ON SOME EXTENSIONS OF THE A-MODEL

RYTIS JURŠENAS

Abstract. The A-model for finite rank singular perturbations of class $\mathcal{H}_{m-2} \setminus \mathcal{H}_{m-1}$, $m \in \mathbb{N}$, is considered from the perspective of boundary relations. Assuming further that the Hilbert spaces $(\mathcal{H}_n)_{n \in \mathbb{Z}}$ admit an orthogonal decomposition $\mathcal{H}_n^- \oplus \mathcal{H}_n^+$, the A-model is modified so that it takes into consideration the functions from the subspaces $\mathcal{H}_n^\pm$. As an example, rank-four singular perturbations of class $\mathcal{H}_{-4} \setminus \mathcal{H}_{-3}$ of the Rashba operator in $L^2(\mathbb{R}^6) \otimes \mathbb{C}^4$ are presented.

1. Introduction

Consider a lower semibounded self-adjoint operator $L$ in the Hilbert space $\mathcal{H}_0$. Let $(\mathcal{H}_n)_{n \in \mathbb{Z}}$ be the scale of Hilbert spaces associated with $L$. Let also $\{\varphi_\sigma\}$ be the family of linearly independent functionals of class $\mathcal{H}_{m-2} \setminus \mathcal{H}_{m-1}$, $m \in \mathbb{N}$, where $\sigma$ ranges over an index set $S$ of dimension $d \in \mathbb{N}$. Then, the symmetric restriction $L_{\min} \subseteq L$ to the set of $f \in \mathcal{H}_{m+2}$ such that $\langle \varphi_\sigma, f \rangle = 0$, for all $\sigma$, is essentially self-adjoint in $\mathcal{H}_0$, and so traditional methods, see e.g. [1, 14], for describing nontrivial extensions of $L_{\min}$ (i.e. perturbations of $L$) in $\mathcal{H}_0$ are insufficient.

To construct nontrivial realizations of $L_{\min}$ in Hilbert or Pontryagin spaces, one considers the so-called cascade (A or B) models [11, 12, 18, 19, 13] and the peak model [17, 20]. In these models the Weyl (or Krein $Q$-) function is the sum of a Nevanlinna function associated with $L_{\min}$ in $\mathcal{H}_m$ and a generalized Nevanlinna function associated with a certain multiplication operator in a reproducing kernel Pontryagin space [3, Theorem 4.10]; more on reproducing kernel spaces can be found in [5, 2, 4, 8]. Successively, singular perturbations are interpreted by means of the compression to the reference space $\mathcal{H}_0$ of the resolvent of an appropriate extension in the model space.

Here we study the cascade A-model for rank-$d$ higher order singular perturbations. More precisely, for a specific choice of model parameters, we extend the main results obtained in [11] to the case of an arbitrary $d \in \mathbb{N}$ (see Theorem 2.2). Then, by assuming that the Hilbert spaces $\mathcal{H}_n$ are expressed as the Hilbert sums $\mathcal{H}_n^- \oplus \mathcal{H}_n^+$ of their subspaces
such that \( \mathcal{F}_n \subset \mathcal{F}_{n+1} \) densely, we examine nontrivial realizations that account for the above described space decompositions (see Theorems 3.2 and 3.5). The exposition utilizes the techniques based on the notion of boundary triples [9, 10, 7, 6].

The motivation for considering the A-model, as opposed to the peak model, arises from an attempt to elude a too restrictive condition imposed on the Gram matrix \( G = (G_{\sigma j, \sigma' j'}) \in \mathbb{C}^{md} \) of the peak model; namely, \( G \) must be diagonal in \( j \in \{1, \ldots, m\} \). Although initially contemplated as an advantageous feature [20], this restriction is not satisfied for some operators \( L \), for \( m > 1 \). The example that we keep in mind is the two-particle Rashba operator in the Hilbert space \( \mathcal{H}_0 = L^2(\mathbb{R}^6) \otimes \mathbb{C}^4 \), combined with spin-orbit and Rashba couplings [16]. In this example the subspaces \( \mathcal{F}_n^- = H^n(\mathbb{R}^6) \otimes \mathbb{C}^1 \) and \( \mathcal{F}_n^+ = H^n(\mathbb{R}^6) \otimes \mathbb{C}^3 \) (where \( H^n \) denotes the \( L^2 \)-Sobolev space of order \( n \)) account for the antisymmetric and symmetric spin states. More details are provided in Section 4.

2. THE A-MODEL FOR FINITE RANK PERTURBATIONS

Let \( (\mathcal{F}_n)_{n \in \mathbb{Z}} \) be the scale of Hilbert spaces associated with a lower semibounded self-adjoint operator \( L \) in the reference Hilbert space \( \mathcal{H}_0 \). The scalar product in \( \mathcal{F}_n \) is defined by \( \langle \cdot, \cdot \rangle_n := \langle \cdot, (L - z_1)^n \cdot \rangle_0 \) for some fixed \( z_1 \in \text{res } L \cap \mathbb{R} \). In the notation of [11], this definition assumes the parameters \( a_j = -z_1 \) for all \( j \in \{1, 2, \ldots, m+1\} \). The action on \( \mathcal{F}_{m+2} \) of linearly independent functionals \( \{\varphi_\sigma\} \) is realized via the duality pairing \( \langle \varphi_\sigma, \cdot \rangle \) in a usual way; we also use the vector notation \( \langle \varphi, \cdot \rangle = ((\varphi_\sigma, \cdot)): \mathcal{F}_{m+2} \to \mathbb{C}^d \).

Let \( L_{\max} \) denote the triplet adjoint of \( L_{\min} \) for the Hilbert triple \( \mathcal{F}_m \subset \mathcal{F}_0 \subset \mathcal{F}_{-m} \); see also [11] Theorem 2.1, [20] Definition 3.1, [17] Proposition 4.2. The operator \( L_{\max} \) extends \( L \mid_{\mathcal{F}_{-m+2}} \) to the domain \( \text{dom}(L_{\max}) = \mathcal{F}_{-m+2} \uplus \mathcal{N}_z(L_{\max}), \ z \in \text{res } L \), where the eigenspace \( \mathcal{N}_z(L_{\max}) \) is a linear span of the singular elements \( \{g_\sigma(z) \in \mathcal{F}_{-m} \\setminus \mathcal{F}_{-m+1}\} \) defined (in the generalized sense) by \( g_\sigma(z) := (L - z)^{-1} \varphi_\sigma \).

Consider an \( md \)-dimensional linear space

\[ \mathfrak{K}_A := \text{span}\{h_\alpha \mid \alpha = (\sigma, j) \in \mathcal{S} \times J\} \]

with \( J := \{1, 2, \ldots, m\} \) and

\[ h_{\sigma j} := (L - z_1)^{-j} \varphi_\sigma \in \mathcal{F}_{-m-2+2j} \setminus \mathcal{F}_{-m-1+2j}. \]

Note that \( h_{\sigma 1} = g_\sigma(z_1) \in \mathcal{N}_{z_1}(L_{\max}) \). An element \( k \in \mathfrak{K}_A \subseteq \mathcal{F}_m \) is thus of the form

\[ k = \sum_\alpha d_\alpha(k) h_\alpha, \quad d_\alpha(k) \in \mathbb{C}. \]

Since the system \( \{h_\alpha\} \) is linearly independent, the Gram matrix

\[ \tilde{G}_A = ([\tilde{G}_A]_{\alpha \alpha'} \in \mathbb{C}^{md}), \quad [\tilde{G}_A]_{\alpha \alpha'} := \langle h_\alpha, h_{\alpha'} \rangle_{-m} \]

is positive definite, and one establishes a bijective correspondence \( \mathfrak{K}_A \ni k \leftrightarrow d(k) \in \mathbb{C}^{md} \). Observe that \( \mathfrak{K}_A \cap \mathcal{F}_{m-1} = \{0\} \).
Define a linear space
\[ \mathcal{H}_A := \mathcal{H}_m \oplus \mathcal{K}_A \]
with an indefinite metric
\[ [f + k, f' + k']_A := \langle f, f' \rangle_m + \langle d(k), G_A d(k') \rangle_{\mathbb{C}^{md}} \]
for \( f, f' \in \mathcal{H}_m \) and \( k, k' \in \mathcal{K}_A \). An Hermitian matrix \( G_A = ([G_A]_{\alpha \alpha'}) \in [\mathbb{C}^{md}] \) is referred to as the Gram matrix of the A-model. Thus \( \mathcal{H}_A \) is a Hilbert space if \( G_A \geq 0 \) and a Pontryagin space otherwise. Let also
\[ \mathcal{H}'_A := \left( \mathcal{H}_m \oplus \mathbb{C}^{md}, \left[ \cdot, \cdot \right]_{\mathcal{H}'_A} \right) \]
with an indefinite metric
\[ [(f, \xi), (f', \xi')]_A := \langle f, f' \rangle_m + \langle \xi, G_A \xi' \rangle_{\mathbb{C}^{md}} \]
for \( f, f' \in \mathcal{H}_m \) and \( \xi, \xi' \in \mathbb{C}^{md} \). The isometric isomorphism from \( \mathcal{H}_A \) onto \( \mathcal{H}'_A \), realized via the above established bijective correspondence \( \mathcal{K}_A \leftrightarrow \mathbb{C}^{md} \), is denoted by \( U_A \).

The construction of nontrivial extensions to \( \mathcal{H}_A \) of \( L_{\text{min}} \) relies upon the following lemma; cf. [11, Eq. (2.3)].

**Lemma 2.1.** The restriction to \( \mathcal{H}_A \) of \( L_{\text{max}} \) is the operator \( A_{\text{max}} \) given by
\[
\begin{align*}
\text{dom } A_{\text{max}} &= \{ f^# + h_{m+1}(c) + k \mid f^# \in \mathcal{H}_{m+2}, k \in \mathcal{K}_A \}; \\
h_{m+1}(c) &= \sum_{\sigma} c_{\sigma} h_{\sigma,m+1}; \quad c = (c_{\sigma}) \in \mathbb{C}^d; \\
h_{\sigma,m+1} &= (L - z_1)^{-m-1} \varphi_\sigma \in \mathcal{H}_m \setminus \mathcal{H}_{m+1}, \\
A_{\text{max}}(f^# + h_{m+1}(c) + k) &= L f^# + z_1 h_{m+1}(c) + \tilde{k}, \quad \tilde{k} \in \mathcal{K}_A, \\
d(\tilde{k}) &= M_d d(k) + \eta(c), \quad \eta(c) := (\delta_{jm} c_{\sigma}) \in \mathbb{C}^{md}
\end{align*}
\]
where the matrix \( M_d := \bigoplus M \cdots \bigoplus M \) (d times) is the matrix direct sum of \( d \) matrices \( M = (M_{jj'}) \in [\mathbb{C}^m] \) defined by
\[
M_{jj'} := \delta_{jj'} z_1 + \delta_{j+1,j'}, \quad j \in J \setminus \{m\}, \quad j' \in \mathbb{J}
\]
and \( M_{mj'} := \delta_{jm} z_1, \quad j' \in J \). For \( m = 1 \) one puts \( M := z_1 \).

**Proof.** By definition, the action of \( L_{\text{max}} \) on \( f + k \in \mathcal{H}_m \oplus \mathcal{K}_A \) is given (in the generalized sense) by
\[
L_{\text{max}}(f + k) = L f + \sum_{\sigma} z_1 d_{\sigma 1}(k) h_{\sigma 1} + \sum_{\sigma} \sum_{j=2}^{m} d_{\sigma j}(k) (L - z_1)^{-j} \varphi_\sigma
\]
\[
= L f + z_1 k + \sum_{\sigma} \sum_{j=1}^{m-1} d_{\sigma,j+1}(k) h_{\sigma j}.
\]
Now \( Lf \in \mathcal{H}_{m-2} \), thus the range restriction \( L_{\text{max}}(f + k) \in \mathcal{H}_{m} + \mathcal{R}_A \) implies that \( f \) is of the form \( f^\# + g \) for some \( f^\# \in \mathcal{H}_{m+2} \) and \( g \in \mathcal{H}_{m} \) such that \( Lg \in \mathcal{H}_A \). By noting that \( Lh_{m+1}(c) = z_1h_{m+1}(c) + h_m(c) \ (h_m(c) \in \mathcal{R}_A \) is defined similar to \( h_{m+1}(c) \)) for an arbitrary \( c \in \mathbb{C}^d \), one concludes that \( g = h_{m+1}(c) \), and the required result follows. \( \Box \)

Now we state the main realization theorem in the A-model.

**Theorem 2.2.** Assume that an invertible Hermitian matrix \( G_A \) satisfies the commutation relation

\[
G_A \mathcal{M}_d = \mathcal{M}_d^* G_A.
\]

Then the triple \((\mathbb{C}^d, \Gamma^A_0, \Gamma^A_1)\), where \( \Gamma^A := (\Gamma^A_0, \Gamma^A_1) : \text{dom } A_{\text{max}} \to \mathbb{C}^d \times \mathbb{C}^d \) is defined by

\[
\Gamma^A_0(f^\# + h_{m+1}(c) + k) := c,
\]

\[
\Gamma^A_1(f^\# + h_{m+1}(c) + k) := \langle \varphi, f^\# \rangle - [G_A d(k)]_m
\]

with

\[
[G_A d(k)]_m := ([G_A d(k)]_{\sigma m}) \in \mathbb{C}^d
\]

and \( f^\# \in \mathcal{H}_{m+2}, k \in \mathcal{R}_A, c \in \mathbb{C}^d \), is an ordinary boundary triple (OBT) for the adjoint \( A_{\text{min}} = A_{\text{max}} \) of a densely defined, closed, and symmetric operator \( A_{\text{min}} = A_{\text{max}} \mid_{\ker \Gamma^A} \) in \( \mathcal{H}_A \).

Moreover, for a (closed) linear relation \( \Theta \) in \( \mathbb{C}^d \), a proper extension \( A_\Theta \) of \( A_{\text{min}} \) is the restriction of \( A_{\text{max}} \) to the set of \( f \in \text{dom } A_{\text{max}} \) such that \( \Gamma^A f \in \Theta \). The Krein–Naimark resolvent formula reads

\[
(A_\Theta - z)^{-1} = (A_0 - z)^{-1} + \gamma_A(z)(\Theta - M_A(z))^{-1}\gamma_A(\overline{z})^*
\]

for \( z \in \text{res } A_0 \cap \text{res } A_\Theta \). The resolvent of a distinguished self-adjoint extension \( A_0 := A_{\{0\} \times \mathbb{C}^d} \) is given by

\[
(A_0 - z)^{-1} = U_A^*[L - z]^{-1} \oplus (\mathcal{M}_d - z)^{-1}]U_A
\]

for \( z \in \text{res } A_0 = \text{res } L \setminus \{z_1\} \). The \( \gamma \)-field \( \gamma_A \) and the Weyl function \( M_A \) associated with \((\mathbb{C}^d, \Gamma^A_0, \Gamma^A_1)\) are given by

\[
\gamma_A(z) \in \mathbb{C}^d = \mathcal{M}_z(A_{\text{max}}) = \left\{ \sum c_\sigma F_\sigma(z) \mid c_\sigma \in \mathbb{C} \right\}, \quad F_\sigma(z) := \frac{g_\sigma(z)}{(z - z_1)^m}
\]

and

\[
M_A(z) = g(z) + r(z) \quad \text{on } \mathbb{C}^d
\]

for \( z \in \text{res } A_0 \). The Krein Q-function \( q \) of \( L_{\text{min}} \) is defined by

\[
q(z) = ([q(z)]_{\sigma \sigma'}) \in [\mathbb{C}^d], \quad [q(z)]_{\sigma \sigma'} := (z - z_1) \langle \varphi_\sigma, (L - z)^{-1} h_{\sigma', m+1} \rangle
\]
for $z \in \text{res } L$, and the generalized Nevanlinna function $r$ is defined by

$$r(z) = ([r(z)]_{\sigma'}) \in [\mathbb{C}^d], \quad [r(z)]_{\sigma'} := - \sum_j \frac{[G_A]_{\sigma m, \sigma' j}}{(z - z_1)^{m-j+1}}$$

for $z \in \mathbb{C} \setminus \{z_1\}$.

**Proof.** By Lemma 2.1, the boundary form of $A_{\text{max}}$ is given by

$$[f, A_{\text{max}}g]_\Lambda - [A_{\text{max}}f, g]_\Lambda = \langle d(k), (G_{2R} - G_{2R}^*)d(k') \rangle_{\mathbb{C}^d}$$

$$+ \langle \Gamma_0^A f, \Gamma_1^A g \rangle_{\mathbb{C}^d} - \langle \Gamma_2^A f, \Gamma_2^A g \rangle_{\mathbb{C}^d}$$

with $G_{2R} := \mathcal{G}_A \mathcal{M}_d$, where $f = f^# + h_{m+1}(c) + k \in \text{dom } A_{\text{max}}$; $g = g^# + h_{m+1}(c') + k' \in \text{dom } A_{\text{max}}$; $f^#, g^# \in \mathfrak{S}_{m+2}; c, c' \in \mathbb{C}^d$; $k, k' \in \mathfrak{K}_A$. Assuming that $\mathcal{G}_A$ is invertible, the adjoint $A_{\text{min}} := A_{\text{max}}^*$ in $\mathcal{H}_A$ is given by

$$\text{dom } A_{\text{min}} = \ker \Gamma^A,$$

$$A_{\text{min}}(f^# + k) = Lf^# + \sum_{\alpha} [\mathcal{G}_A^{-1} \mathcal{M}_d^2 \mathcal{G}_A d(k)]_\alpha h_\alpha$$

and hence the boundary form of $A_{\text{min}}$ reads

$$[f, A_{\text{min}}g]_\Lambda - [A_{\text{min}}f, g]_\Lambda = \langle d(k), (G_{2R} - G_{2R}^*)d(k') \rangle_{\mathbb{C}^d}$$

with $f = f^# + k \in \text{dom } A_{\text{min}}$ and $g = g^# + k' \in \text{dom } A_{\text{min}}$ as above. One verifies that the adjoint $A_{\text{min}}^* = A_{\text{max}}$, and hence $A_{\text{max}}$ is closed in $\mathcal{H}_A$.

If (2.3) holds, the boundary form of $A_{\text{min}}^*$ satisfies an abstract Green identity. Thus, since $\Gamma^A$ is single-valued and surjective, the triple $(\mathbb{C}^d, \Gamma^A, \Gamma^A_1)$ is an OBT for $A_{\text{min}}^*$.

The eigenvalue equation for $A_{\text{max}}$ yields

$$f^# = (z - z_1)(L - z)^{-1} h_{m+1}(c), \quad d(k) = -(\mathcal{M}_d - z)^{-1} \eta(c)$$

for $f^# + h_{m+1}(c) + k \in \text{dom } A_{\text{max}}$ as above. Now

$$[(\mathcal{M}_d - z)^{-1} \eta(c)]_{\sigma j} = \sum_{\sigma'} [(\mathcal{M}_d - z)^{-1}]_{\sigma j, \sigma' m} c_{\sigma'}$$

with $c = (c_{\sigma}) \in \mathbb{C}^d$ and with

$$[(\mathcal{M}_d - z)^{-1}]_{\sigma j, \sigma' m} = \delta_{\sigma \sigma'}[(\mathcal{M}_d - z)^{-1}]_{jm}, \quad [(\mathcal{M} - z)^{-1}]_{jm} = \frac{-1}{(z - z_1)^{m-j+1}}.$$ 

Thus, by noting that

$$(L - z)^{-1}(L - z_1)^{-m} + \sum_j (L - z_1)^{-j}(z - z_1)^{-m+j-1} = (L - z)^{-1}(z - z_1)^{-m}$$

one concludes that the eigenvector $f^# + h_{m+1}(c) + k \in \mathcal{M}_z(A_{\text{max}})$ is given as stated in the theorem.
Finally, the Weyl function

$$M_A(z)c = \langle \varphi, f^\# \rangle - [G_A d(k)]_m$$

for $f^\#$ and $k$ as in (2.4). The first term on the right-hand side defines $q(z)c$ and the second term defines $r(z)c$. \hfill \Box

Let us mention that the $Q$-function $q$ is actually the Weyl function associated with a certain boundary triple for $L^*_\min$; see Corollary 3.3 below. While $q$ is a Nevanlinna function, $r$ is a generalized Nevanlinna function, and the Nevanlinna class $[5, 2]$ depends on the particular choice of $G_A$.

The matrix $G_{2r} := G_A \mathcal{M}_d$ is Hermitian iff

(2.5) \quad $[G_A]_{\sigma j, \sigma' j'} = 0$,

$[G_A]_{\sigma j, \sigma' m} = [G_A]_{\sigma' m, \sigma j} = [G_A]_{\sigma j+1, \sigma' m-1}$,

$\quad j, j' \in J \setminus \{m\}$

for $m \geq 2$. For $m = 1$, however, the matrix $G_{2r} = z_1 G_A$ is automatically Hermitian.

Due to (2.5), several remarks are in order. First one verifies that $r$ is symmetric with respect to the real axis, that is, $r(z)^* = r(\overline{z})$, because $[G_A]_{\sigma m, \sigma' j} = [G_A]_{\sigma j, \sigma' m}$ ($j \in J$) by (2.5). Note that $q(z)^* = q(\overline{z})$ is clear from the definition. Next, one observes that the Gram matrix $\tilde{G}_A$ does not satisfy (2.3) for $m \geq 2$, because $[\tilde{G}_A]_{\sigma_1, \sigma_1} > 0$. This shows that, in order use Theorem 2.2 for $m \geq 2$, one cannot define the Gram matrix of the A-model in a way that is done in the peak model.

**Remark 2.6.** Let us recall that in the peak model the parameters $\{a_j\}$ are all necessarily distinct. However, putting $a_j = -z_1 + \delta_{j-1}$ for $\delta_j \neq 0$ and $j \in J \setminus \{1\}$ and $m \geq 2$, and formally taking the limits $\delta_j \to \delta_{j-1}$, as well as $\delta_1 \to 0$, one can show by induction that the $Q$-function associated with the Gram matrix $G$ of the peak model approaches $r$, up to $O(\delta_1)$, with $[G_A]_{\sigma m, \sigma' j} = [G_A]_{\sigma j, \sigma' m}$. Notice that $[\tilde{G}_A]_{\sigma j, \sigma' j}$ with $m \geq 2$, satisfies the second relation in (2.5). On the other hand, taking the above described limits, the matrix element $G_{\sigma_1, \sigma_2} = [\tilde{G}_A]_{\sigma_1, \sigma_1} + O(\delta_1)$, so the requirement that $G$ must be diagonal in $j$—which is essential in applying the extension theory of symmetric operators in the peak model—fails for $m \geq 2$. For $m = 1$, both models produce the same Nevanlinna function $r(z) = G_A/\langle z_1 - z \rangle$, that is $G_A = \tilde{G}_A(\in [\mathbb{C}^d])$.

### 3. Restrictions to the Hilbert subspaces

In this section we assume that the Hilbert spaces $\mathcal{H}_n$ are expressed as the Hilbert sums $\mathcal{H}_n = \mathcal{H}_n^- \oplus \mathcal{H}_n^+$ of their subspaces $\mathcal{H}_n^- := P^- \mathcal{H}_n$, where $P^-$ (resp. $P^+$) is the orthogonal projection in $\mathcal{H}_n$ to $\mathcal{H}_n^-$ (resp. $\mathcal{H}_n^+$), and it satisfies $\mathcal{H}_{n+1}^- \subset \mathcal{H}_n^-$, with the inclusion being dense. According to the above decomposition, each element $f \in \mathcal{H}_n$ splits into the (unique) sum of elements $f^- \in \mathcal{H}_n^-$ and $f^+ \in \mathcal{H}_n^+$. The above situation frequently occurs in quantum mechanical applications, for example when $L$ is the two-particle operator, where each particle separately has spin
In this case typically $\mathcal{H}_0 = L^2(\mathbb{R}^\nu) \otimes \mathbb{C}^4$, with some $\nu \in \mathbb{N}$; see also Section 1 for the two-particle Rashba operator. The space $\mathbb{C}^4$ is identified with $\mathbb{C}^1 \oplus \mathbb{C}^3$, where the space $\mathbb{C}^1$ is associated with the antisymmetric (or singlet) $\mathfrak{su}_2$ representation $1$, with the basis $\{|00\rangle\}$, while the space $\mathbb{C}^3$ is associated with the symmetric (or triplet) $\mathfrak{su}_2$ representation $3$, with the basis $\{|1s\rangle \mid s \in \{-1,0,1\}\}$. Thus, given $f = \sum_{\sigma} f_{\sigma} \otimes |\sigma\rangle$, $f_{\sigma} \in H^m(\mathbb{R}^\nu)$, the function $f^- = f_{00} \otimes |00\rangle$ is antisymmetric with respect to the spin-exchange transformation, while the function $f^+ = \sum_{\sigma} f_{\sigma} \otimes |1s\rangle$ is symmetric with respect to the spin-exchange transformation. Let us recall that the spin-exchange transformation acts on $|\sigma\rangle = |Ss\rangle \in \mathbb{C}^4$ as the operator of multiplication by $(-1)^{S+1}$.

We are going to derive an analogue of Theorem 2.2 for the operator whose domain accounts for the above described Hilbert space decomposition.

Consider the operator $A'$ in $\mathcal{H}_{A}'$, which is a counterpart of the operator $A_{\max}$ in $\mathcal{H}_A$ obtained by applying $U_A$. Let $A^\pm$ be the restriction of $A'$ to the domain $\Pi^\pm$ dom $A'$. The operator $\Pi^\pm := P^\pm \oplus I$ is bounded and self-adjoint in $\mathcal{H}_A'$, and it leaves dom $A'$ invariant. Note that dom $A^- \cap$ dom $A^+ = \{0\} \otimes \mathbb{C}^{md}$.

An element $f^-$ from dom $A^-$ is of the form $(f^#_+ + h_{m+1}^- (c), \xi)$, where $f^#_+ \in \mathcal{H}_{m+2}$, $h_{m+1}^- (c) := P^- h_{m+1} (c)$, $c \in \mathbb{C}^d$, and $\xi \in \mathbb{C}^{md}$. The similar form applies to $f^+ \in$ dom $A^+$, with the subscript “minus” replaced by “plus”. Thus the boundary form of $A^-$ is given by

$$[f^-, A^- g^-]'_A - [A^- f^-, g^-]'_A = \langle \xi, (G_{2\mathbb{R}} - G_{2\mathbb{R}}^*) \xi \rangle_{\mathbb{C}^{md}}$$

(3.1)

(and similarly for $A^+$) with $f^- \in \text{dom } A^-$ as above, and with $g^- \in \text{dom } A^-$ of the form $(g^#_+ + h_{m+1}^- (c'), \xi')$, where $g^#_+ \in \mathcal{H}_{m+2}$, $c' \in \mathbb{C}^d$, and $\xi' \in \mathbb{C}^{md}$. The operator $\Gamma^- := (\Gamma_0^-, \Gamma_1^-) \colon \text{dom } A^- \to \mathbb{C}^d \times \mathbb{C}^d$ is defined by

$$\Gamma_0^-(f^#_+ + h_{m+1}^- (c), \xi) := c,$n

$$\Gamma_1^-(f^#_+ + h_{m+1}^- (c), \xi) := \langle \varphi^-, f^#_- \rangle - [G_{A} \xi]_m.$$

The duality pairing $\langle \varphi^-, \cdot \rangle = (\langle \varphi^-, \cdot \rangle) : \mathcal{H}_{m+2} \to \mathbb{C}^d$, where the functional

$$\varphi^- := (L - zI)^{m+1} h_{\sigma,m+1}^- \in \mathcal{H}_{-m-2} \oplus \mathcal{H}_{-m-1}, \quad h_{\sigma,m+1}^- := P^- h_{\sigma,m+1}.$$

Note that $L$ does not necessarily commute with $P^\pm$.

Assuming that $G_{A}$ is invertible, the adjoint $A^-_{\min} := A^{*-} \in \mathcal{H}_A'$ is given by

$$\text{dom } A^-_{\min} = \ker \Gamma^-,$n

$$A^-_{\min}(f^#_+, \xi) = (Lf^#, G_{A}^{-1} M_{\mathbb{R}} G_{A} \xi)$$

with $f^#_+ \in \mathcal{H}_{m+2}$ and $\xi \in \mathbb{C}^{md}$. The extension $\Gamma^- := (\Gamma_0^-, \Gamma_1^-)$ of $\Gamma^-$ is defined by

$$\Gamma_0^- (f^#_+ + h_{m+1}^- (c), \xi) := c.$$
It follows that the $A$-model is not applicable directly to $A^-$ (resp. $A^+$), but rather to its closure $A_{\text{max}}^-$ (resp. $A_{\text{max}}^+$), which is given by

$$\text{dom} A_{\text{max}}^- = \{(f^# + h_{m+1}(c), \xi) \mid f^# \in \mathcal{S}_{m+2}; c \in \mathbb{C}^d; \xi \in \mathbb{C}^{md}\},$$

$$A_{\text{max}}^-(f^# + h_{m+1}(c), \xi) = (Lf^# + z_1^*h_{m+1}(c), \mathcal{M}_\xi \eta(c)).$$

The boundary form of $A_{\text{max}}^-$ is as in (3.1), with $\Gamma^-$ replaced by $\tilde{\Gamma}^-$ and with $f^-, g^-$ from dom $A_{\text{max}}^-$.

One concludes that the operator $A_{\text{min}}^-$ is a densely defined, closed restriction of $A_{\text{max}}^-$ to ker $\tilde{\Gamma}^-$, and it is symmetric in $\mathcal{H}'$ iff an invertible matrix $\mathcal{G}_A$ satisfies the commutation relation (2.3). If (2.3) holds, the boundary form of $A_{\text{min}}^-$ satisfies an abstract Green identity as described above. Thus, since $\tilde{\Gamma}^-$ is single-valued and surjective, the triple $(\mathbb{C}^d, \tilde{\Gamma}_0^-, \tilde{\Gamma}_1^-)$ is an OBT for $A_{\text{min}}^* = A_{\text{max}}^-.$

**Theorem 3.2.** Assume that an invertible Hermitian matrix $\mathcal{G}_A$ satisfies the commutation relation (2.3). Then the triple $(\mathbb{C}^d, \tilde{\Gamma}_0^-, \tilde{\Gamma}_1^-)$ is an OBT for the adjoint $A_{\text{min}}^* = A_{\text{max}}^-$ of a densely defined, closed, and symmetric operator $A_{\text{min}}^- \in \mathcal{H}'_\lambda$. For a (closed) linear relation $\Theta$ in $\mathbb{C}^d$, a proper extension $A_{\Theta}^-$ of $A_{\text{min}}^-$ is the restriction of $A_{\text{max}}^-$ to the set of $f \in \text{dom} A_{\text{max}}^-$ such that $\tilde{\Gamma}^- f \in \Theta$. The Krein-Naimark resolution formula reads

$$(A_{\Theta}^- - z)^{-1} = (A_0^- - z)^{-1} + \gamma^{-\lambda}_A(z)(\Theta - M_A^{-\lambda}(z))^{-1}\gamma_A^{-\lambda}(z)^*$$

for $z \in \text{res} A_0 \cap \text{res} A_{\Theta}^-$, with a distinguished self-adjoint extension $A_0^\Theta := U^\lambda A_0 U^\lambda$. The $\gamma$-field $\gamma_A^-$ and the Weyl function $M_A^-$ associated with $(\mathbb{C}^d, \tilde{\Gamma}_0^-, \tilde{\Gamma}_1^-)$ are given by

$$\gamma_A^-(z) \mathbb{C}^d = \mathcal{H}_z(A_{\text{max}}^-) = \{(L - z)^{-1}(L - z_1)h_{m+1}(c), -(\mathcal{M}_d - z)^{-1}\eta(c)) \mid c \in \mathbb{C}^d\}$$

and

$$M_A^-(z) = q^-(z) + r(z) \quad \text{on} \quad \mathbb{C}^d$$

for $z \in \text{res} A_0$. The function $q^-$ is defined by

$$q^-(z) = ([q^-(z)]_{\sigma\sigma'}) \in \mathbb{C}^d, \quad [q^-(z)]_{\sigma\sigma'} := (z - z_1)(\varphi, (L - z)^{-1}h_{\varphi',m+1})$$

for $z \in \text{res} L$, and it is the Weyl function associated with the OBT $(\mathbb{C}^d, \tilde{\Gamma}_{m0}^-, \tilde{\Gamma}_{m1}^-),$

$$\tilde{\Gamma}_{m0}^{-}(f^# + h_{m+1}(c)) := c, \quad \tilde{\Gamma}_{m1}^{-}(f^# + h_{m+1}(c)) := \langle \varphi, f^# \rangle$$

$(f^# \in \mathcal{S}_{m+2}, c \in \mathbb{C}^d)$, for the adjoint $L_{\text{min}}^*$ of a densely defined, closed, and symmetric operator $L_{\text{min}}^- := L \{f \in \mathcal{S}_{m+2} \mid \varphi, f = 0\}$ in $\mathcal{S}_m$; the adjoint operator extends $L|_{\mathcal{S}_{m+2}}$ to the domain $\text{dom} L_{\text{min}}^- = \mathcal{S}_{m+2} + \mathcal{H}_z(L_{\text{min}}^-), \quad z \in \text{res} L$, where the eigenspace $\mathcal{H}_z(L_{\text{min}}^-) = \pi_m \mathcal{H}_z(A_{\text{max}}^-), \quad \pi_m$ denotes an orthogonal projection from $\mathcal{S}_m \oplus \mathbb{C}^{md}$ onto $\mathcal{S}_m$. The corresponding $\gamma$-field is $\pi_m \gamma_A^-.$
An analogous theorem can be formulated for $A^+_{\min}$.

**Proof.** The proof of the first part of the theorem is analogous to that of Theorem 2.2. The (last) part of the theorem concerning the Weyl function $q^-$ is verified by direct computation, by observing that

$$f^# + (L - z)^{-1}(L - z_1)h_{m+1}^-(c) = \hat{f}^# + h_{m+1}(c)$$

with $\hat{f}^# \in \mathcal{H}_{m+2}$ given by $f^# + (z - z_1)(L - z)^{-1}h_{m+1}^-(c)$. Using the latter one also verifies that $\mathcal{H}_{m+2} \cap \mathcal{N}_z(L_{\min}^-) = \{0\}$. \hfill \□

In particular, putting $P^- = I$ (hence $P^+ = 0$), one deduces the following:

**Corollary 3.3.** The Krein Q-function $q$ is the Weyl function associated with the OBT $(\mathbb{C}^d, \Gamma_{m0}, \Gamma_m)$,

$$\Gamma_{m0}(f^# + h_{m+1}(c)) := c, \quad \Gamma_m(f^# + h_{m+1}(c)) := \langle \varphi, f^# \rangle$$

$(f^# \in \mathcal{H}_{m+2}, c \in \mathbb{C}^d)$, for the adjoint $L_{\min}^*$ on $\text{dom} L_{\min}^*$, $\mathcal{H}_{m+2} = \mathcal{H}_{m+2} \cap \mathcal{N}_z(L_{\min}^*)$, where the eigenspace $\mathcal{N}_z(L_{\min}^-) = (L - z)^{-1}h_m(\mathbb{C}^d)$, $z \in \text{res} L$. \hfill \□

The Weyl functions $q^\pm$ can be further decomposed as follows.

**Proposition 3.4.** It holds $q^- = q^{-} + q^{+-}$ on $\text{res} L$, where

$$[q^-(z)]_{\sigma\sigma'} := (z - z_1)\langle \varphi_\sigma, P^-(L - z)^{-1}h_{\sigma',m+1} \rangle,$$

$$[q^{+-}(z)]_{\sigma\sigma'} := (z - z_1)\langle \varphi_\sigma, P^+(L - z)^{-1}h_{\sigma',m+1} \rangle$$

and similarly for $q^+ = q^{++} + q^{+-}$:

$$[q^{++}(z)]_{\sigma\sigma'} := (z - z_1)\langle \varphi_\sigma, P^+(L - z)^{-1}h_{\sigma',m+1} \rangle,$$

$$[q^{+-}(z)]_{\sigma\sigma'} := (z - z_1)\langle \varphi_\sigma, P^-(L - z)^{-1}h_{\sigma',m+1} \rangle.$$

**Proof.** Define $L^- := P^- L |_{\mathcal{D}_0^-}$. Then $L^-$ is self-adjoint in $\mathcal{H}_0^-$, and by the spectral mapping theorem

$$P^- (L - z)^{-1} |_{\mathcal{D}_0^-} = (L^--z)^{-1}.$$

Thus

$$\langle \varphi_\sigma, (L - z)^{-1}h_{\sigma',m+1} \rangle$$

$$= \langle (L - z_1)^{m+1}(L^- - z_1)^{-m-1}\varphi_\sigma, (L - z)^{-1}(L^- - z_1)^{-m-1}\varphi_\sigma \rangle$$

$$= \langle (L - z_1)^{m+1}(L^- - z_1)^{-m-1}\varphi_\sigma, P^-(L - z)^{-1}(L^- - z_1)^{-m-1}\varphi_\sigma \rangle$$

$$+ \langle (L - z_1)^{m+1}(L^- - z_1)^{-m-1}\varphi_\sigma, P^+(L - z)^{-1}(L^- - z_1)^{-m-1}\varphi_\sigma \rangle$$

$$= \langle \varphi_\sigma, (L^--z)^{-1}(L^- - z_1)^{-m-1}\varphi_\sigma \rangle + \langle \varphi_\sigma^+, P^+(L - z)^{-1}h_{\sigma',m+1} \rangle.$$

But, by the functional calculus

$$\langle \varphi_\sigma, (L^--z)^{-1}(L^- - z_1)^{-m-1}\varphi_\sigma \rangle = \langle \varphi_\sigma, P^-(L - z)^{-1}(L - z_1)^{-m-1}\varphi_\sigma \rangle$$
and one deduces the decomposition for \( q^- \) as stated in the proposition. The proof for \( q^+ \) is similar. \( \square \)

Thus \( q^- + q^{++} = q \). If in particular \( L \) commutes with \( P^\pm \), then the functions \( q^- \) and \( q^{++} \) vanish.

Next, one shows that an extension \( \hat{A}_{\hat{\Theta}} \) is the closure of the operator \( \hat{A}_{\hat{\Theta}} \) in \( \mathcal{H}_\Lambda \), which is the restriction of \( A^- \) to the set of \( f^- \in \text{dom } A^- \) such that \( \Gamma^- f^- \in \Theta \). The operator \( \hat{A}_{\hat{\Theta}} \) is densely defined, and it is symmetric iff so is \( \Theta \). In particular, if \( \Theta \) is self-adjoint in \( \mathbb{C}^d \), then \( \hat{A}_{\hat{\Theta}} \) is essentially self-adjoint in \( \mathcal{H}_\Lambda \). One notices that dom \( \hat{A}_{\hat{\Theta}} \) (resp. dom \( \hat{A}_{\hat{\Theta}}^* \)) contains the functions from \( \mathcal{S}_{m} \) (resp. \( \mathcal{S}_{m}^\prime \)), while dom \( \hat{A}_{\hat{\Theta}}^\prime \) also contains the functions from the whole \( \mathcal{S}_{m+2} \), i.e. the functions from both subspaces \( \mathcal{S}_{m+2}^\prime \) and \( \mathcal{S}_{m+2}^+ \).

**Theorem 3.5.** Assume that an invertible Hermitian matrix \( G_\Lambda \) satisfies the commutation relation (2.3). For a (closed) linear relation \( \Theta \) in \( \mathbb{C}^d \), let \( \hat{A}_{\hat{\Theta}} \) in \( \mathcal{H}_\Lambda \) be the restriction of \( A^- \) to the set of \( f^- \in \text{dom } A^- \) such that \( \Gamma^- f^- \in \Theta \). The operator \( \hat{A}_{\hat{\Theta}} \) is densely defined, and its adjoint \( \hat{A}_{\hat{\Theta}}^* \) in \( \mathcal{H}_\Lambda \) is the operator \( \hat{A}_{\hat{\Theta}}^* \). In particular: (a) if \( \Theta \) is symmetric, then so is \( \hat{A}_{\hat{\Theta}} \); (b) if \( \Theta \) is self-adjoint, then \( \hat{A}_{\hat{\Theta}} \) is essentially self-adjoint.

**Proof.** We identify the operators with their graphs. Thus the adjoint \( \hat{A}_{\hat{\Theta}}^* \) consists of the pairs \((y, x) \in H'_\Lambda \times H'_\Lambda\) such that \( \forall f^- \in \text{dom } \hat{A}_{\hat{\Theta}} \) \( [f^-, x]'_\Lambda = [\hat{A}_{\hat{\Theta}} f^-, y]'_\Lambda \). Using the representation of \( f^- \) as in (3.1), as well as putting \( x = (x^y, \xi_x) \in \mathcal{S}_m \oplus \mathbb{C}^{md} \) and \( y = (y^z, \xi_y) \in \mathcal{S}_m \oplus \mathbb{C}^{md} \), one finds that

\[
\langle c, (h^-_{m+1}, x^y - z_1 y^z)'_m \rangle_{\mathcal{C}^d} = \langle \hat{\Theta}^{\#}, Ly^z - x^y \rangle_m - \langle \xi, G_\Lambda (x^- - m d \xi_y) \rangle_{\mathbb{C}^{md}}
\]

where one also uses the vector notation \( \langle h^-_{m+1}, \xi_x \rangle_m = \langle h^-_{m+1}, \xi_m \rangle_m \). On the other hand, the boundary condition \( \Gamma^- f^- \in \Theta \) implies that \( \exists (r, s) \in \Theta^* \)

\[
\langle c, s \rangle_{\mathcal{C}^d} = \langle \hat{\Theta}^{\#}, \omega r \rangle = \langle \xi, G_\Lambda \eta(r) \rangle_{\mathbb{C}^{md}}
\]

with \( \omega r := \sum_{\sigma} r \varphi_{\sigma}^r, r = (r_{\sigma}) \). Thus it follows that

\[
s = \langle \hat{\Theta}^{\#}, L - z_1 \rangle^{-1} (x^y - z_1 y^z) - [G_\Lambda \xi_y]'_m, \quad \omega r = \langle L - z_1 \rangle^{m} (Ly^z - x^y)
\]

and \( \xi_x = M_d \xi_y + \eta(r) \). Since \( \langle L - z_1 \rangle^{-m-1} \omega r = h^-_{m+1}(r) \), one finds that

\[
(L - z_1)^{-1} (x^y - z_1 y^z) = y^z - h^-_{m+1}(r)
\]

and concludes that \( y^z - h^-_{m+1}(r) =: y^\# \in \mathcal{S}_{m+2} \); hence \( \hat{A}_{\hat{\Theta}}^* = A_{\hat{\Theta}}^* \).

In particular, if \( \Theta \subseteq \Theta^* \) then \( (\hat{A}_{\hat{\Theta}} \subseteq A_{\hat{\Theta}} \subseteq A_{\hat{\Theta}}^* \), i.e. \( \hat{A}_{\hat{\Theta}} \) is symmetric; if \( \Theta = \Theta^* \) then the closure \( \hat{A}_{\hat{\Theta}}^* = A_{\hat{\Theta}}^* \) is self-adjoint. \( \square \)

Observe that the if argument in the theorem can be strengthened to the iff argument due to the bijective correspondence \( \Theta \leftrightarrow \hat{A}_{\hat{\Theta}} \). An analogous theorem can be formulated for \( \hat{A}_{\hat{\Theta}}^* \).

The next proposition describes the eigenspace of \( \hat{A}_{\hat{\Theta}} \subseteq A_{\hat{\Theta}} \).
Proposition 3.6. Assume the conditions in Theorem 3.5. The eigenspace

$$\mathfrak{N}_2(\mathcal{A}_0) = \{(L - z)^{-1}(L - z_1)h_{m+1}(c), -(\mathcal{M}_d - z)^{-1}\eta(c) | h_{m+1}(c) \in \mathcal{R}^z_2; c \in \mathfrak{N}_0(\Theta - M_\Lambda^-(z))\}$$

for \( z \in \text{res} \, A_0 \). The set \( \mathcal{R}^z_2 := (L - z)\mathcal{D}^- \), where the set \( \mathcal{D}^- \) consists of \( f^- \in \mathfrak{H}^{-2} \) such that \( Lf^- \in \mathfrak{H}^- \).

Proof. For \( f^- \) as in (3.1), the eigenvalue equation yields \( Lf^\#^- \in \ker P^+ = \mathfrak{H}_m^- \) and

$$\begin{align*}
(L - z)f^\#^- &= (z - z_1)h_{m+1}(c) + h^+, \quad h^+ \in \ker P^- = \mathfrak{H}_m^+
\end{align*}$$

and \( \xi = -(\mathcal{M}_d - z)^{-1}\eta(c) \), with \( z \in \text{res} \, A_0 \). Thus \( f^\#^- \in \mathcal{D}^- \) and \( h^+ = 0 \). But then the condition \( f^\#^- \in \mathcal{D}^- \) is equivalent to \( h_{m+1}(c) \in \mathcal{R}^z_2 \). \( \square \)

One verifies that

$$\mathfrak{N}_2(\mathcal{A}_0) \subseteq \Pi^-(\mathfrak{N}_2(\mathcal{A}_0)) \quad \text{where} \quad \mathfrak{N}_2(\mathcal{A}_0) = \gamma_\Lambda(z)\mathfrak{N}_0(\Theta - M_\Lambda^-(z))$$

with \( z \in \text{res} \, A_0 \). To compute the eigenspace \( \mathfrak{N}_2(\mathcal{A}_0^-) \) one uses Theorem 3.2 from which it follows that each element from \( \mathfrak{N}_2(\mathcal{A}_0^-) \) is given by \( \gamma_\Lambda(z)c \), where \( c \) is found from the boundary condition, which is \( (c, M_\Lambda^-(z)c) \in \Theta \).

4. Example: Two-particle Rashba operator

In the present section we apply the A-model to the spectral analysis of the self-adjoint two-particle Rashba operator \( L \) in the Hilbert space \( \mathfrak{H}_0 = L^2(\mathbb{R}^6) \otimes \mathbb{C}^4 \), written in the center-of-mass coordinate system \( K = (x, X) \) (where \( x \in \mathbb{R}^3 \) is the relative coordinate and \( X \in \mathbb{R}^3 \) is the center-of-mass coordinate) and combined with weak spin-orbit coupling of strength \( \varepsilon \gg 0 \) and Rashba coupling (or else magnetic field) of strength \( \beta \gg 0 \); by saying “weak” we mean that \( \varepsilon \ll \sqrt{2\beta} \) is arbitrarily small; hence \( L \gg -2\beta \).

Let us recall from [16] that \( L \) is unitarily equivalent to \( \tilde{L} := A \otimes I + I \otimes B + \varepsilon D \) in the space \( (L^2(\mathbb{R}^3) \otimes \mathbb{C}^2)^2 \), where \( A = A(\varepsilon, \beta) \) (resp. \( B = B(\varepsilon, \beta) \)) represents the differential expression in the relative (resp. center-of-mass) coordinate \( x \) (resp. \( X \)), while \( D \) is the differential expression in both \( x \) and \( X \). For \( \varepsilon = 0 \), \( A(0, \beta) \otimes I + I \otimes B(0, \beta) \) admits the separation of variables, i.e. the two-particle case reduces to the single-particle case for the \( x \)-dependent interaction potential. We assume that the interaction is point-like, and so in this case one can apply the classical extension theory of symmetric operators (see e.g. [1] Theorem 5.2.1). For \( \varepsilon > 0 \), however, \( \tilde{L} \) is no longer separable in the center-of-mass coordinate system \( K \), and the point-like perturbation is of class \( \mathfrak{H}_{-4} \setminus \mathfrak{H}_{-3} \) ([16, Theorem 11]).
We now consider singular perturbations of \( L \) more rigorously. Since \( \mathbb{C}^4 \) is identified with \( \mathbb{C}^1 \oplus \mathbb{C}^3 \) (recall the discussion in Section [3]), the index set

\[
(4.1) \quad \mathcal{S} = \{(0, 0), (1, 0), (1, 1), (1, -1)\}
\]

and each \( \sigma \in \mathcal{S} \) is represented by the pair \((S, s)\). At some point it will be convenient to interpret \( \mathcal{S} \) as an ordered set, but at the present moment this is inessential. The action of \( \varphi_\sigma \in \mathcal{H}_{-4} \setminus \mathcal{H}_{-3} \) on \( f = \sum f_\sigma \otimes |\sigma| \), \( f_\sigma \in H^4(\mathbb{R}^6) \), is realized via the duality pairing \( \langle \varphi_\sigma, f \rangle = N_\sigma f_\sigma(K_0) \) with some fixed \( K_0 = (0, X_0) \in \mathbb{R}^6 \). The normalization constant \( N_\sigma > 0 \) is chosen such that \((L^2 + I)^{-1} \varphi_\sigma \) is the unit vector in \( \mathcal{H}_0 \). Then according to [16] Theorem 11

\[
N_\sigma^2 = \frac{1}{\mu_\sigma} - \varepsilon^2 \frac{\mu_\sigma}{\nu_\sigma^2} + O(\varepsilon^4)
\]

with the positive numbers

\[
\mu_\sigma := \frac{1}{512 \pi^3} \left( \delta_{s0} \pi + 2 \delta_S \left[ \delta_s (-2 \beta + \theta_\beta (1 + 4 \beta^2)) 
+ \delta_{s,-1} (2 \beta + (\pi - \theta_\beta)(1 + 4 \beta^2)) \right] \right)
\]

and

\[
\nu_\sigma := \frac{1}{1536 \pi^3 \beta^2} \left\{ \frac{1}{4} \delta_{s0} \left[ 2 \beta \left[ \pi (5 + 4 \beta^2) - 11 \theta_\beta + 4 \beta (2 - 3 \beta \theta_\beta) \right] 
- 4 \log(1 + 4 \beta^2) + \beta \sqrt{1 + 4 \beta^2} \left[ (4 \beta (\pi - \theta_\beta) - \log(1 + 4 \beta^2)) \cos \theta_\beta 
+ 2 \left( \pi - \theta_\beta + \beta \log(1 + 4 \beta^2) \right) \sin \theta_\beta \right] 
+ \delta_S \left[ 8 \beta^2 (1 - 2 \beta \theta_\beta) + \log(1 + 4 \beta^2) \right] 
+ \delta_{s,-1} \left[ 8 \beta^2 (1 + 2 \beta (\pi - \theta_\beta)) + \log(1 + 4 \beta^2) \right] \right\}
\]

and \( \theta_\beta := \arg(2 \beta + i) \).

Throughout, \( \log \) of a nonzero complex number \( z \) is defined by \( \log z := \log |z| + i \arg z \), where \( \arg \) is the principal value of the argument; hence \( \arg z = - \arg z \). For \( z = x \in \mathbb{R} \setminus \{0\} \), we assume that \( \arg z := \arg(x + i0) \); hence \( \arg x = 0 \) for \( x > 0 \) and \( \arg x = \pi \) for \( x < 0 \). With this definition, \( \arg(x - i0) = - \arg x \) for \( x \) as before.

Remark 4.2. One can show that the non-diagonal element of the Gram matrix \( G \) in the peak model is given, for example, by

\[
G_{(S,0)^1,(S,0)^2} = C \frac{2a_1a_2 \log(a_1/a_2) - a_1^2 + a_2^2}{(a_2 - a_1)^3}
\]

for \( \varepsilon = 0 \) and \( a_1, a_2 > 2 \beta \ (a_1 \neq a_2) \) and some normalization constant \( C > 0 \). The formula indicates that \( G \) is non-diagonal in \( j \in J = \{1, 2\} \), so the peak model is not applicable for \( \varepsilon > 0 \) arbitrarily small (but nonzero).
4.1. Weyl function $q$. Putting $z_1 \in \text{res} \ L \cap \mathbb{R} = (-\infty, -2\beta)$ and applying [16] Propositions 8, 9, A.1, one finds that the Weyl function $q$ is the matrix valued Nevanlinna function given by

$$q(z) = q^0(z) + \varepsilon^2 q^1(z) + O(\varepsilon^4)$$

with the diagonal matrices in $\mathbb{C}^4$

$$q^t(z) := \text{diag}\left\{ \frac{\varphi_\sigma}{(z - z_1)^2} \left( \sum_{p=0}^2 q^t_{\sigma p} z^p - \psi_\sigma(z) \right) \right\}, \quad t \in \{0, 1\}$$

defined for $z \in \mathbb{C} \setminus \{z_1\}$. The normalization constant $\varphi_\sigma := (128 \pi^3 \mu_\sigma)^{-1} > 0$, the (real valued) coefficients

$$q^0_{\sigma 0} := \frac{1}{2} z_1(4\beta_\sigma + z_1) + 4\beta_\sigma^2 \log(2\beta_\sigma - z_1),$$

$$q^0_{\sigma 1} := -2[1 + \beta_\sigma(1 + 2 \log(2\beta_\sigma - z_1))],$$

$$q^0_{\sigma 2} := \frac{3}{2} + \log(2\beta_\sigma - z_1)$$

and

$$q^1_{\sigma 0} := \frac{1}{6\beta_\sigma^2} (-\psi_\sigma(z_1) + z_1\psi'_\sigma(z_1) - \frac{1}{2} z_1^2 \psi''_\sigma(z_1)) - \frac{\mu_\sigma^2}{\nu_\sigma^2} q^0_{\sigma 0},$$

$$q^1_{\sigma 1} := \frac{1}{6\beta_\sigma^2} (-\psi'_\sigma(z_1) + z_1\psi''_\sigma(z_1)) - \frac{\mu_\sigma^2}{\nu_\sigma^2} q^0_{\sigma 1},$$

$$q^1_{\sigma 2} := -\frac{1}{12\beta_\sigma^2} \psi''_\sigma(z_1) - \frac{\mu_\sigma^2}{\nu_\sigma^2} q^0_{\sigma 2}$$

with

$$\beta_\sigma := \begin{cases} 0, & \sigma \in \{(0, 0), (1, 0)\}, \\ \beta_s := \beta s, & \sigma = (1, s), s \in \{-1, 1\}. \end{cases}$$

The logarithmic functions

$$\psi^0_\sigma(z) := \chi^0(2\beta_\sigma - z), \quad \chi^t(z) := \begin{cases} z^{t+2} \log z, & z \in \mathbb{C} \setminus \{0\}, \\ 0, & z = 0 \end{cases}$$

and

$$\psi^1_\sigma(z) := -\frac{1}{6\beta_\sigma^2} \psi_\sigma(z) - \frac{\mu_\sigma^2}{\nu_\sigma^2} \psi^0_\sigma(z),$$

$$\psi_\sigma(z) := (-1)^{s+1} \chi^1(-z) + \omega_\sigma(4\beta_\sigma + z) \psi^0_\sigma(z) + \frac{\delta_{s0}}{2} \sum_{s'=\pm 1} \chi^1(2\beta_{s'} - z)$$

with $\omega_\sigma := \delta_{s1}(\delta_{s1} + \delta_{s,-1})$.

We assume that $P^-$ (resp. $P^+$) projects $\mathcal{H}_n = H^a(\mathbb{R}^6) \otimes \mathbb{C}^4$ onto $\mathcal{H}_n^- = H^a(\mathbb{R}^6) \otimes \mathbb{C}^1$ (resp. $\mathcal{H}_n^+ = H^a(\mathbb{R}^6) \otimes \mathbb{C}^3$). Then one also verifies that $q^{-+}$ and $q^{+-}$ vanish up to $O(\varepsilon^4)$. 
Thus by Proposition 3.4, \( q \) is approximated by \( q^{-} + q^{+} \) up to \( O(\varepsilon^{4}) \). The matrices \( q^{\pm}(z) \) are diagonal with the same accuracy \( O(\varepsilon^{4}) \), and the diagonal elements
\[
[q^{-}(z)]_{\sigma \sigma} = \delta_{\sigma, 00} |q(z)|_{00, 00} + O(\varepsilon^{4}), \quad [q^{+}(z)]_{\sigma \sigma} = \delta_{S1} [q(z)]_{1s, 1s} + O(\varepsilon^{4}).
\]

4.2. Weyl function \( M_{A} \). Interval of decrease. Next we list some properties of the Weyl functions \( M_{A} \) and \( M_{A}^{\perp} \) that we use later on.

**Lemma 4.3.** Let \( \lambda \in \mathbb{R} \setminus \{z_1\} \). Then, for \( \varepsilon > 0 \) arbitrarily small, \( \Im[M_{A}(\lambda)]_{\sigma \sigma} = O(\varepsilon^{4}) \) iff \( \lambda \in \mathcal{D}_{\sigma}^{\varepsilon} \), where
\[
\mathcal{D}_{\sigma}^{\varepsilon} := (-\infty, \Sigma_{\sigma}] \setminus \{z_1\}, \quad \Sigma_{\sigma} := \begin{cases} -2\beta, & \sigma = (S, 0) \\ \min\{0, 2\beta_{\sigma}\}, & \sigma = (1, \pm 1) \end{cases}
\]
while for \( \varepsilon = 0 \), \( \Im[M_{A}(\lambda)]_{\sigma \sigma} = 0 \) iff \( \lambda \in \mathcal{D}_{\sigma}^{0} := (-\infty, 2\beta_{\sigma}] \setminus \{z_1\} \).

**Proof.** Because \( r(\lambda)^{*} = r(\lambda) \), one has that \( \Im[M_{A}(\lambda)] = \Im[q(\lambda)] \), and \( \Im[q(\lambda)] \neq 0 \) in general, because by hypothesis \( \lambda \in \mathbb{R} \setminus \{z_1\} \supset \text{res} A_0 \cap \mathbb{R} \). On the other hand, \( \Im[q'(\lambda)]_{\sigma \sigma} = 0 \) iff \( \Im[\psi'_{\sigma}(\lambda)] = 0 \); for \( \varepsilon > 0 \), the latter must hold for both \( t = 0 \) and \( t = 1 \). The statements of the lemma then follow from the definition of \( \psi'_{\sigma} \). \( \square \)

Since \( M_{A} \) is a generalized Nevanlinna function, there exists an interval in \( \mathbb{R} \setminus \{z_1\} \), on which it is (possibly) decreasing. The function \( \lambda \mapsto [r(\lambda)]_{\sigma \sigma} \) is strictly decreasing on the interval \( l_{\sigma} \), which is given by:
\[
l_{\sigma} := \{\lambda \in \mathbb{R} \setminus \{z_1\} | \frac{2[G_{A}]_{\sigma2, \sigma1} + (\lambda - z_1)[G_{A}]_{\sigma2, \sigma2}}{(\lambda - z_1)^3} < 0\}.
\]

By Lemma 4.3, the function \( \lambda \mapsto [M_{A}(\lambda)]_{\sigma \sigma} \) is strictly decreasing on the set, denoted \( \chi_{\sigma}^{z} \), which consists of \( \lambda \in l_{\sigma} \cap \mathcal{D}_{\sigma}^{\varepsilon} \) such that the derivatives satisfy \( [r(\lambda)]_{\sigma \sigma}' < -[q(\lambda)]_{\sigma \sigma}' \leq 0 \) (recall that the Nevanlinna function \( \lambda \mapsto [q(\lambda)]_{\sigma \sigma} \) is monotonically nondecreasing). If \( z_{\varepsilon}^{z} \) solves \( [r(\lambda)]_{\sigma \sigma}' = -[q(\lambda)]_{\sigma \sigma}' \) with respect to \( \lambda \), then \( \chi_{\sigma}^{z} \) can be represented as the union \( l_{\sigma} \cap \mathcal{D}_{\sigma}^{\varepsilon} \cap (z_{\varepsilon}^{z}, \infty) \). The interval \( \chi_{\sigma}^{z} \) can be further narrowed depending on the specific form of \( G_{A} \). Subsequently, \( \lambda \mapsto [M_{A}^{-}(\lambda)]_{00, 00} \) is strictly decreasing on \( \chi_{\sigma}^{00} \), and \( \lambda \mapsto [M_{A}^{\perp}(\lambda)]_{1s, 1s} \) is strictly decreasing on \( \chi_{\sigma}^{1s} \).

4.3. Spectrum. General remarks. We discuss some spectral properties in the case when \( \Theta \) is self-adjoint. By Theorems 3.2 and 5.2 the spectrum
\[
\sigma(A_{0}^{\perp}) = \sigma(A_{0}) \cup \hat{\sigma}_{\Theta}^{\pm}, \quad \hat{\sigma}_{\Theta}^{\pm} := \{\lambda \in \mathbb{R} \setminus \{z_1\} | 0 \in \sigma(\Theta - M_{A}^{\pm}(\lambda))\}.
\]

The subscript “\( \pm \)” indicates that the formulas apply to \( A_{\Theta} \) and \( A_{\Theta}^{\perp} \). Since the spectrum of the self-adjoint extension \( A_{0} \) is \( \{z_1\} \cup [-2\beta, \infty] \), in what follows we shall be interested in the set \( \hat{\sigma}_{\Theta}^{\pm} \), with some Hermitian matrix \( \Theta \). In this case the singular point \( \lambda \in \hat{\sigma}_{\Theta}^{\pm} \) solves \( \text{det}(\Theta - M_{A}^{\pm}(\lambda)) = 0 \). Moreover, \( \sigma_{p}(A_{\Theta}^{\pm}) \setminus \{z_1\} = \hat{\sigma}_{\Theta}^{\pm} \), where \( \sigma_{p}(A_{\Theta}^{\pm}) \) denotes the point spectrum of a self-adjoint extension \( A_{\Theta}^{\pm} \).
**Theorem 4.4.** Let $\Theta$ be an Hermitian matrix.

(a) The point spectrum of $A_\Theta$ is empty above 0 for $\varepsilon > 0$ arbitrarily small and above $2\beta$ for $\varepsilon = 0$.

(b) The eigenvalues of $A_\Theta$ corresponding to the spin state $(0,0)$ have the upper bound $-2\beta$ for $\varepsilon > 0$ arbitrarily small and 0 for $\varepsilon = 0$.

(c) The eigenvalues of $A_\Theta^\pm$ corresponding to the spin state $(1,s)$ have the upper bound $\Sigma_{1s} \leq 0$ for $\varepsilon > 0$ arbitrarily small and $2\beta s$ for $\varepsilon = 0$.

**Proof.** Let $\lambda$ be an eigenvalue from $\mathbb{R}\setminus\{z_1\}$ and $f_\lambda = \gamma_\lambda^z(\lambda)c$ the corresponding eigenvector; $c = (c_\sigma) \in \mathcal{A}_0(\Theta - M_\lambda^z(\lambda))$. Using the relation

$$\frac{M_\lambda^z(z) - M_\lambda^z(w)^*}{z - w} = \gamma_\lambda^z(w)^*\gamma_\lambda^z(z); \quad z, w \in \mathbb{C}\setminus\{z_1\}$$

one finds that ([,]_\lambda^z denotes either [,]_A or [,]_\lambda)

$$[f_\lambda, f_\lambda]^z_\lambda = \langle c, P^z(\lambda)c \rangle \mathcal{C}_\mathcal{D}, \quad P^z(\lambda) := \lim_{y \to 0} y^{-1} \Im M_\lambda^z(\lambda + iy).$$

Since $\lambda \in \mathbb{R}\setminus\{z_1\}$, one has that

$$P^z(\lambda) = \lim_{y \to 0} y^{-1} \Im q^z(\lambda + iy) + r^z(\lambda).$$

Since $f_\lambda \in \mathcal{H}_\Lambda$ (or $f_\lambda \in \mathcal{H}_\Lambda'$ for $A_\Theta^\pm$), and $q^z(\lambda + iy)$ is diagonal (up to $O(\varepsilon^4)$), it must hold

$$\lim_{y \to 0} y^{-1} \Im[q^z(\lambda + iy)]_{\sigma\sigma} < \infty$$

for $\sigma$ such that $c_\sigma \neq 0$. By Lemma 1.3, the above inequality holds iff: (a) $\lambda \in D^z_\sigma$ for $A_\Theta$; (b) $\lambda \in D_{00}^\varepsilon$ and $\sigma = (0,0)$ or $\lambda \in \mathbb{R}\setminus\{z_1\}$ and $\sigma \neq (0,0)$ for $A_\Theta$; (c) $\lambda \in D_{1s}^\varepsilon$ and $\sigma = (1,s)$ or $\lambda \in \mathbb{R}\setminus\{z_1\}$ and $\sigma \neq (1,s)$ for $A_\Theta^\pm$.

Since $D^z_\sigma \subseteq D_{11}^\varepsilon$ for $\varepsilon \geq 0$, (a) implies that the eigenvalue of $A_\Theta$ does not exceed the upper bound of $D_{11}^\varepsilon$. The upper bounds of the eigenvalues of $A_\Theta^\pm$ corresponding to a given spin state follow directly from (b) and (c).

We emphasize that there are at most two singular points corresponding to the same spin state, since $M_\lambda^z(\lambda)$ contains the terms which are quadratic in $\lambda$.

**Remark 4.5.** Let us recall from [15] that, for the single-particle Rashba operator, the point spectrum is empty above the threshold $-\beta$ for $\varepsilon > 0$ small and above $\beta$ for $\varepsilon = 0$.

### 4.4. Asymptotics of eigenvalues.

Having discussed the location of eigenvalues, now we study their specific representation. For simplicity, we assume that the matrix $r(z)$ is diagonal. For example, if (see Remark 2.6) $[G_\Lambda]_{\sigma\sigma'} = [\tilde{G}_\Lambda]_{\sigma\sigma'}$, one can show that in this case $r(z)$ is diagonal up to $O(\varepsilon^4)$, and it is the matrix valued generalized Nevanlinna function of class $\mathcal{N}_4(\mathcal{C}^4)$. 


We examine the singular point \( \lambda \in \hat{\sigma}_\Theta^0 \) of the form \( \lambda^0 + \omega(\varepsilon) \) for some \( \lambda^0 \) from \( \hat{\sigma}_\Theta^0 \) and some real valued \( \omega \), which satisfies \( \omega(0) = 0 \) and is smooth in the neighborhood of the origin:

\[
\omega(\varepsilon) = \sum_{l=1}^{3} \varepsilon^l \omega_l + O(\varepsilon^4); \quad \omega_1 := \omega'(0), \quad \omega_2 := \frac{\omega''(0)}{2}, \quad \omega_3 := \frac{\omega'''(0)}{6}.
\]

The defining equation for the singular point \( \lambda \) reads

\[
\det \left( \Theta - M^{0z}_A(\lambda^0) - \sum_{l=1}^{3} \varepsilon^l H^{l}_l(\lambda^0; \omega_1, \ldots, \omega_l) + O(\varepsilon^4) \right) = 0
\]

with \( M^{0z}_A := q^{0z} + r \) (\( q^{\pm} \), \( t \in \{0, 1\} \), are defined similar to \( q^{\pm} \), but with \( q \) replaced by \( q^t \)) and with the diagonal matrices (the primes denote the derivatives)

\[
H^0_1(\lambda^0; \omega_1) := \omega_1 M^{0z}_A(\lambda^0)', \quad H^0_2(\lambda^0; \omega_1, \omega_2) := q^{1z}(\lambda^0) + \omega_2 M^{0z}_A(\lambda^0)' + \frac{\omega_2^2}{2} M^{0z}_A(\lambda^0)'' ,
\]

\[
H^0_3(\lambda^0; \omega_1, \omega_2, \omega_3) := \omega_1 q^{1z}(\lambda^0)' + \omega_3 M^{0z}_A(\lambda^0)' + \omega_1 \omega_2 M^{0z}_A(\lambda^0)' + \frac{\omega_1^2}{6} M^{0z}_A(\lambda^0)''.
\]

Considering \( S \) in (4.11) as an ordered set, let \( S_{\sigma} \) be the position of \( \sigma \) in \( S \); e.g. \( S_{11} = 3 \). We use the order relation \( \sigma < \sigma' \) iff \( S_{\sigma} < S_{\sigma'} \) for \( \sigma, \sigma' \in S \). Then, the determinant can be written in the form

\[
- \sum_{l=1}^{3} \varepsilon^l D^l(\lambda^0; \omega_1, \ldots, \omega_l) + O(\varepsilon^4)
\]

with the numbers

\[
D^1_1(\lambda^0; \omega_1) := \sum_{\sigma} [H^0_1(\lambda^0; \omega_1)]_{\sigma} m^{0z}_\sigma(\lambda^0),
\]

\[
D^1_2(\lambda^0; \omega_1, \omega_2) := \sum_{\sigma} [H^0_2(\lambda^0; \omega_1, \omega_2)]_{\sigma} m^{0z}_\sigma(\lambda^0)
- \sum_{\sigma < \sigma'} [H^0_1(\lambda^0; \omega_1)]_{\sigma} [H^0_2(\lambda^0; \omega_1)]_{\sigma} [H^0_2(\lambda^0; \omega_1)]_{\sigma} m^{0z}_{\sigma'}(\lambda^0),
\]

\[
D^1_3(\lambda^0; \omega_1, \omega_2, \omega_3) := \sum_{\sigma} [H^0_3(\lambda^0; \omega_1, \omega_2, \omega_3)]_{\sigma} m^{0z}_\sigma(\lambda^0)
- \sum_{\sigma < \sigma'} ([H^0_1(\lambda^0; \omega_1)]_{\sigma} [H^0_2(\lambda^0; \omega_1, \omega_2)]_{\sigma} [H^0_2(\lambda^0; \omega_1)]_{\sigma} m^{0z}_{\sigma'}(\lambda^0)
+ [H^0_2(\lambda^0; \omega_1, \omega_2)]_{\sigma} [H^0_1(\lambda^0; \omega_1)]_{\sigma} m^{0z}_{\sigma'}(\lambda^0)
+ \sum_{\sigma} [\Theta - M^{0z}_A(\lambda^0)]_{\sigma} \prod_{\sigma' \neq \sigma} [H^0_1(\lambda^0; \omega_1)]_{\sigma} m^{0z}_{\sigma'}(\lambda^0).
\]
where $m_{\sigma\sigma}^{\Theta z}(\lambda^0) = m_{\sigma\sigma}^{\Theta z}(\lambda^0)$ is the minor of the matrix $\Theta - M^0_A(\lambda^0)$ obtained by deleting the $S_{\sigma}$th and the $S_{\sigma'}$th rows and columns, and $m_{\sigma\sigma}^{\Theta z}(\lambda^0) := m_{\sigma\sigma}^{\Theta z}(\lambda^0)$.

Thus one arrives at the following proposition.

**Proposition 4.6.** Let $r(z)$ be diagonal. For $\varepsilon > 0$ arbitrarily small, $\hat{\sigma}_{\Theta,1}^{\pm} \supseteq \hat{\sigma}_{\Theta,1}^{\pm} \supseteq \hat{\sigma}_{\Theta,2}^{\pm}$ where

$$\hat{\sigma}_{\Theta,1}^{\pm} := \{ \lambda^0 + \sum_{l=1}^{3} \varepsilon \omega_l + O(\varepsilon^4) \mid \lambda^0 \in \hat{\sigma}_{\Theta}^{0z} ; (\forall l) D^{0z}_1(\lambda^0; \omega_1, \ldots, \omega_l) = 0 \}$$

and

$$\hat{\sigma}_{\Theta,2}^{\pm} := \{ \lambda^0 + 2\lambda^1 + O(\varepsilon^4) \mid \lambda^0 \in \hat{\sigma}_{\Theta}^{0z} ; \lambda^1 := -\sum_{\sigma} [q^{\pm z} (\lambda^0)]_{\sigma\sigma} m_{\sigma\sigma}^{\Theta z}(\lambda^0) \in \mathbb{R} ; \sum_{\sigma} [M^0_A(\lambda^0)]_{\sigma\sigma} m_{\sigma\sigma}^{\Theta z}(\lambda^0) \neq 0 \}.$$  

If, in addition, $\Theta$ is diagonal, then $\hat{\sigma}_{\Theta,2}^{\pm} \supseteq \hat{\sigma}_{\Theta,3}^{\pm}$ where

$$\hat{\sigma}_{\Theta,3}^{\pm} := \bigcup_{\sigma} \{ \lambda^0_\sigma + \varepsilon \lambda^1 \sigma + O(\varepsilon^4) \mid \Theta_{\sigma\sigma} - [M^0_A(\lambda^0)]_{\sigma\sigma} = 0 ; \lambda^0_\sigma \in D^{\pm z}_\sigma ; \lambda^1 := -[q^{\pm z}(\lambda^0_\sigma)]_{\sigma\sigma} \}.$$  

Here $D^{\pm z}_\sigma := D^{\pm z}_\sigma \setminus \{ z^0_0 \}$ for $A_\sigma$; $D^{+ z}_0 := D^{++ z}_0 \setminus \{ z^0_{00} \}$ if $\sigma = (0,0)$ and $D^{+ z}_\sigma := D^{+ z}_0$ if $\sigma \neq (0,0)$ for $A_\sigma$; $D^{\pm z}_1 := D^{\pm z}_1 \setminus \{ z^0_{1s} \}$ if $\sigma = (1,s)$ and $D^{\pm z}_\sigma := D^{\pm z}_0$ if $\sigma \neq (1,s)$ for $A_\sigma$.

**Proof.** The first inclusion $\hat{\sigma}_{\Theta}^{\pm} \supseteq \hat{\sigma}_{\Theta,1}^{\pm}$ is due to our hypothesis imposed on the singular point for $\varepsilon > 0$ small, and the formula for the determinant. The subset $\hat{\sigma}_{\Theta,2}^{\pm}$ is the set of $\lambda^0 + \eta(\varepsilon)$ from $\hat{\sigma}_{\Theta,1}^{\pm}$ such that $\sum_{\sigma} [M^0_A(\lambda^0)]_{\sigma\sigma} m_{\sigma\sigma}^{\Theta z}(\lambda^0) \neq 0$ for $\lambda^0 \in \hat{\sigma}_{\Theta}^{0z}$; hence $\omega_1 = 0$ implies that $\omega_2 = \lambda^1$ and $\omega_3 = 0$. For $\Theta$ and $r$ diagonal, the matrix $\Theta - M^0_A(\lambda^0)$ is diagonal, so $\hat{\sigma}_{\Theta,2}^{\pm}$ contains the subset $\hat{\sigma}_{\Theta,3}^{\pm}$, which is the set of $\lambda^0 + 2\lambda^1 + O(\varepsilon^4)$ from $\hat{\sigma}_{\Theta,2}^{\pm}$ such that $[\Theta - M^0_A(\lambda^0)]_{\sigma\sigma} = 0$ has the solutions only for $\sigma = \sigma'$. The condition implies that $m_{\sigma\sigma}^{\Theta z}(\lambda^0) = \delta_{\sigma\sigma} m_{\sigma\sigma}^{\Theta z}(\lambda^0)$ and $m_{\sigma\sigma}^{\Theta z}(\lambda^0) = 0$, as well as $m_{\sigma\sigma}^{\Theta z}(\lambda^0) = \delta_{\sigma\sigma} m_{\sigma\sigma}^{\Theta z}(\lambda^0) + \delta_{\sigma\sigma} m_{\sigma\sigma}^{\Theta z}(\lambda^0)$, with $\sigma \neq \sigma''$, and $m_{\sigma\sigma}^{\Theta z}(\lambda^0) \neq 0$. The point $\lambda^0_\sigma$ from $\hat{\sigma}_{\Theta}^{\pm}$ belongs to $D^{\pm z}_\sigma$ excluding the point $z^0_\sigma$ for which $[M^0_A(z^0_\sigma)]_{\sigma\sigma} = 0$. The same applies to the points from $\hat{\sigma}_{\Theta}^{0z}$ provided that $\sigma = (0,0)$ (resp. $\sigma = (1,s)$) in the antisymmetric (resp. symmetric) case; otherwise $\lambda^1_\sigma$ vanishes.

In the closing remarks we mention that the eigenvectors are constructed starting from [16 Eq. (4.3)] and in particular

$$g_{\sigma}(z) = N_{\sigma} \sum_{\sigma'} R_{\sigma\sigma}^{c}(z)(\cdot - K_0) \otimes |\sigma'\rangle , \quad \exists z \neq 0$$
\( (R^c_{\sigma_\sigma}(z) \) is the entry of the integral kernel of the resolvent \((L - z)^{-1}\). Here we only compute the “probability density” \([f_\lambda, f_\lambda]_A\) for the eigenvalue \(\lambda \in \mathbb{R} \setminus \{z_1\}\) and the corresponding eigenvector \(f_\lambda = \gamma_\lambda(\lambda)c\), \(c = (c_\sigma) \in \mathfrak{H}_0(\Theta - M_\lambda(\lambda)):\)
\[
[f_\lambda, f_\lambda]_A = \sum_{\sigma} |c_\sigma|^2 \langle p_\sigma^0(\lambda) + \varepsilon^2 p_\sigma^1(\lambda) + \langle c, r'(\lambda)c \rangle_{C^d} + O(\varepsilon^4) \]
\]
with
\[
p_\sigma^t(\lambda) := \lim_{y \to 0} y^{-1} \Im[q_t(\lambda + iy)]_{\sigma\sigma} = \frac{\psi_\sigma}{(\lambda - z_1)^t} \left( \sum_{p=0}^2 q_{\sigma p} \lambda^{1-p} (-2\lambda + p(\lambda - z_1)) \right) + 2\psi_\sigma^t(\lambda) - (\lambda - z_1)\psi_\sigma^t(\lambda), \ t \in \{0, 1\}
\]
where the primes denote the derivatives with respect to \(\lambda\); see the proof of Theorem 4.4.

In particular, for \(r(\lambda)\) diagonal, the eigenvector \(f_\lambda\) belongs to the negative subspace of \(H_A\), that is \([f_\lambda, f_\lambda]_A < 0\), if \(\lambda\) belongs to \(\bigcup_{\sigma} \mathcal{X}_\sigma\), where the union is taken over \(\sigma\) such that \(c_\sigma \neq 0\).

Finally, for the numerical illustration, let \(\varepsilon = 0.4\), \(\beta = 1.4\), and \(z_1 = -5\). Assume also that \(\Theta\) and \(r(z)\) are the diagonal matrices. We compute the eigenvalues, up to \(O(\varepsilon^4)\), corresponding to the spin state \(\sigma = (0, 0)\) by putting \([G_\lambda]_{\sigma_2, \sigma_2} = -1.4\), \([G_\lambda]_{\sigma_2, \sigma_1} = 2.6\), and \(\Theta_{\sigma\sigma} = -1.2\). Then the sets \(l_\sigma = (-\infty, z_1) \cup (\lambda_+, \infty)\), with \(\lambda_+ = -1.28571\), and \(\mathcal{X}_\sigma = (z_\sigma^-, z_1)\), with \(z_\sigma^- = -11.4566\). The eigenvalues \(\lambda = \lambda_\sigma\) solve \(\Theta_{\sigma\sigma} - \{M_\lambda(\lambda)\}_{\sigma\sigma} = 0\), and the numerical solutions are given by \([-7.43299, -4.02215\]) without spin-orbit coupling, and respectively by \([-7.43436, -4.02240\]) with spin-orbit-coupling. The computed correction terms \(\lambda_\sigma^1\) in \(\tilde{\sigma}^{\varepsilon}_{\Theta, 3}\) are thus: \(-0.0084818\) for the lower eigenvalue and \(-0.00156083\) for the upper one. Since the lower eigenvalue belongs to \(\mathcal{X}_\sigma\), the corresponding eigenvector \(f_\lambda\) is an element of the negative subspace of the Pontryagin space \(H_A\). Indeed, an indefinite inner product reads
\[
[f_{\lambda_\sigma}, f_{\lambda_\sigma}]_\lambda = p_\sigma^0(\lambda) + \varepsilon^2 p_\sigma^1(\lambda) + [r(\lambda)]_{\sigma\sigma}^+ + O(\varepsilon^4)
\]
for \(c = (\delta_{\sigma,0}, 0)\), and the leading term is given by \(-0.527914\) for the lower eigenvalue, and by 4.19659 for the upper one.

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Vilnius University, Institute of Theoretical Physics and Astronomy, Saulėtekio Ave. 3, LT-10257 Vilnius, Lithuania

E-mail address: Rytis.Juršenas@tfai.vu.lt