BOUNDARY TRIPLES AND WEYL FUNCTIONS FOR SINGULAR PERTURBATIONS OF SELF-ADJOINT OPERATORS

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ABSTRACT. Given the symmetric operator $A_N$ obtained by restricting the self-adjoint operator $A$ to $N$, a linear dense set, closed with respect to the graph norm, we determine a convenient boundary triple for the adjoint $A_N^*$ and the corresponding Weyl function. These objects provide us with the self-adjoint extensions of $A_N$ and their resolvents.

1. Introduction

Let $A : D(A) \subseteq \mathcal{H} \to \mathcal{H}$ be a self-adjoint operator on the Hilbert space $\mathcal{H}$. Another self-adjoint operator $\hat{A}$ is said to be a singular perturbation of $A$ if the set $\mathcal{N} := \{ \phi \in D(\hat{A}) \cap D(A) : \hat{A}\phi = A\phi \}$ is dense in $\mathcal{H}$ (see e.g. [11]). Since $\mathcal{N}$ is closed with respect to the graph norm on $D(A)$, the linear operator $A_N$, obtained by restricting $A$ to $\mathcal{N}$, is a densely defined closed symmetric operator. Thus $\hat{A}$ is a singular perturbation of $A$ if and only if it is a self-adjoint extension of $A_N$ such that $D(\hat{A}) \cap D(A) = \mathcal{N}$, where $\mathcal{N} \subset D(A)$ is any dense set which is closed with respect to the graph norm on $D(A)$. Therefore all singular perturbations of $A$ could be determined by using von Neumann’s theory [14]. By such a theory, given a closed densely defined symmetric operator $S$, one has

$$D(S^*) = D(S) \oplus \mathcal{K}_+ \oplus \mathcal{K}_-,$$

$$S^*(\phi_0 + \phi_+ + \phi_-) = S\phi_0 + i\phi_+ - i\phi_-,$$

where the direct sum decomposition is orthogonal with respect to the graph inner product of $S^*$ and $\mathcal{K}_\pm := \text{Ker}(-S^* \pm i)$ denotes the deficiency spaces. Any self-adjoint extension $A_U$ of $S$ is then obtained by restricting $S^*$ to a subspace of the kind $D(S) \oplus \text{Graph } U$, where $U : \mathcal{K}_+ \to \mathcal{K}_-$ is unitary. Alternatively one could determine the singular perturbations of $A$ by Krein’s resolvent formula (see [12], [13], [18] for the cases where $\dim \mathcal{K}_\pm = 1$, $\dim \mathcal{K}_+ < +\infty$, $\dim \mathcal{K}_- = +\infty$ respectively; also see [9]). This approach gives the resolvent difference
of any pair (in our situation \(A\) and \(\hat{A}\)) of self-adjoint extensions of \(S\), thus allowing for a better understanding of the spectral properties of such extensions. Like in von Neumann’s theory, also in Krein’s one a main role is played by the defect spaces, through the orthogonal projections onto \(K_+\). This is a consequence of the fact that both these theories regard self-adjoint extensions of an arbitrary closed densely defined symmetric operator with equal defect indices. However in the case of singular perturbation the situation is simpler. Indeed here \(A_N\) is not an arbitrary symmetric operator but is the restriction to \(N\) of a given self-adjoint operator \(A\). Thus, instead of the orthogonal projections onto \(K_\pm\), one can use the orthogonal projection \(\pi: \mathcal{H}_+ \to N^\perp\), where \(\mathcal{H}_+\) denotes the Hilbert space given by the set \(D(A)\) equipped with the scalar product \(\langle \phi_1, \phi_2 \rangle_+ := \langle A\phi_1, A\phi_2 \rangle + \langle \phi_1, \phi_2 \rangle\), and the orthogonal decomposition \(\mathcal{H}_+ = N \oplus N^\perp\) is used, being \(N\) closed in \(\mathcal{H}_+\). More generally, since this gives advantages in concrete applications where usually a variant of \(\pi\) is what is known in advance, one can consider a bounded linear map \(\tau: \mathcal{H}_+ \to \mathfrak{h}\), an auxiliary Hilbert space, such that \(N := \text{Ker}(\tau)\) is dense in \(\mathcal{H}\) and \(\text{Ran}(\tau) = \mathfrak{h}\), so that \(\mathcal{H}_+ \simeq \text{Ker}(\tau) \oplus \mathfrak{h}\). This alternative approach has been developed in [15] as regards Krein’s formula and in [17], where an additive decomposition of any singular perturbation is given and the explicit connection with von Neumann’s theory is found. The approach contained in [15], [16], [17], looks simpler than the original ones (for example no knowledge of either \(A_N^*\) or \(K_+\) is needed), allows for a natural formulation in terms of (abstract) boundary conditions and makes easier to work out concrete applications where \(\tau\) is the trace (restriction) map along some null subset of \(\mathbb{R}^d\) and \(A\) is a (pseudo-)differential operator (see the examples contained in the quoted references).

Another approach, different from both von Neumann’s and Krein’s theories, has been used to obtain self-adjoint extensions of a given symmetric operator \(S\) with equal defect indices: this is the theory of boundary triplets introduced by Bruk and Kochubei [4], [10] and then successively developed in many papers and books (see e.g. [9], [6], [7] and references therein). Here one needs to find a boundary triple \(\{\mathfrak{h}, \gamma_1, \gamma_2\}\) for \(S^*\), i.e. one needs a Hilbert space \(\mathfrak{h}\) (with scalar product \(\langle \cdot, \cdot \rangle\)) and two linear maps \(\gamma_1\) and \(\gamma_2\) on \(D(S^*)\) to \(\mathfrak{h}\) such that \(\phi \mapsto (\gamma_1\phi, \gamma_2\phi)\) is surjective and

\[
\langle S^*\phi, \psi \rangle - \langle \phi, S^*\psi \rangle = [\gamma_1 \phi, \gamma_2 \psi] - [\gamma_2 \phi, \gamma_1 \psi].
\]

Once a boundary triple is known, any self-adjoint extensions of \(S\) is then obtained by restricting \(S^*\) to the set of \(\phi\)’s such that the couple \((\gamma_2\phi, \gamma_1\phi)\) belongs to a self-adjoint relation.
Boundary triples theory, thanks to the concept of Weyl function successively introduced in [5], generalizing a concept earlier used by Weyl in the study of Sturm-Liouville problems, allows for a spectral analysis of the self-adjoint extensions of $S$ (see e.g. [6], [3] and references therein).

The scope of this paper is to work out the theory of boundary triples and Weyl functions in the case of singular perturbations, making use of the orthogonal projection $\pi : \mathcal{H}_+ \to \mathcal{N}^\perp$ or better of its generalization given by a map $\tau : \mathcal{H}_+ \to \mathfrak{h}$. This is done in section 3, after that, in section 2, we have given a concise review (we refer to [6], [9] for the proofs) of the theory of boundary triples. In particular a convenient boundary triple for $A_N^\star$, and the corresponding Weyl function are given in Theorem 3.1. The successive Corollary 3.2 characterizes all singular perturbations of $A$ in terms of (abstract) boundary conditions of the kind $\Theta \phi = \tau \phi$, where $\Theta$ is self-adjoint on $\mathfrak{h}$. As we already said, in the case $A$ is a differential operator, these are indeed concrete boundary conditions since usually $\tau$ is the (trace) evaluation map along some null subset. Finally in Theorem 3.4 we determine the possible eigenvectors (and their multiplicity) of the singular perturbations of a self-adjoint operator.

2. Boundary triples and Weyl Functions.

Let $S : D(S) \subseteq \mathcal{H} \to \mathcal{H}$ be a densely defined closed symmetric operator on the Hilbert space $\mathcal{H}$ with inner product $\langle \cdot, \cdot \rangle$ and corresponding norm $\| \cdot \|$. We will suppose that $S$ has equal defect indices $n_+ = n_-$, where $n_\pm := \text{dim} \mathcal{K}_\pm$ and $\mathcal{K}_\pm := \text{Ker}(-S^* \pm i)$.

A triple $\{\mathfrak{h}, \gamma_1, \gamma_2\}$, where $\mathfrak{h}$ is a Hilbert space with inner product $[\cdot, \cdot]$ and

\[
\gamma_1 : D(S^*) \to \mathfrak{h}, \quad \gamma_2 : D(S^*) \to \mathfrak{h},
\]

are two linear maps such that

\[
\gamma : D(S^*) \to \mathfrak{h} \oplus \mathfrak{h}, \quad \gamma \phi := (\gamma_1 \phi, \gamma_2 \phi)
\]

is surjective and

\[
\langle S^* \phi, \psi \rangle - \langle \phi, S^* \psi \rangle = [\gamma_1 \phi, \gamma_2 \psi] - [\gamma_2 \phi, \gamma_1 \psi].
\]

The definition of boundary triple is well posed. Indeed let

\[
P_\pm : D(S^*) \to \mathcal{K}_\pm
\]

denotes the orthogonal projection given the decomposition

\[
D(S^*) = D(S) \oplus \mathcal{K}_+ \oplus \mathcal{K}_-,
\]
where the direct sum is orthogonal with respect to the graph inner product of $S^*$. Then
\[ \gamma_1 := iP_+ - iUP_-, \quad \gamma_2 := P_+ + UP_-, \]
where $\mathfrak{h} = \mathcal{K}_+$ and $U : \mathcal{K}_- \to \mathcal{K}_+$ is an isometry, give a boundary triple for $S^*$. This also shows, since $U$ is arbitrary, that a boundary triple is not unique.

A closed subspace $\mathcal{G} \subset \mathfrak{h} \oplus \mathfrak{h}$ is said to be a symmetric closed relation if
\[ \forall (f_1, g_1), (f_2, g_2) \in \mathcal{G} \quad [f_1, g_2] = [g_1, f_2]. \]
$\mathcal{G}$ is then said to be a self-adjoint relation if it is maximal symmetric, i.e. if it does not exists a closed symmetric relation $\hat{\mathcal{G}}$ such that $\mathcal{G} \subset \hat{\mathcal{G}}$. Of course the graph of a self-adjoint operator is a particular case of self-adjoint relation.

The main result of boundary triples theory is given in the following

**Theorem 2.1.** \cite{9}, Theorem 1.6, chapter 3 \textit{Let $\{\mathfrak{h}, \gamma_1, \gamma_2\}$ be a boundary triple for $S^*$. Then any self-adjoint extension of $S$ is of the kind $S^*\mathcal{G}$, where $S^*\mathcal{G}$ denotes the restriction of $S^*$ to the subspace $\{\phi \in D(S^*) : (\gamma_2\phi, \gamma_1\phi) \in \mathcal{G}\}$, $\mathcal{G}$ being a self-adjoint relation.}

Form now on we will denote by $A_\Theta$ the self-adjoint extension which corresponds to $\mathcal{G} = \text{graph}(-\Theta)$, where $\Theta$ is a self-adjoint operator on $\mathfrak{h}$, and by $A$ the self-adjoint extension corresponding to the self-adjoint relation $\mathcal{G} = \{0\} \times \mathfrak{h}$.

Given the boundary triple $\{\mathfrak{h}, \gamma_1, \gamma_2\}$ for $S^*$, the Weyl function of $S$ corresponding to $\{\mathfrak{h}, \gamma_1, \gamma_2\}$ is defined as the unique map
\[ \Gamma : \rho(A) \to \mathcal{B}(\mathfrak{h}) \]
such that
\[ \forall \phi_z \in \mathcal{K}_z := \text{Ker}(-S^* + z), \quad \Gamma(z)\gamma_2\phi_z = \gamma_1\phi_z. \]
Since, for any $z \in \rho(A)$, $\gamma_1$ and $\gamma_2$ are bijections on $\mathcal{K}_z$ to $\mathfrak{h}$, one can define
\[ G(z) := (\gamma_2|_{\mathcal{K}_z})^{-1}, \]
and thus
\[ \Gamma(z) = \gamma_1G(z). \]
Moreover
\[ \Gamma(z) - \Gamma(w)^* = (z - \bar{w})G(w)^*G(z), \]
i.e. $\Gamma$ is a $Q$-function of $S$ belonging to the extension $A$ in the sense of Krein.
Weyl functions can be used to deduce spectral properties of the extensions:
Theorem 2.2. ([6], Propositions 1 and 2, section 2)
\[ z \in \rho(A_\Theta) \cap \rho(A) \iff 0 \in \rho(\Theta + \Gamma(z)) \]
and
\[ \lambda \in \sigma_i(A_\Theta) \cap \rho(A) \iff 0 \in \sigma_i(\Theta + \Gamma(\lambda)), \quad i = p, c, r, \]
where \( \sigma_p(A_\Theta), \sigma_c(A_\Theta), \sigma_r(A_\Theta) \) denote the point, continuous and residual spectrum respectively. Moreover one has the Krein's formula
\[ (-A_\Theta + z)^{-1} = (-A + z)^{-1} + G(z)(\Theta + \Gamma(z))^{-1}G(z)^*. \]

The Weyl function \( \Gamma \) is a Herglotz or Nevanlinna operator-valued function. This means that \( \Gamma \) is holomorphic in the upper half complex plane \( \mathbb{C}_+ \) and the operator \( \Gamma(z) \) is dissipative, i.e.
\[ \forall z \in \mathbb{C}_+, \quad \frac{1}{2i} (\Gamma(z) - \Gamma(z)^*) \geq 0. \]
Thus, by the celebrated Nevanlinna-Riesz-Herglotz decomposition, one has
\[ \Gamma(z) = C + \int_{\mathbb{R}} d\Sigma(t) \left( \frac{1}{t - z} - \frac{t}{1 + t^2} \right), \]
where \( C \in \mathcal{B}(\mathfrak{h}) \) is self-adjoint and the \( \mathcal{B}(\mathfrak{h}) \)-valued measure \( \Sigma \) is self-adjoint and such that
\[ \int_{\mathbb{R}} \frac{d\Sigma(t)}{1 + t^2} \in \mathcal{B}(\mathfrak{h}). \]
Given a (unbounded) self-adjoint operator \( \Theta \) on \( \mathfrak{h} \) and a \( \mathcal{B}(\mathfrak{h}) \)-valued Herglotz function \( \Gamma : \mathbb{C}_+ \to \mathcal{B}(\mathfrak{h}) \), \( \Theta + \Gamma(z) \) is boundedly invertible for any \( z \in \mathbb{C}_+ \) (see [15], Proposition 2.1) and \( (\Theta + \Gamma)^{-1} \) is again a \( \mathcal{B}(\mathfrak{h}) \)-valued Herglotz function.

Lemma 2.3. ([3], Lemma 3.2) The spectral measure of \( A_\Theta \) is equivalent to the self-adjoint measure appearing in the Nevanlinna-Riesz-Herglotz decomposition of \( (\Theta + \Gamma)^{-1} \).

3. Singular Perturbations

Let \( A : D(A) \subseteq \mathcal{H} \to \mathcal{H} \) be a self-adjoint operator on the Hilbert space \( (\mathcal{H}, \langle \cdot, \cdot \rangle) \). We denote by \( (\mathcal{H}_+, \langle \cdot, \cdot \rangle_+) \) the Hilbert space given by the set \( D(A) \) equipped with the scalar product \( \langle \cdot, \cdot \rangle_+ \) leading to the graph norm, i.e. \( \langle \phi_1, \phi_2 \rangle_+ := \langle (A^2 + 1)^{1/2} \phi_1, (A^2 + 1)^{1/2} \phi_2 \rangle \).

Let \( \mathcal{N} \subseteq D(A) \) be a linear dense set which is closed with respect to the graph norm. Being \( \mathcal{N} \) closed we have \( \mathcal{H}_+ = \mathcal{N} \oplus \mathcal{N}^\perp \) and we can then consider the orthogonal projection \( \pi : \mathcal{H}_+ \to \mathcal{N}^\perp \). More generally, since this gives advantages in concrete applications, we will consider a bounded linear map \( \tau : \mathcal{H}_+ \to \mathfrak{h} \), where \( (\mathfrak{h}, [\cdot, \cdot]) \) is a Hilbert space.
We suppose that $\tau$ is surjective and that $\mathcal{N} := \text{Ker}(\tau)$ is dense in $\mathcal{H}$. Note that, by the surjectivity hypothesis, $\mathfrak{h} \simeq \mathcal{H}_+/\mathcal{N} \simeq \mathcal{N}^\perp$, so that $\mathcal{H}_+ \simeq \mathcal{N} \oplus \mathfrak{h}$.

Denoting by $\rho(A)$ the resolvent set of $A$, for any $z \in \rho(A)$ we define the two bounded linear operators
\[ R(z) : \mathcal{H} \to \mathcal{H}_+, \quad R(z) := (-A + z)^{-1} \]
and
\[ G(z) : \mathcal{H} \to \mathfrak{h}, \quad G(z) := (\tau R(\bar{z}))^*. \]

By [17], Lemma 2.1 (see also [1], Theorem A.1, for an analogous result), the denseness hypothesis on $\mathcal{N}$ is equivalent to
\[ \tag{3.1} \text{D}(A) \cap \text{Ran}(G(z)) = \{0\} \]
and, as an immediate consequence of the first resolvent identity for $R(z)$ (see [15], Lemma 2.1),
\[ \tag{3.2} (z - w) R(w) G(z) = G(w) - G(z). \]

These relations imply
\[ \text{D}(A) \cap \text{Ran}(G(w) + G(z)) = \{0\} \]
and
\[ \text{D}(A) \supseteq \text{Ran}(G(w) - G(z)). \]

**Theorem 3.1.** Defining
\[ R := R(i), \quad G := G(-i), \quad G_s := \frac{1}{2} (G(i) + G(-i)), \]
one has
\[ A_N^* \phi = A\phi_s + RG\zeta_\phi, \]
\[ \text{D}(A_N^*) = \{ \phi \in \mathcal{H} : \phi = \phi_s + G_s\zeta_\phi, \ \phi_s \in \text{D}(A), \ \zeta_\phi \in \mathfrak{h} \}. \]

Defining
\[ \gamma_1 : \text{D}(A_N^*) \to \mathfrak{h}, \quad \gamma_1 \phi := -\tau\phi_s, \]
\[ \gamma_2 : \text{D}(A_N^*) \to \mathfrak{h}, \quad \gamma_2 \phi := \zeta_\phi, \]
the triple $\{ \mathfrak{h}, \gamma_1, \gamma_2 \}$ is a boundary triple for $A_N^*$. The corresponding Weyl function of $A_N^*$ is
\[ \Gamma : \rho(A) \to \mathcal{B}(\mathfrak{h}), \quad \Gamma(z) = \tau(G_s - G(z)). \]

**Proof.** The form of $\text{D}(A_N^*)$ was obtained in [17], Theorems 3.4 and 4.1. By (3.2)
\[ \tag{3.3} RG = \frac{i}{2} (G(i) - G(-i)). \]

Thus the action of $A_N^*$ on its domain follows from [17], Theorem 2.2.
Since $A$ is self-adjoint
\[
\langle A^*_N \phi, \psi \rangle - \langle \phi, A^*_N \psi \rangle = \langle A \phi, \psi \rangle - \langle \phi, A \psi \rangle = 0.
\]
By (3.3)
\begin{equation}
(3.4) \quad G_* = -iRG + G.
\end{equation}
Therefore one has
\[
\langle A^*_N G_* \zeta \phi, G_* \zeta \psi \rangle - \langle G_* \zeta \phi, A^*_N G_* \zeta \psi \rangle
= \langle (2i + (A + i))G_* \zeta \phi, G_* \zeta \psi \rangle = 0,
\]
\[
\langle A^*_N \phi, G_* \zeta \psi \rangle - \langle \phi, A^*_N G_* \zeta \psi \rangle
= \langle A^*_N \phi, G_* \zeta \psi \rangle - \langle \phi, G_* \zeta \psi \rangle
= \langle G^*(A - i) \phi, G_* \zeta \psi \rangle - \langle \phi, G_* \zeta \psi \rangle.
\]
\[
\langle A^*_N \phi, G_* \zeta \psi \rangle - \langle \phi, A^*_N G_* \zeta \psi \rangle
= \langle G^*(A - i) \phi, G_* \zeta \psi \rangle - \langle \phi, G_* \zeta \psi \rangle
= -\langle G^*(A - i) \phi, G_* \zeta \psi \rangle - \langle \phi, G_* \zeta \psi \rangle.
\]

In conclusion
\[
\langle A^*_N \phi, \psi \rangle - \langle \phi, A^*_N \psi \rangle = \langle A^*_N \phi, \psi \rangle - \langle \phi, A^*_N \psi \rangle = 0.
\]

By the above theorem we can characterize all the singular perturbations of $A$ by (abstract) boundary conditions of the kind $\Theta \zeta_\phi = \tau \phi$:
Corollary 3.2. Any singular perturbations $\hat{A}$ of the self-adjoint operator $A$ is of the kind
\[ \hat{A}\phi = A\phi + R\zeta, \]
where $D(\hat{A}) = \{ \phi \in H : \phi = \phi + G\zeta, \phi \in D(A), \zeta \in \mathfrak{h} \}$, $\Theta \zeta = \tau \phi$, and $\Theta$ is a self-adjoint operator on the Hilbert space $\mathfrak{h}$. Moreover
\[ z \in \rho(\hat{A}) \cap \rho(A) \iff 0 \in \rho(\Theta + \tau(G - G(z))). \]

Remark 3.3. The above corollary was already obtained in [17] as a direct consequence of the results contained in [15], without making use of the theory of boundary triples.

We conclude by determining the eigenvectors (and their multiplicity) of the singular perturbations of $A$. A similar result was obtained in [2] in the case of form-bounded (hence weakly singular) perturbations.

Theorem 3.4. For any $\lambda \in \sigma_p(\hat{A}) \cap \rho(A)$, the map $\zeta \mapsto G(\lambda)\zeta$ is a bijection on $\text{Ker}(\Theta + \Gamma(\lambda))$ to $\text{Ker}(-\hat{A} + \lambda)$.

Proof. At first let us note that
\[ G(\lambda)\zeta \in D(\hat{A}) \iff \tau(G(\lambda) - G_s)\zeta = \Theta\zeta \iff (\Theta + \Gamma(\lambda))\zeta = 0. \]
We also note that, by (3.2) and (3.4),
\[ G(\lambda) - G_s = R(\lambda)(-\lambda G_s + RG), \]
i.e.
\[ (-A + \lambda)(G(\lambda) - G_s) = -\lambda G_s + RG. \]
Suppose now that $\zeta \in \text{Ker}(\Theta + \Gamma(\lambda))$. Then $G(\lambda)\zeta \in D(\hat{A})$ and
\[ (-\hat{A} + \lambda)G(\lambda)\zeta = (-\hat{A} + \lambda)((G(\lambda) - G_s)\zeta + G_s\zeta) \]
\[ = (-A + \lambda)(G(\lambda) - G_s)\zeta - RG\zeta + \lambda G_s\zeta \]
\[ = -\lambda G_s\zeta + RG\zeta - RG\zeta + \lambda G_s\zeta = 0. \]
Conversely suppose that $\phi \in \ker(-\hat{A} + \lambda)$. Then
\[ 0 = (-\hat{A} + \lambda)\phi = (-A + \lambda)\phi_s - RG\zeta + \lambda G_s\zeta \]
\[ = (-A + \lambda)\phi_s - (-A + \lambda)(G(\lambda) - G_s)\zeta_s \]
\[ = (-A + \lambda)(\phi_s + (G_s - G(\lambda))\zeta_s). \]
Since \( \lambda \in \rho(A) \), this implies \( \phi_\ast + (G_\ast - G(\lambda))\zeta_\phi = 0 \), which is equivalent to \( \phi = G(\lambda)\zeta_\phi \).

\[ \square \]

**Remark 3.5.** We know that the choice of a boundary triple is not unique. Therefore a different (from the one given in Theorem 3.1) choice leads to a different parametrization of the family of the singular perturbations of \( A \). In particular the resolvents will depend on a different Weyl function \( \tilde{\Gamma} \). In [15] it was obtained a Krein-like formula which, in the terminology of the present paper, gives singular perturbations of \( A \) in terms of an arbitrary choice of a Weyl function. Since, given any Weyl function \( \tilde{\Gamma} \), one has that \( \tilde{\Gamma}(z) - \Gamma(z) \) is a \( z \)-independent self-adjoint operator (see [15], remark 2.3), if we denote by \( \tilde{A} \) a singular perturbations of \( A \) given by a Weyl function \( \tilde{\Gamma} \), we have that \( \tilde{A} = \hat{A} \), where \( \hat{A} \) is the singular perturbation given in Corollary 3.2 with \( \Theta := \hat{\Theta} + \tilde{\Gamma}(z) - \Gamma(z) \), \( \hat{\Theta} \) self-adjoint. Therefore Theorem 3.4 holds true independently of the Weyl function (or, equivalently, of the boundary triple) one uses to describe the singular perturbations of \( A \).

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