$B_{\min} := B^+_{\max} = \{\{U, B_{\max}U\} \mid U \in \operatorname{dom} B_{\max}, u_1 = 0, F_\beta(U) = 0\}.$$

By Theorem 4.1 it is a densely defined symmetric operator on $\mathcal{H}_B$. The element

$$\Phi_B(z) = \begin{pmatrix} \vec{b}(z) \\ \dfrac{1}{L-z}\dfrac{b_{n-2}(z)}{b_{n-2}(L)}\varphi \end{pmatrix} \in \operatorname{dom} B_{\max}, \quad z \in \rho(L), \tag{4.14}$$

satisfies the equation

$$(B_{\max} - z)\Phi_B(z) = 0,$$

and so it is a defect element for $B_{\min}$. As in the A-model,

$$\Phi_B(z) = \mathbf{j}_1\,\varphi(z), \quad \varphi(z) = \frac{1}{L-z}\,\varphi \in \mathbf{H}.$$

Berezin's approach in [6] can be applied to describe all self-adjoint extensions B (self-adjoint in the sense $B^+ = B$) of $B_{\min}$ as a one-parameter family. Although $\mathcal{H}_B$ is a pre-Pontryagin space, the parametrization formula is the same as Krein's resolvent formula. To prepare for it we define a self-adjoint extension B_0 of $B_{\min}$, show that $\Phi_B(z)$ is a defect function for B_0 and construct a Q-function for $B_{\min}$ and B_0.
The self-adjoint extension B_0 of $B_{\min}$ which we choose to play the key role in the resolvent formula is given by

$$\operatorname{dom}\, B_0 = \{U \in \operatorname{dom}\, B_{\max} \,|\, u_1 = 0\}$$

and

$$B_0 \begin{pmatrix} 0 \\ u_2 \\ \vdots \\ u_{n-2} \\ u_r + u_{n-1}\varphi_{n-1} \end{pmatrix} = \begin{pmatrix} u_2 \\ u_3 - a_2 u_2 \\ \vdots \\ u_{n-1} - a_{n-2}u_{n-2} \\ Lu_r - a_{n-1}u_{n-1}\varphi_{n-1} \end{pmatrix}.$$

Then $B_{\min}$ can be interpreted as the one-dimensional restriction of B_0 to the domain

$$\{U \in \text{dom } B_0 \,|\, \langle (B_0 + a_1)U, \Phi_B(-a_1)\rangle_B = 0\}$$

Note that

$$\Phi_B(-a_1) = \begin{pmatrix} \vec{e}_1 \\ 0 \end{pmatrix}.$$

We have $\rho(B_0) = \rho(L)$ and, for z in this set, $\Phi_B(z)$ in (4.14) can be represented as

$$\Phi_B(z) = \Phi_B(-a_1) + (z + a_1)\frac{1}{B_0 - z}\,\Phi_B(-a_1).$$

This implies the Hilbert identity

$$\Phi_B(z) - \Phi_B(\zeta) = (z - \zeta)\frac{1}{B_0 - z}\,\Phi_B(\zeta),$$

which together with the property $\Phi_B(z) \in \ker\,(B_{\max} - z)$ yield that $\Phi_B(z)$ is a defect function and

$$Q_B(z) = (z + a_1)\,\langle \Phi_B(z), \Phi_B(-a_1)\rangle_B\,, \tag{4.15}$$

is a Q–function for $B_{\min}$ and B_0. Note that $Q_B(z)$ is normalized by the condition $Q_B(-a_1) = 0$. Substituting the coordinates of $\Phi_B(z)$ in (4.15) we obtain that

$$Q_B(z) = b_{n-2}(z)\left\langle \frac{z + a_{n-1}}{L - z}\,\varphi, \frac{1}{b_{n-1}(L)}\,\varphi\right\rangle + p_{n-2}(z),$$

where with β_j as in (4.4) the polynomial $p_{n-2}(z)$ is given by

$$p_{n-2}(z) = \sum_{j=1}^{n-2} \beta_j b_j(z).$$

Using B_0, $\Phi_B(z)$ and $Q_B(z)$ we can now formulate the Berezin-Krein theorem which describes all self-adjoint extensions of $B_{\min}$ as a one-parameter family. The proof is similar to that of Theorem 3.3 and is therefore omitted.

Theorem 4.2. (i) *The relation*

$$\frac{1}{B_\theta - z} = \frac{1}{B_0 - z} - \frac{1}{Q_B(z) + \cot\theta}\,\langle\,\cdot\,, \Phi_B(z^*)\rangle_B \Phi_B(z).$$

defines a one-to-one correspondence between all self-adjoint extensions B_θ of $B_{\min}$ in $\mathcal{H}_B$ and the numbers $\theta \in [0, \pi)$.
(ii) *The self-adjoint operator B_θ is the restriction of $B_{\max}$ described by the formula*

$$B_\theta = \{\{U, B_{\max}U\} \mid U \in \operatorname{dom} B_{\max},\ \sin\theta F_\beta(\mathbf{U}) = -\cos\theta\, u_1\}. \tag{4.16}$$

The analogs of the formulas following Theorem 3.3 are

$$B_{\max} = B_0 \dot{+} \text{span}\,\{\Phi_B(-a_1), -a_1\Phi_B(-a_1)\}$$

and

$$\begin{aligned} B_\theta &= \{\{U + u_1\Phi_B(-a_1), B_0U - a_1u_1\Phi_B(-a_1)\} \mid U \in \operatorname{dom} B_0, \\ &\quad u_1 \in \mathbb{C},\ \langle (B_0 + a_1)U, \Phi_B(-a_1)\rangle_B = -u_1 \cot\theta\}\,. \end{aligned}$$

4.2. Compressions of the resolvent of B_θ

The following formula for the skew-compressed resolvent is valid

$$\mathbf{j}_1^{-1} \frac{1}{B_\theta - z}|_{\mathcal{H}_{n-2}} = \frac{1}{L-z} - \frac{1}{Q_B(z) + \cot\theta} \left\langle \cdot\,, \frac{1}{L-z^*}\,\varphi \right\rangle \frac{1}{L-z}\,\varphi,$$

which is an analog of formula (3.13).

The formula for the compression of the resolvent $\frac{1}{B_\theta - z}$ to the subspace $\mathcal{H}_{n-2} \subset \mathcal{H}_B$ reads as follows:

$$\begin{aligned} P_{\mathcal{H}_{n-2}} \frac{1}{B_\theta - z}|_{\mathcal{H}_{n-2}} &= \frac{1}{L-z} \\ &- \frac{1}{\left\langle \dfrac{z + a_{n-1}}{(L-z)b_{n-1}(L)}\,\varphi, \varphi \right\rangle + \dfrac{p_{n-2}(z) + \cot\theta}{b_{n-2}(z)}} \left\langle \cdot\,, \frac{1}{L-z^*}\,\varphi \right\rangle \frac{1}{L-z}\,\varphi_{n-2}. \end{aligned}$$

It implies that the spectral problem for the operator B_θ is equivalent to the following explicit eigenvalue depending "boundary value" problem:

$$\begin{aligned} (L-z)u &= c\varphi_{n-1}, \quad u \in \mathcal{H}_n,\ c \in \mathbb{C}, \\ b_{n-1}(z)\langle u, \varphi\rangle &= -c\,(p_{n-2}(z) + \cot\theta)\,. \end{aligned}$$

4.3. Pontryagin space completion and the self-adjoint realizations $\widehat{B}_\theta$

We set $\kappa = [(n-1)/2]$. The inner product (4.1) on $\mathcal{H}_B$ can be written also in the form

$$\begin{aligned} \left\langle \begin{pmatrix} \vec{u} \\ u \end{pmatrix}, \begin{pmatrix} \vec{v} \\ v \end{pmatrix} \right\rangle_B &= \left\langle \begin{pmatrix} \vec{u}\,' \\ P_\kappa \vec{u} \end{pmatrix}, \begin{pmatrix} 0 & I_{\mathbf{C}^\kappa} \\ I_{\mathbf{C}^\kappa} & \{\beta_{j,k}\}_{j,k=1}^\kappa \end{pmatrix} \begin{pmatrix} \vec{v}\,' \\ P_\kappa \vec{v} \end{pmatrix} \right\rangle_{\mathbb{C}^\kappa \oplus \mathbb{C}^\kappa} \\ &\quad + \left\langle (u + \textstyle\sum_{j=\kappa+1}^{n-2} u_j\varphi_j), (v + \sum_{j=\kappa+1}^{n-2} v_j\varphi_j) \right\rangle, \end{aligned} \tag{4.17}$$

where

$$P_\kappa \vec{u} = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_\kappa \end{pmatrix},$$

$$\begin{aligned} \vec{u}\,' &= \sum_{j=1}^{\kappa} \left(\langle u, \varphi_j\rangle + \sum_{k=\kappa+1}^{n-2} u_k\beta_{j,k} \right) \vec{e}_j, \\ \vec{v}\,' &= \sum_{j=1}^{\kappa} \left(\langle v, \varphi_j\rangle + \sum_{k=\kappa+1}^{n-2} v_k\beta_{j,k} \right) \vec{e}_j, \end{aligned}$$

and $\vec{e}_1, \dots, \vec{e}_\kappa$ now stand for the standard basis in $\mathbb{C}^\kappa$. As the Gram matrix in the first inner product in (4.17) has κ negative eigenvalues, the inner product on $\mathcal{H}_B$ has κ negative squares. The Pontryagin space completion of $\mathcal{H}_B$ with respect to this inner product is the Pontryagin space $\widehat{\mathcal{H}}_B = (\mathbb{C}^\kappa \dot{+} \mathbb{C}^\kappa) \oplus \mathcal{H}$ with inner product, still be denoted by $\langle \cdot, \cdot \rangle_B$, defined by Gram operator

$$G_B = \begin{pmatrix} 0 & I_{\mathbf{C}^\kappa} \\ I_{\mathbf{C}^\kappa} & \{\beta_{j,k}\}_{j,k=1}^\kappa \end{pmatrix} \oplus I_{\mathcal{H}}.$$

The natural isometric embedding $\mathbf{j}_2$ from $\mathcal{H}_B$ into its completion $\widehat{\mathcal{H}}_B$ is described by the formula

$$\mathbf{j}_2 \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-2} \\ u \end{pmatrix} = \begin{pmatrix} \left(\langle u, \varphi_j \rangle + \sum_{k=\kappa+1}^{n-2} u_k \beta_{j,k} \right)_{j=1}^\kappa \\ (u_j)_{j=1}^\kappa \\ u + \sum_{j=\kappa+1}^{n-2} u_j \varphi_j \end{pmatrix}.$$

The results proved for the operators in the pre-Pontryagin space $\mathcal{H}_B$ can be carried over to the closures of these operators in the Pontryagin space $\widehat{\mathcal{H}}_B$; see [31, 17, 13].

Theorem 4.3. (i) *The closure $\widehat{B}_{\min}$ of $\mathbf{j}_2\, B_{\min}\, \mathbf{j}_2^{-1}$ in $\widehat{\mathcal{H}}_B$ is a non-densely defined symmetric operator with defect indices $(1,1)$. Its adjoint $\widehat{B}_{\max}$ is the closure of $\mathbf{j}_2\, B_{\max}\, \mathbf{j}_2^{-1}$ in $\widehat{\mathcal{H}}_B$.*
(ii) *The closure $\widehat{B}_0$ of $\mathbf{j}_2\, B_0\, \mathbf{j}_2^{-1} in \widehat{\mathcal{H}}_B$ is a self-adjoint relation with multi-valued part $\widehat{B}_0(0) = \mathrm{span}\, \{0 \oplus \vec{e}_1 \oplus 0\}$. It is an extension of $\widehat{B}_{\min}$.*
(iii) *The function $\mathbf{j}_2\, \Phi_B(z)$ is the defect function and the function*

$$Q_B(z) = (z + a_1) \langle \Phi_B(z), \Phi_B(-a_1) \rangle_B$$

is the Q-function for the operators $\widehat{B}_{\min}$ and $\widehat{B}_0$.
(iv) *The formula*

$$\frac{1}{\widehat{B}_\theta - z} = \frac{1}{\widehat{B}_0 - z} - \frac{1}{Q_B(z) + \cot\theta} \langle \cdot, \mathbf{j}_2\, \Phi_B(z^*) \rangle_B\, \mathbf{j}_2\, \Phi_B(z).$$

gives a one-to-one correspondence between all selfadjoint extensions $\widehat{B}_\theta$ of $\widehat{B}_{\min}$ in $\widehat{\mathcal{H}}_B$ and $\theta \in [0, \pi)$. Each $\widehat{B}_\theta$ is the closure of $\mathbf{j}_2\, B_\theta\, \mathbf{j}_2^{-1}$ in $\widehat{\mathcal{H}}_B$.

4.4. On properties of the function $Q_B(z)$

The function $Q_B(z)$ is a generalized Nevanlinna function which belongs to the class N_κ, $\kappa = [(n-1)/2]$. More precisely, $Q_B(z)$ belongs to the subclass $N_\kappa^\infty \subset N_\kappa$ considered in [13]: N_κ^∞ consists of the functions $Q(z) \in N_\kappa$ which are holomorphic on $\mathbf{C} \setminus \mathbf{R}$ and admit the representation

$$Q(z) = (z+1)^{2\kappa} Q_0(z) + p_{2\kappa-1}(z), \tag{4.18}$$

where $Q_0(z) \in N_0$,

$$\lim_{y\to\infty} \frac{\operatorname{Im} Q_0(iy)}{y} = 0, \quad \lim_{y\to\infty} y\operatorname{Im}Q_0(iy) = \infty,$$

and $p_{2\kappa-1}(z)$ is a real polynomial of degree at most $2\kappa - 1$.
In this case, since L is a nonnegative operator, one can say more, see [14]: The function $Q_0(z)$ is holomorphic on $\mathbf{C}\backslash\mathbf{R}^+$ and its asymptotic behavior at $-\infty$ along the negative real axis is given by

$$\lim_{x\to-\infty} Q_0(x) = \begin{cases} 0, & \text{if } n \text{ is odd,} \\ -\infty, & \text{if } n \text{ is even.} \end{cases}$$

Writing $Q_B(z) + \cot\theta$ in the form (4.18):

$$Q_B(z) + \cot\theta = (z+1)^{2\kappa} Q_0(z) + p_{2\kappa-1}(z),$$

one can show that

$$Q_0(z) = \begin{cases} \left\langle \dfrac{1}{(L-z)(L+1)^\kappa}\,\varphi, \dfrac{1}{(L+1)^\kappa}\,\varphi \right\rangle, & \text{if } n \text{ is odd,} \\[2ex] \left\langle \dfrac{z+1}{(L-z)(L+1)^\kappa}\,\varphi, \dfrac{1}{(L+1)^{\kappa+1}}\,\varphi \right\rangle + g_{2\kappa+1}, & \text{if } n \text{ is even,} \end{cases}$$

is independent of θ and

$$p_{2\kappa-1}(z) = \sum_{j=0}^{2\kappa-1} g_{j+1}(z+1)^j.$$

Here

$$g_1 = Q_B(-1) + \cot\theta, \quad g_k = \frac{1}{(k-1)!}\, Q_B^{(k-1)}(-1),\ k = 2, 3, \dots, 2\kappa+1,$$

and by calculating the derivatives these numbers can be expressed in terms of the normalization points a_j and the parameters $\beta_{1,j}$, $j = 1, 2, \dots, n-2$.

4.5. Compression of the resolvent of $\widehat{B}_\theta$

The function $Q_B(z)$ admits not only the representation (4.18) but also the representation (see [13, Section 6], where the relations between various representations are described):

$$Q_B(z) = b_\kappa(z)^2\, \widehat{Q}_0(z) + \widehat{p}_{2\kappa-1}(z), \tag{4.19}$$

with Nevanlinna function

$$\widehat{Q}_0(z) = \begin{cases} \left\langle \dfrac{1}{(L-z)b_\kappa(L)}\,\varphi, \dfrac{1}{b_\kappa(L)}\,\varphi \right\rangle, & n = 2\kappa+1, \\[2ex] \left\langle \dfrac{z+a_{\kappa+1}}{(L-z)b_\kappa(L)}\,\varphi, \dfrac{1}{b_{\kappa+1}(L)}\,\varphi \right\rangle + \beta_{\kappa+1,\kappa}, & n = 2\kappa+2, \end{cases}$$

and polynomial

$$\widehat{p}_{2\kappa-1}(z) = \sum_{j=1}^{\kappa} \beta_{1,j}(z+a_1)b_{j-1}(z) + \sum_{j=2}^{\kappa} \beta_{\kappa,j} b_{j-1}(z) b_\kappa(z).$$

Then by Krein's formula in Theorem 4.2 (i), the formula for the compression of the resolvent of $\widehat{B}_\theta$ to $\mathcal{H}$ takes the form

$$P_{\mathcal{H}} \frac{1}{\widehat{B}_\theta - z}|_{\mathcal{H}} = \frac{1}{L-z} - \frac{1}{\widehat{Q}_0(z) + \tau_\theta(z)} \left\langle \cdot\,, \frac{1}{L-z^*}\,\widehat{\varphi} \right\rangle \frac{1}{L-z}\,\widehat{\varphi},$$

where $\widehat{\varphi} := \dfrac{1}{b_\kappa(L)}\,\varphi$, and

$$\tau_\theta(z) := \frac{\widehat{p}_{2\kappa-1}(z) + \cot\theta}{b_\kappa(z)^2}.$$

This compressed resolvent is a generalized resolvent of the one-dimensional restriction of L in $\mathcal{H}$:

$$\widehat{B}_{\min} := \{\{u, Lu\} \mid u \in \mathcal{H}_2, \langle u, \widehat{\varphi}\rangle = 0\}.$$

The adjoint of this restriction is given by

$$\widehat{B}_{\max} := \widehat{B}^*_{\min} = \left\{ \left\{ u + c\frac{1}{L+a_{\kappa+1}}\,\widehat{\varphi}, Lu - c\frac{a_{\kappa+1}}{L+a_{\kappa+1}}\,\widehat{\varphi} \right\} \mid u \in \mathcal{H}_2,\, c \in \mathbb{C} \right\}.$$

It implies that the spectral problem for the operator $\widehat{B}_\theta$ is equivalent to the following explicit eigenvalue depending "boundary value" problem in $\mathcal{H}$:

$$\begin{aligned} (L-z)u &= c\frac{1}{L+a_{\kappa+1}}\,\varphi, \quad u \in \mathcal{H}_2,\ c \in \mathbb{C}, \\ (z+a_{\kappa+1})\langle u, \widehat{\varphi}\rangle &= -c(\widehat{Q}_0(-a_{\kappa+1}) + \tau_\theta(z)). \end{aligned}$$

5. Comparison of the models

Evidently, there is a close relation between the A- and B- models. The aim of this section is to describe what the two have in common and to point out their differences. Among other things we discuss the dependence of the models on the parameters and compare aspects of the negative point spectra of the self-adjoint operators.

5.1. Minimality of the models

The operator representations of the functions $Q_A(z)$ and $Q_B(z)$ in the models are unique up to unitary equivalence if

$$\mathcal{H}_A = \overline{\operatorname{span}}\,\{\Phi_A(z) \mid z \in \rho(L)\}$$

and

$$\widehat{\mathcal{H}}_B = \overline{\operatorname{span}}\,\{\mathbf{j}_2\Phi_B(z) \mid z \in \rho(L)\},$$

respectively. These minimality conditions can be achieved simultaneously by requiring that the interaction is cyclic with respect to L, that is,

$$\mathcal{H} = \overline{\text{span}} \left\{ \frac{1}{(L-z)b_{n-1}(L)} \varphi \mid z \in \rho(L) \right\}.$$

This implies also that

$$\mathbf{H} = \overline{\text{span}} \left\{ \frac{1}{L-z} \varphi \mid z \in \rho(L) \right\}.$$

5.2. The parameters of the models

We first list the parameters used in the two models:

Model A :
- the normalization points $a_1, a_2, ..., a_{n-1}$,
- the real numbers $\alpha_{1,n-2}, \alpha_{2,n-2}, ..., \alpha_{n-2,n-2}$ in the last column of Γ_α,
- the self-adjoint extension parameter $\theta_A \in [0, \pi)$.

Model B:
- the normalization points $a_1, a_2, ..., a_{n-1}$,
- the real numbers $\beta_{1,1}, \beta_{1,2}, ..., \beta_{1,n-2}$ in the first row of Γ_β,
- the self-adjoint extension parameter $\theta_B \in [0, \pi)$.

For a given set of normalization points the other parameters are independent and parameterize the models in an unique way. Therefore the two models will be compared in the case where the sets of normalization points are the same.

Since the functions in the denominators in Krein's formulas determine the corresponding operators uniquely up to a unitary transformation, it is enough to compare these two functions

$$Q_A(z) + \cot \theta_A \quad \text{and} \quad Q_B(z) + \cot \theta_B.$$

Indeed, for $\theta \neq 0$, the functions

$$-\frac{1}{Q_A(z) + \cot \theta}, \quad -\frac{1}{Q_B(z) + \cot \theta}$$

are the Q-functions of A_θ and $A_{\min}$ and B_θ and $B_{\min}$ respectively. It is more convenient to compare the following two functions instead:

$$\begin{aligned} &b_{n-2}(z) \left(Q_A(z) + \cot \theta_A \right) \\ &\quad = b_{n-2}(z) \left\langle \frac{z + a_{n-1}}{L-z} \varphi, \frac{1}{b_{n-1}(L)} \varphi \right\rangle - \sum_{k=1}^{n-2} \alpha_{k,n-2} b_{k-1}(z) - \alpha b_{n-2}(z), \end{aligned} \tag{5.1}$$

where

$$\alpha = \cot \theta_A + \sum_{k=1}^{n-2} \alpha_{k,n-2} \frac{b_{k-1}(-a_{n-1})}{b_{n-2}(-a_{n-1})},$$

and

$$Q_B(z) + \cot\theta_B \tag{5.2}$$
$$= b_{n-2}(z)\left\langle \frac{z+a_{n-1}}{L-z}\,\varphi, \frac{1}{b_{n-1}(L)}\,\varphi\right\rangle + \sum_{k=1}^{n-2} \beta_j b_j(z) + \cot\theta_B.$$

These two functions coincide if and only if the parameters are related as follows

$$\begin{pmatrix} \cot\theta_B \\ \beta_1 \\ \vdots \\ \beta_{n-3} \\ \beta_{n-2} \end{pmatrix} = \operatorname{diag}\,(-1,-1,\dots,-1,1)\begin{pmatrix} \alpha_{1,n-2} \\ \alpha_{2,n-2} \\ \vdots \\ \alpha_{n-2,n-2} \\ \cot\theta_A \end{pmatrix}. \tag{5.3}$$

Recall that the numbers β_j, $j = 1, 2, \dots, n-2$ given by (4.4). This formula shows that there is a one-to-one correspondence between these numbers and the $n-2$ entries of the first row of the matrix Γ_β:

$$\begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_{n-3} \\ \beta_{n-2} \end{pmatrix} = \begin{pmatrix} 1 & a_1-a_2 & \dots & 0 & 0 \\ 0 & 1 & \ddots & & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & & \ddots & 1 & a_1-a_{n-3} \\ 0 & 0 & \dots & 0 & 1 \end{pmatrix}\begin{pmatrix} \beta_{1,1} \\ \beta_{1,2} \\ \vdots \\ \beta_{1,n-3} \\ \beta_{1,n-2} \end{pmatrix} + \beta_{1,n-1}\begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ a_1-a_{n-1} \end{pmatrix}. \tag{5.4}$$

In the last summand on the righthand side

$$\beta_{1,n-1} = \langle \frac{1}{b_{n-1}(L)}\,\varphi, \frac{1}{L+a_1}\,\varphi\rangle$$

and, since the matrix in (5.4) is invertible, the formulas (5.3) and (5.4) describe a one-to-one correspondence between the parameters in the models A and B, except in the cases where $\theta_A = 0$ or $\theta_B = 0$. In these exceptional cases, the self-adjoint operator A_0 has no counterpart in the B-model and the self-adjoint relation $\widehat{B}_0$ has no counterpart in the A-model.

Theorem 5.1. *Assume that the normalization points in the A- and B-models are the same and that the parameters $\alpha_{j,n-2}$ and $\theta_A \neq 0$ and the parameters $\beta_{1,j}$'s and $\theta_B \neq 0$ of the two models are related by the equations* (5.3)*and* (5.4)*. Then the identification map $T = \mathbf{j}_1\,\mathbf{i} : \mathcal{H}_A \to \mathcal{H}_B$ intertwines the self -adjoint operators A_{θ_A} in Theorem* 3.3 *and B_{θ_B} in Theorem* 4.2*:*

$$B_{\theta_B}T = TA_{\theta_A}. \tag{5.5}$$

Remark 5.2. If we provide $\mathcal{H}_B$ with a new norm that makes $\mathbf{j}_1$ an isomorphism, then the operators $B_{\max}$ and its self-adjoint restrictions are closed, T is a similarity operator, that is, bounded and boundedly invertible, and the intertwining relation (5.5) shows that the operators A_{θ_A} and B_{θ_B} are similar.

Proof of Theorem 5.1. By definition,

$$TA_{\max} = \mathbf{j}_1 \mathbf{L}_{\max} \mathbf{i} = B_{\max} T.$$

The relations (5.3) and (5.4) readily imply $T \operatorname{dom} A_{\theta_A} \subset \operatorname{dom} B_{\max}$ and that the restriction (3.11) describing A_{θ_A} which can be written as

$$\langle u_r, \varphi \rangle + \cot \theta_A \, u_{n-1} - \sum_{j=1}^{n-2} \alpha_{j,n-2} u_j = 0$$

is equivalent to the restriction

$$\langle u_r, \varphi \rangle + \sum_{k=1}^{n-2} \beta_j u_{j+1} + \cot \theta_B \, u_1 = 0$$

in the formula for (4.16) for B_{θ_B}. Hence $T \operatorname{dom} A_{\theta_A} = \operatorname{dom} B_{\theta_B}$, and now the intertwining formula (5.5) easily follows. □

5.3. The spectra of the realizations

Assume the conditions of Theorem 5.1 and assume that φ is a cyclic generalized element for L. Then Theorem 5.1 implies that

$$\rho(A_{\theta_A}) = \rho(B_{\theta_B}), \quad \sigma_c(A_{\theta_A}) = \sigma_c(B_{\theta_B}), \quad \sigma_p(A_{\theta_A}) = \sigma_p(B_{\theta_B}).$$

As the resolvent $(\widehat{B}_{\theta_B} - z)^{-1}$, $z \in \rho(B_{\theta_B})$, coincides with the closure in $\widehat{\mathcal{H}}_B$ of the resolvent $(B_{\theta_B} - z)^{-1}$ it follows that $\rho(\widehat{B}_{\theta_B}) = \rho(B_{\theta_B})$, and, therefore the spectra of $\widehat{B}_{\theta_B}$ and B_{θ_B} coincide. Also for the essential spectrum of $\widehat{B}_{\theta_B}$ we have the equalities

$$\sigma_{\text{ess}}(\widehat{B}_{\theta_B}) = \sigma_{\text{ess}}(\widehat{B}_0) = \sigma_{\text{ess}}(L) = \sigma_{\text{ess}}(A_0) = \sigma_{\text{ess}}(A_{\theta_A}),$$

and hence $\sigma_{\text{ess}}(\widehat{B}_{\theta_B}) \subset \overline{\mathbb{R}^+}$. These equalities follow from the fact that the resolvents of A_{θ_A} and $\widehat{B}_{\theta_B}$ are rank one perturbations of the resolvents of A_0 and $\widehat{B}_0$, respectively. Hence the parts in $\mathbb{C} \setminus \overline{\mathbb{R}^+}$ of $\sigma(\widehat{B}_{\theta_B})$ and $\sigma(A_{\theta_A})$ are the same. Recall that for $\theta_A, \theta_B \neq 0$,

$$-\left(Q_A(z) + \cot \theta_A\right)^{-1} = -b_{n-2}(z) \left(Q_B(z) + \cot \theta_B\right)^{-1} \tag{5.6}$$

where the functions

$$-\left(Q_A(z) + \cot \theta_A\right)^{-1}, \quad -\left(Q_B(z) + \cot \theta_B\right)^{-1} \tag{5.7}$$

are the Q-functions of A_{θ_A} and $A_{\min}$ and $\widehat{B}_{\theta_B}$ and $B_{\min}$, respectively, which determine the extensions A_{θ_A} and $\widehat{B}_{\theta_B}$ up to unitary equivalence. We apply to both sides of (5.6) Langer's criterion [23, Theorem 1], which characterizes the eigenvalues of non-positive and positive type of A_{θ_A} and $\widehat{B}_{\theta_B}$ in terms of certain non-tangential limits for the generalized Nevanlinna functions in (5.7); the multiplier $b_{n-2}(z)$ on the righthand side of (5.6) plays no role in these limits, because $b_{n-2}(x) > 0$ for $x \geq 0$. We obtain that the eigenvalues of non-positive (positive) type of $\widehat{B}_{\theta_B}$ in

$\overline{\mathbb{R}^+}$ are the eigenvalues of non-positive type (positive type, respectively) of A_{θ_A}. It follows that the continuous and point spectra of A_{θ_A} and $\widehat{B}_{\theta_B}$ coincide:

$$\sigma_c(A_{\theta_A}) = \sigma_c(\widehat{B}_{\theta_B}), \quad \sigma_p(A_{\theta_A}) = \sigma_p(\widehat{B}_{\theta_B}).$$

We consider the case where $\mathcal{H}_A$ is a Hilbert space in more detail.

Theorem 5.3. *Assume that the normalization points are mutually different and ordered such that* $0 < a_1 < a_2 < \ldots < a_{n-2}$, $\Gamma_\alpha > 0$, *and that the conditions of Theorem* 5.1 *hold. Then* $\sigma_p(A_{\theta_A}) = \sigma_p(\widehat{B}_{\theta_B})$ *contains at least* $n-2$ *simple eigenvalues* z_j *with* $-a_{j+1} < z_j < -a_j$, $j = 1, 2, \ldots, n-3$ *and* $z_{n-2} < a_{n-2}$. *The ones with an even index are of positive type and those with an odd index are of negative type for the operator* $\widehat{B}_\theta$.

Proof. The function $Q_A(z)$ is a Nevanlinna function of the form

$$Q_A(z) = \left\langle \frac{z + a_{n-1}}{L - z}\,\varphi, \frac{1}{b_{n-1}(L)}\,\varphi \right\rangle - \sum_{j=1}^{n-2} \frac{\sigma_j}{z + a_j},$$

which has only real zeros. Introduce the disjoint intervals

$$I_{n-2} = (-\infty, -a_{n-2}), I_{n-3} = (-a_{n-2}, -a_{n-3}), \ldots, I_1 = (-a_2, -a_1).$$

As each point $-a_j$, $j = 1, 2, \ldots, n-2$ is a pole of the function $Q_A(z) + \cot\theta_A$ and $\lim_{x\to-\infty} Q_A(x) = -\infty$, this function has exactly one zero, say z_j, in each interval I_j, $j = 1, 2, \ldots, n-2$. Hence $\sigma_p(A_{\theta_A}) = \sigma_p(\widehat{B}_{\theta_B})$ contains at least $n-2$ negative simple eigenvalues, namely $z_1, z_2, \ldots, z_{n-2}$. We prove that for the generalized Nevanlinna function $Q_B(z) + \cot\theta_B$ the zeros z_{2k} with even index are zeros of positive type and the exactly κ zeros z_{2k-1} with odd index are zeros of negative type, $k = 1, 2, \ldots, [(n-2)/2]$. Indeed, since $z_1, z_2, \ldots, z_{n-2}$ are simple eigenvalues of $\widehat{B}_{\theta_B}$ and by [13, Theorem 3.3], the vectors $\mathbf{j}_2\Phi_B(z_1), \mathbf{j}_2\Phi_B(z_2), \ldots, \mathbf{j}_2\Phi_B(z_{n-2})$ are the corresponding eigenvectors and

$$\langle \mathbf{\Phi}_B(z_j), \mathbf{\Phi}_B(z_j)\rangle_B = Q'_B(z_j),$$

where $Q'_B(z)$ means derivative of $Q_B(z)$ in z. According to (5.1) and (5.2),

$$Q'_B(z_j) = \prod_{k=1}^{j} (a_k - z_j) \prod_{k=j+1}^{n-2} (a_k - z_j)\, Q'_A(z_j).$$

As $Q_A(z) \in N_0$ we have that $Q'_A(z_j) > 0$ for $j = 1, 2, \ldots, n-2$. Since $z_j < -a_j$, the second product is positive and the first product is positive, if j is even, and it is negative, if j is odd. □

Further, according to a theorem of L.S. Pontryagin each self-adjoint operator B in Pontryagin space Π_κ with κ negative squares has a κ–dimensional non-positive invariant subspace $\mathcal{M}(B)$ such that the spectrum $\sigma(B|_{\mathcal{M}(B)})$ of the restriction of B to $\mathcal{M}(B)$ is in the closed upper half plane. In the case of the Theorem 5.3,

$$\mathcal{M} = \operatorname{span}\{\mathbf{j}_2\Phi_B(z_1), \mathbf{j}_2\Phi_B(z_3), \ldots, \mathbf{j}_2\Phi_B(z_{2\kappa-1})\}$$

and the space $\widehat{\mathcal{H}}_B$ admits the orthogonal decomposition

$$\widehat{\mathcal{H}}_B = \mathcal{H}_+ \oplus \mathcal{M}, \tag{5.8}$$

where $\mathcal{H}_+$ is a $\widehat{B}_{\theta_B}$–invariant Hilbert subspace of $\widehat{\mathcal{H}}_B$. The restriction $B_+ := \widehat{B}_{\theta_B}\,|_{\mathcal{H}_+}$ is a self-adjoint operator in $\mathcal{H}_+$ and describes the Hilbert space part of the B-model. This operator is not similar to A_{θ_A}, since

$$\sigma(B_+) = \sigma(A_{\theta_A}) \setminus \{z_1, z_3, \ldots, z_{2\kappa-1}\}.$$

The paper concerns the realization problem for highly singular perturbations and we describe two different models: A and B. In the situation of Theorem 5.3 the A-model is a Hilbert space realization and the B-model is a Pontryagin realization. The negative type spectrum of $\widehat{B}_{\theta_B}$ in the B-model consists of simple isolated eigenvalues and hence $\widehat{B}_{\theta_B}$ is similar to a Hilbert space operator. In fact, the decomposition (5.8) implies that the operator $\widehat{B}'_{\theta_B} := \widehat{B}_{\theta_B}|_{\mathcal{H}_+} \oplus \widehat{B}_{\theta_B}|_{\mathcal{M}}$ is self-adjoint in the space $\widehat{\mathcal{H}}_B$ equipped with the positive scalar product

$$\langle\,\cdot\,,\,\cdot\,\rangle' = \langle\,\cdot\,,\,\cdot\,\rangle_{\mathcal{H}_+} - \langle\,\cdot\,,\,\cdot\,\rangle_{\mathcal{M}},$$

which makes it a Hilbert space. The operator $\widehat{B}'_{\theta_B}$ however, is not a solution of the realization problem and, from the point of view of scattering theory, its restriction to $\mathcal{H}_+$, that is, the operator B_+ considered above, is the more appropriate Hilbert space operator.

6. Examples

Here we illustrate the main points in the correspondence between the A-model and the B-model in the simplest cases when $\varphi \in \mathcal{H}_{-n} \setminus \mathcal{H}_{-n+1}$ with $n = 3$ and $n = 4$. Concrete examples with $n = 3$ are point-like perturbations of the Laplacian $L = -\Delta$ in $\mathcal{H} = L^2(\mathbb{R}^4)$ and $\mathcal{H} = L^2(\mathbb{R}^5)$ with the interaction $\varphi = \delta(x)$. Then the regularized Q–functions are of the form

$$Q(z) = -\frac{1}{16\pi^2}\, z \ln\,(-z) + c_1 z + c_0,$$

and

$$Q(z) = \frac{1}{24\pi^2}(-z)^{3/2} + c_1 z + c_0,$$

respectively, with real parameters c_0, c_1.
Examples with $n = 4$ are point-like perturbations of $L = -\Delta$ in $\mathcal{H} = L^2(\mathbb{R}^6)$ and $\mathcal{H} = L^2(\mathbb{R}^7)$ also with the interaction $\varphi = \delta(x)$. Now the regularized Q–functions are

$$Q(z) = -\frac{1}{128\pi^3}\, z^2 \ln\,(-z) + c_2 z^2 + c_1 z + c_0,$$

and

$$Q(z) = -\frac{1}{240\pi^3}(-z)^{5/2} + c_2 z^2 + c_1 z + c_0,$$

respectively, where c_0, c_1, c_2 are real parameters. In all four cases the functions $Q(z)$ are generalized Nevanlinna functions from the class N_1^∞, that is, with 1 negative square and with the only one pole of non-positive type at $z = \infty$.

6.1. Derivation of the formulas

For $d = 1, 2, \ldots$, let L be the self-adjoint realization of the Laplacian $-\Delta$ in $\mathcal{H} = L^2(\mathbb{R}^d)$ and let $\varphi = \delta(x)$. Observe that $\varphi \in \mathcal{H}_{-n} \setminus \mathcal{H}_{1-n}$, where $n = 2 + [(d-2)/2]$. This can be checked by using the spectral representation of L in $L^2(\mathbb{R}^+) \otimes L^2(S_{d-1})$ (S_{d-1} denotes the unit sphere in $\mathbb{R}^d$), where L is realized as the operator of multiplication by the independent variable, say λ, and $\varphi = \delta(x)$ is represented by the function

$$\widetilde{\varphi}(\lambda) = \left(\frac{1}{2^d \pi^{d/2} \Gamma(d/2)} \right)^{1/2} \lambda^{(d-2)/4}.$$

Here $\Gamma(\lambda)$ is the Euler gamma-function. Applying the regularization procedure from Subsection 1.4 with equal normalization points $a_1 = a_2 = \ldots = a_{n-1} = a > 0$ to the formal expression $\langle \frac{1}{L-z} \varphi, \varphi \rangle$, we obtain the regularization

$$Q(z) = (z+a)^{n-1} \left\langle \frac{1}{L-z}\,\varphi, \frac{1}{(L+a)^{n-1}}\,\varphi \right\rangle + \sum_{j=0}^{n-2} p_j (z+a)^j,$$

where the p_j's are real numbers. By the spectral representation of L, the first summand can be written as

$$(z+a)^{n-1} \left\langle \frac{1}{L-z}\,\varphi, \frac{1}{(L+a)^{n-1}}\,\varphi \right\rangle = \frac{(z+a)^{n-1}}{2^d \pi^{d/2} \Gamma(\frac{d}{2})} \int_0^\infty \frac{\lambda^{(d-2)/2}\, d\lambda}{(\lambda - z)(\lambda + a)^{n-1}}.$$

For the integral, using a calculation as in the proof of [14, Proposition 2.1], we find

$$(z+a)^{n-1} \int_0^\infty \frac{\lambda^{(d-2)/2}\, d\lambda}{(\lambda - z)(\lambda + a)^{n-1}} = F(z) - \sum_{j=0}^{n-1} \frac{(z+a)^j}{j!} F^{(j)}(-a),$$

where

$$F(z) = \begin{cases} -\pi \dfrac{(-z)^{(d-2)/2}}{\sin(\pi(d-2)/2)}, & \text{if } d \text{ is odd,} \\[2ex] -z^{(d-2)/2} \ln(-z), & \text{if } d \text{ is even .} \end{cases}$$

Inserting these results in the expression of $Q(z)$ we see that

$$Q(z) = \begin{cases} -\dfrac{1}{2^d \pi^{(d-2)/2} \Gamma(d/2)} \dfrac{(-z)^{(d-2)/2}}{\sin(\pi(d-2)/2)} + p_{[(d-2)/2]}(z), & \text{if } d \text{ is odd,} \\[2ex] -\dfrac{1}{2^d \pi^{d/2} \Gamma(d/2)} z^{(d-2)/2} \ln(-z) + p_{(d-2)/2}(z), & \text{if } d \text{ is even,} \end{cases}$$

where $p_\ell(z)$ stands for a polynomial of degree at most ℓ with real coefficients. The formulas for $Q(z)$ mentioned in the beginning of this section correspond to the cases $d = 4, 5, 6$, and 7, respectively.

6.2. The case $n = 3$

In this case $\varphi \in \mathcal{H}_{-3} \setminus \mathcal{H}_{-2}$ and there are two normalization points $a_1, a_2 > 0$. We set

$$b_1(z) = z + a_1,\ b_2(z) = (z + a_1)(z + a_2), \quad \varphi_j = \frac{1}{b_j(L)}\varphi,\ j = 1, 2. \tag{6.1}$$

The A-model. The function $Q_A(z) + \cot\theta_A$ has the form

$$Q_A(z) + \cot\theta_A = \left\langle \frac{z + a_2}{L - z}\varphi_2, \varphi \right\rangle - \frac{\alpha}{z + a_1} + \cot\theta_A,$$

where $\alpha \in \mathbb{R}$ and $\theta_A \in [0, \pi)$. The space of the self-adjoint realization of the singular perturbation is

$$\mathcal{H}_A = \mathbb{C} \oplus \mathcal{H}_1$$

with Gram operator $G_A = \alpha \oplus I_{\mathcal{H}_1}$. G_A is non-degenerate only if $\alpha \neq 0$, $\mathcal{H}_A$ is a Hilbert space if $\alpha > 0$, and it is a Pontryagin space with negative index 1 if $\alpha < 0$. The self-adjoint realization in the A-model is the self-adjoint operator in the representation of the function $-(Q_A(z) + \cot\theta_A)^{-1}$ and this is the operator A_{θ_A} in $\mathcal{H}_A$ which is the restriction of

$$A_{\max}\begin{pmatrix} u_1 \\ u_r + u_2\varphi_2 \end{pmatrix} = \begin{pmatrix} u_2 - a_1 u_1 \\ L u_r - a_2 u_2 \varphi_2 \end{pmatrix}, \quad u_r \in \mathcal{H}_3,\ u_1, u_2 \in \mathbb{C},$$

by the self-adjoint "boundary" condition

$$\langle u_r, \varphi\rangle - \alpha u_1 = -\cot\theta_A u_2.$$

The B-model. The function $Q_B(z) + \cot\theta_B$ has the form

$$Q_B(z) + \cot\theta_B = b_2(z)\left\langle \frac{1}{L - z}\varphi_2, \varphi \right\rangle + \beta_1(z + a_1) + \cot\theta_B,$$

where $\beta_1 \in \mathbb{R}$ and $\theta_B \in [0, \pi)$. The space of the realization is

$$\widehat{\mathcal{H}}_B = \mathbb{C} \oplus \mathbb{C} \oplus \mathcal{H}$$

with Gram operator

$$G_B = \begin{pmatrix} 0 & 1 \\ 1 & \beta_{11} \end{pmatrix} \oplus I_{\mathcal{H}}, \quad \beta_{11} = \beta_1 + (a_2 - a_1)\langle \varphi_2, \varphi_1\rangle.$$

It is a Pontryagin space with negative index 1 and the completion of the pre-Pontryagin space $\mathcal{H}_B = \mathbb{C}\dot{+}\mathcal{H}_1$ with elements of the form $U = \begin{pmatrix} u_1 \\ u \end{pmatrix}$, where $u_1 \in \mathbb{C}$ and $u \in \mathcal{H}_1$, and inner product

$$\langle U, V\rangle_B = \langle u, v\rangle + u_1\langle \varphi_1, v\rangle + v_1^*\langle u, \varphi_1\rangle + \beta_{11} v_1^* u_1.$$

The self-adjoint realization of the singular perturbation in the B-model is the self-adjoint operator in the representation of the function $-(Q_B(z) + \cot\theta_B)^{-1}$, and this operator is the closure in $\widehat{\mathcal{H}}_B$ of the operator B_{θ_B} in $\mathcal{H}_B$. The operator B_{θ_B} is the restriction of the operator

$$B_{\max}\begin{pmatrix} u_1 \\ u_r + u_2\varphi_2 \end{pmatrix} = \begin{pmatrix} u_2 - a_1u_1 \\ Lu_r - a_2u_2\varphi_2 \end{pmatrix}, \quad u_r \in \mathcal{H}_3,\ u_1, u_2 \in \mathbb{C},$$

determined by the self-adjoint "boundary" condition

$$\langle u_r, \varphi\rangle + \beta_1 u_2 = -\cot\theta_B u_1.$$

The correspondence between the A- and B-models can be seen from the relation

$$Q_B(z) + \cot\theta_B = (z + a_1)\,(Q_A(z) + \cot\theta_A)$$

and it implies the correspondence between parameters

$$\beta_1 = \cot\theta_A, \quad \cot\theta_B = -\alpha.$$

6.3. The case $n = 4$

Now $\varphi \in \mathcal{H}_{-4} \setminus \mathcal{H}_{-3}$ and there are three normalization points $a_1, a_2, a_3 > 0$. Besides (6.1) we set

$$b_3(z) = (z + a_1)(z + a_2)(z + a_3), \quad \varphi_3 = \frac{1}{b_3(L)}\,\varphi.$$

The A-model. The function $Q_A(z) + \cot\theta_A$ is of the form

$$Q_A(z) + \cot\theta_A = \langle\frac{z + a_3}{L - z}\,\varphi_3, \varphi\rangle - \frac{\alpha_1 + \alpha_2(z + a_1)}{(z + a_1)(z + a_2)} + \cot\theta_A,$$

where $\alpha_1, \alpha_2 \in \mathbb{R}$ and $\theta_A \in [0, \pi)$. The space of the realization is

$$\mathcal{H}_A = \mathbb{C}^2 \oplus \mathcal{H}_2$$

with Gram operator

$$G_A = \Gamma_\alpha \oplus I_{\mathcal{H}_2}, \quad \Gamma_\alpha = \begin{pmatrix} (a_1 - a_2)\alpha_1 & \alpha_1 \\ \alpha_1 & \alpha_2 \end{pmatrix}.$$

G_A is non-degenerate only if

$$\det\,\Gamma_\alpha = (a_1 - a_2)\alpha_1\alpha_2 - \alpha_1^2 \neq 0.$$

The last condition is a restriction on the admissible parameters in the A-model. As to the signature of the space $\mathcal{H}_A$:
a) $\mathcal{H}_A$ is a Hilbert space if $a_1 \neq a_2$ and

$$\frac{\alpha_1}{a_2 - a_1} > 0, \quad \alpha_2 + \frac{1}{a_2 - a_1} > 0.$$

b) $\mathcal{H}_A$ is a Pontryagin space with negative index $= 1$ if either $a_1 \neq a_2$ and one of the following three alternatives are satisfied

$$\frac{\alpha_1}{a_2 - a_1} > 0,\ \alpha_2 + \frac{1}{a_2 - a_1} < 0 \quad \text{or} \quad \frac{\alpha_1}{a_2 - a_1} < 0,\ \alpha_2 + \frac{1}{a_2 - a_1} > 0,$$

or $a_1 = a_2$ and $\alpha_1 \neq 0$.

c) $\mathcal{H}_A$ is a Pontryagin space with negative index 2 if $a_1 \neq a_2$ and

$$\frac{\alpha_1}{a_2 - a_1} < 0, \quad \alpha_2 + \frac{1}{a_2 - a_1} < 0.$$

The self-adjoint realization of the singular perturbation in the A-model now is the operator A_{θ_A} in $\mathcal{H}_A$ defined as the restriction of the operator

$$A_{\max} \begin{pmatrix} u_1 \\ u_2 \\ u_r + u_3\varphi_3 \end{pmatrix} = \begin{pmatrix} u_2 - a_1 u_1 \\ u_3 - a_2 u_2 \\ L u_r - a_3 u_3 \varphi_3 \end{pmatrix}, \quad u_r \in \mathcal{H}_4,\ u_1, u_2, u_3 \in \mathbb{C},$$

by the self-adjoint "boundary" condition

$$\langle u_r, \varphi\rangle - \alpha_1 u_1 - \alpha_2 u_2 = -\cot\theta_A u_3.$$

The B-model. The function $Q_B(z) + \cot\theta_B$ has the form

$$Q_B(z) + \cot\theta_B = b_3(z)\langle\frac{1}{L - z}\,\varphi_3, \varphi\rangle + \beta_2(z + a_1)(z + a_2) + \beta_1(z + a_1) + \cot\theta_B,$$

where $\beta_1, \beta_2 \in \mathbb{R}$ and $\theta_B \in [0, \pi)$. The space of the realization is

$$\widehat{\mathcal{H}}_B = \mathbb{C} \oplus \mathbb{C} \oplus \mathcal{H}$$

with Gram operator

$$G_B = \begin{pmatrix} 0 & 1 \\ 1 & \beta_{11} \end{pmatrix} \oplus I_{\mathcal{H}},$$

$$\beta_{11} = \beta_1 + (a_2 - a_1)\beta_2 + (a_3 - a_1)(a_2 - a_1)\langle\varphi_3, \varphi_1\rangle$$

and $\widehat{\mathcal{H}}_B$ is a Pontryagin space with negative index $= 1$.
The space $\widehat{\mathcal{H}}_B$ is the completion of the pre-Pontryagin space $\mathcal{H}_B$ which is the linear space of the elements $U = \begin{pmatrix} \vec{u} \\ u \end{pmatrix}$, where $\vec{u} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \in \mathbb{C}^2$ and $u \in \mathcal{H}_2$, and endowed with the inner product

$$\langle U, V\rangle_B = \langle u, v\rangle + \sum_{j=1}^{2} \big(u_j\langle\varphi_j, v\rangle + v_j^*\langle u, \varphi_j\rangle\big) + \sum_{j=1}^{2}\sum_{k=1}^{2} \beta_{jk} v_j^* u_k,$$

where

$$\beta_{12} = \beta_{21} = \beta_2 + (a_3 - a_1)\langle\varphi_3, \varphi_1\rangle, \quad \beta_{22} = \langle\varphi_2, \varphi_2\rangle.$$

The self-adjoint realization of the singular perturbation in the B-model is the self-adjoint operator in the representation of the function $-(Q_B(z) + \cot\theta_B)^{-1}$, and this is the closure in $\widehat{\mathcal{H}}_B$ of the operator B_{θ_B} in $\mathcal{H}_B$. The operator B_{θ_B} is the restriction of the operator

$$B_{\max} \begin{pmatrix} u_1 \\ u_2 \\ u_r + u_3\varphi_3 \end{pmatrix} = \begin{pmatrix} u_2 - a_1 u_1 \\ u_3 - a_2 u_2 \\ L u_r - a_3 u_3 \varphi_3 \end{pmatrix}, \quad u_r \in \mathcal{H}_4,\ u_1, u_2, u_3 \in \mathbb{C},$$

by the self-adjoint "boundary" condition

$$\langle u_r, \varphi\rangle + \beta_1 u_2 + \beta_2 u_3 = -\cot\theta_B u_1.$$

The correspondence between the A- and B-models is given via the relations

$$Q_B(z) + \cot\theta_B = (z + a_1)(z + a_2)\,(Q_A(z) + \cot\theta_A)$$

which imply that

$$\beta_1 = -\alpha_2,\ \beta_2 = \cot\theta_A,\ \cot\theta_B = -\alpha_1.$$

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