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***J*-self-adjoint operators with \mathcal{C} -symmetries: an extension theory approach**

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Abstract

A well-known tool in conventional (von Neumann) quantum mechanics is the self-adjoint extension technique for symmetric operators. It is used, e.g., for the construction of Dirac–Hermitian Hamiltonians with point-interaction potentials. Here we reshape this technique to allow for the construction of pseudo-Hermitian (J -self-adjoint) Hamiltonians with complex point interactions. We demonstrate that the resulting Hamiltonians are bijectively related to the so-called hypermaximal neutral subspaces of the defect Krein space of the symmetric operator. This symmetric operator is allowed to have arbitrary but equal deficiency indices $\langle n, n \rangle$. General properties of the \mathcal{C} operators for these Hamiltonians are derived. A detailed study of \mathcal{C} -operator parametrizations and Krein type resolvent formulae is provided for J -self-adjoint extensions of symmetric operators with deficiency indices $\langle 2, 2 \rangle$. The technique is exemplified on 1D pseudo-Hermitian Schrödinger and Dirac Hamiltonians with complex point-interaction potentials.

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1. Introduction

The use of non-Hermitian operators and indefinite Hilbert space structures in quantum mechanics dates back to the early 1940s [1, 2]. The interest in this subject strongly increased after it was discovered in 1998 that complex Hamiltonians possessing \mathcal{PT} -symmetry (the product of parity and time reversal) can have a real spectrum (such as self-adjoint operators)

[3]. This gave rise to a mathematically consistent complex extension of conventional quantum mechanics (CQM) into \mathcal{PT} quantum mechanics (PTQM), see e.g. the review paper [4] and references therein.

During the past ten years PTQM models have been analyzed with a wealth of technical tools (for an overview see [5–8]). Most prominent ones concern Bethe Ansatz techniques (to prove the reality of the spectrum for the Hamiltonian with a complex cubic potential ix^3 which originated a lot of interest) [9], various global approaches based on the extension of differential operators into the complex coordinate plane [10–13], SUSY approaches [14–17], \mathcal{PT} -symmetric perturbations of Hermitian operators [18], Moyal product [19, 20] and Lie algebraic [21] techniques. We would also like to mention more recent considerations on spectral degeneracies [22–25].

Apart from these techniques and applications, one of the most important concepts to place \mathcal{PT} -symmetry in a general mathematical context remains the concept of *pseudo-Hermiticity* [26]. A linear densely defined operator A acting in a Hilbert space \mathfrak{H} with the inner product (\cdot, \cdot) is called pseudo-Hermitian if its adjoint A^* satisfies the condition

$$A^*\eta = \eta A, \quad (1.1)$$

where η is an invertible bounded self-adjoint operator in \mathfrak{H} . Since a Hilbert space \mathfrak{H} endowed with an indefinite metric $[f, g]_\eta = (\eta f, g)$ is an example of a Krein space with a fundamental symmetry $J = \eta|\eta|^{-1}$ (here $|\eta| = \sqrt{\eta^2}$ is the modulus of η) [27, 28], one can reduce the investigation of pseudo-Hermitian operators to the study of J -self-adjoint operators in a Krein space [29–33].

We recall that a linear densely defined operator A acting in a Krein space $(\mathfrak{H}, [\cdot, \cdot]_J)$ with a fundamental symmetry J (i.e., $J = J^*$ and $J^2 = I$) and an indefinite metric $[\cdot, \cdot]_J = (J\cdot, \cdot)$ is called J -self-adjoint if $A^*J = JA$. Obviously, J -self-adjoint operators are pseudo-Hermitian ones in the sense of (1.1). We note that there exists an alternative rigorous approach to \mathcal{PT} -symmetric problems where J is assumed to be an *antilinear* involution (conjugation) [34–38].

In contrast to self-adjoint operators in Hilbert spaces (which necessarily have a purely real spectrum), self-adjoint operators in Krein spaces, in general, have a spectrum which is only symmetric with respect to the real axis [27, 28]. Pairwise complex conjugate eigenvalues, as part of the discrete spectrum, are connected with spontaneously broken \mathcal{PT} -symmetry. This means that although the Hamiltonian will have \mathcal{PT} -symmetry, its eigenfunctions will not be \mathcal{PT} -symmetric. The real discrete spectrum corresponds to the sector of the so-called exact \mathcal{PT} -symmetry where in addition to the Hamiltonian also its eigenfunctions are \mathcal{PT} -symmetric.

One of the key points in PTQM is the description of a hidden symmetry \mathcal{C} [39] which is present for a given \mathcal{PT} -symmetric Hamiltonian A in the sector of exact \mathcal{PT} -symmetry.

By analogy with [4], the definition of \mathcal{C} -symmetry for the case of J -self-adjoint operators can be formalized as follows.

Definition 1.1. *A J -self-adjoint operator A has the property of \mathcal{C} -symmetry if there exists a bounded linear operator \mathcal{C} in \mathfrak{H} such that (i) $\mathcal{C}^2 = I$; (ii) $J\mathcal{C} > 0$; (iii) $A\mathcal{C} = \mathcal{C}A$.*

The operator \mathcal{C} shows some rough analogy with the charge conjugation operator in quantum field theory. The existence of \mathcal{C} provides an inner product $(\cdot, \cdot)_\mathcal{C} = [\mathcal{C}\cdot, \cdot]_J$ whose associated norm is positive definite and the dynamics generated by A is therefore governed by a unitary time evolution. However, the operator \mathcal{C} depends on the choice of A and its finding is a nontrivial problem [40–43]. A generalization from bounded to unbounded \mathcal{C} operators has been recently discussed in [44]. Another kind of generalized \mathcal{C} operator can arise in

connection with model classes of interacting relativistic quantum fields with indefinite metrics and satisfying all Morchio–Strocchi axioms, see, e.g. [46] (and references therein).

In this paper, we are going to study J -self-adjoint operators with \mathcal{C} -symmetries within an extension theory approach. This is motivated by the well-known fact that not all \mathcal{PT} -symmetric operators are \mathcal{P} -self-adjoint in a Krein space $(\mathcal{K}_{\mathcal{P}}, [\cdot, \cdot]_{\mathcal{P}})$, but rather that they will be J -self-adjoint in $(\mathcal{K}_J, [\cdot, \cdot]_J)$ with suitably adapted involution operators J . Therefore, we choose J -self-adjointness as the basic (fundamental) starting point and develop a corresponding most general technical framework. Subsequently, the technique is applied to models with concrete \mathcal{PT} -symmetric boundary conditions, i.e. the complex potential, typical for PTQM Hamiltonians, is induced via point interactions which are described by an operator extension technique. The extension technique is a standard mathematical tool [45] in CQM and is widely used to efficiently describe point interactions [47, 48]. PTQM-related considerations based on this technique can be found in [30, 49, 50].

The paper is organized as follows. Section 2 contains an abstract study of \mathcal{C} -symmetries in a Krein space approach and has an auxiliary character. In section 3, we describe all J -self-adjoint extensions of a given symmetric operator A_{sym} (under the condition $A_{\text{sym}}J = JA_{\text{sym}}$) and, for the case of deficiency indices $(2, 2)$, we propose a general method allowing us: (i) to describe the set of J -self-adjoint extensions $A_{M(U)}$ of A_{sym} with \mathcal{C} -symmetries; (ii) to construct the corresponding \mathcal{C} -symmetries in a simple explicit form (family of $C_{\theta, \omega}$ -symmetries); (iii) to establish a Krein-type resolvent formula for J -self-adjoint extensions $A_{M(U)}$ with \mathcal{C} -symmetries. Section 4 illustrates the obtained results on the examples of a Schrödinger operator with general zero-range potential and a one-dimensional Dirac Hamiltonian with point perturbation.

Let us briefly comment on the used notations. $\mathcal{D}(A)$ and $\mathcal{R}(A)$ denote the domain and the range of a linear operator A , respectively. $A \upharpoonright \mathcal{D}$ means the restriction of A on a set \mathcal{D} .

2. J -self-adjoint operators with \mathcal{C} -symmetries

2.1. Elements of Krein space theory

Here all necessary results of Krein space theory are presented in a form convenient for our exposition. Their proofs and detailed analysis can be found in [27, 28].

Let \mathfrak{H} be a Hilbert space with an inner product (\cdot, \cdot) and with a fundamental symmetry (involution) J (i.e., $J = J^*$ and $J^2 = I$). The corresponding orthoprojectors $P_+ = 1/2(I+J)$, $P_- = 1/2(I - J)$ determine the fundamental decomposition of \mathfrak{H} :

$$\mathfrak{H} = \mathfrak{H}_+ \oplus \mathfrak{H}_-, \quad \mathfrak{H}_- = P_- \mathfrak{H}, \quad \mathfrak{H}_+ = P_+ \mathfrak{H}. \quad (2.1)$$

The space \mathfrak{H} endowed with the indefinite inner product (indefinite metric)

$$[x, y]_J := (Jx, y), \quad \forall x, y \in \mathfrak{H} \quad (2.2)$$

is called a *Krein space* $(\mathfrak{H}, [\cdot, \cdot]_J)$.

A subspace $\mathfrak{L} \subset \mathfrak{H}$ is called hypermaximal neutral if \mathfrak{L} coincides with its J -orthogonal complement: $\mathfrak{L} = \mathfrak{L}^{\perp J} = \{x \in \mathfrak{H} : [x, y]_J = 0, \forall y \in \mathfrak{L}\}$. Hypermaximal neutral subspaces exist only in the case where $\dim \mathfrak{H}_+ = \dim \mathfrak{H}_-$.

A subspace $\mathfrak{L} \subset \mathfrak{H}$ is called *non-negative*, *positive*, *uniformly positive* if, respectively, $[x, x]_J \geq 0$, $[x, x]_J > 0$, $[x, x]_J \geq \alpha^2 \|x\|^2$, $\alpha \in \mathbb{R}$ for all $x \in \mathfrak{L} \setminus \{0\}$. Non-positive, negative and uniformly negative subspaces are introduced similarly. The subspaces \mathfrak{H}_{\pm} in (2.1) are examples of uniformly positive and uniformly negative subspaces and they possess the property of maximality in the corresponding classes (i.e., \mathfrak{H}_+ (\mathfrak{H}_-) does not belong as a subspace to any uniformly positive (negative) subspace).

Let a subspace \mathfrak{L}_+ be maximal uniformly positive. Then its J -orthogonal complement $\mathfrak{L}_- = \mathfrak{L}_+^{\perp J}$ is a maximal uniformly negative subspace of \mathfrak{H} , and the direct J -orthogonal sum

$$\mathfrak{H} = \mathfrak{L}_+ \dot{+}_J \mathfrak{L}_- \tag{2.3}$$

gives the decomposition of \mathfrak{H} onto its positive \mathfrak{L}_+ and negative \mathfrak{L}_- parts (the brackets $[\cdot]_J$ mean the orthogonality with respect to the indefinite metric).

The subspaces \mathfrak{L}_+ and \mathfrak{L}_- in (2.3) can be described as $\mathfrak{L}_+ = (I + K)\mathfrak{H}_+$ and $\mathfrak{L}_- = (I + Q)\mathfrak{H}_-$, where $K : \mathfrak{H}_+ \rightarrow \mathfrak{H}_-$ is a contraction and $Q = K^* : \mathfrak{H}_- \rightarrow \mathfrak{H}_+$ is the adjoint of K .

The self-adjoint operator $T = K P_+ + K^* P_-$ acting in \mathfrak{H} is called an operator of transition from the fundamental decomposition (2.1) to (2.3). Obviously,

$$\mathfrak{L}_+ = (I + T)\mathfrak{H}_+, \quad \mathfrak{L}_- = (I + T)\mathfrak{H}_-. \tag{2.4}$$

Furthermore, the projectors $P_{\mathfrak{L}_\pm} : \mathfrak{H} \rightarrow \mathfrak{L}_\pm$ onto \mathfrak{L}_\pm with respect to the decomposition (2.3) have the form

$$P_{\mathfrak{L}_-} = (I - T)^{-1}(P_- - T P_+), \quad P_{\mathfrak{L}_+} = (I - T)^{-1}(P_+ - T P_-). \tag{2.5}$$

The collection of operators of transition admits a simple ‘external’ description. Namely, a self-adjoint operator T in \mathfrak{H} is an operator of transition if and only if

$$\|T\| < 1 \quad \text{and} \quad J T = -T J. \tag{2.6}$$

2.2. J -self-adjoint operators with \mathcal{C} -symmetries

The following statement characterizes the structure of J -self-adjoint operators with \mathcal{C} -symmetries.

Theorem 2.1 ([30]). *A J -self-adjoint operator A acting in a Krein space $(\mathfrak{H}, [\cdot, \cdot]_J)$ has the property of \mathcal{C} -symmetry if and only if A admits the decomposition*

$$A = A_+ \dot{+}_J A_-, \quad A_+ = A \upharpoonright \mathfrak{L}_+, \quad A_- = A \upharpoonright \mathfrak{L}_- \tag{2.7}$$

with respect to a certain choice of the J -orthogonal decomposition (2.3) of \mathfrak{H} . In that case

$$\mathcal{C} = P_{\mathfrak{L}_+} - P_{\mathfrak{L}_-} = (I + T)(I - T)^{-1} J, \tag{2.8}$$

where T is the operator of transition from the fundamental decomposition (2.1) to (2.3).

Remark 2.1. Since T is a self-adjoint operator and $\|T\| < 1$, formula (2.8) can be rewritten as $\mathcal{C} = e^Q J$, where $Q (= \ln(I + T)(I - T)^{-1})$ is a bounded self-adjoint operator in \mathfrak{H} . Then the condition $\mathcal{C}^2 = I$ takes the form $e^Q J = J e^{-Q}$ which implies $Q J = -J Q$. Therefore, one can rewrite (2.8) as

$$\mathcal{C} = e^Q J = e^{Q/2} J e^{-Q/2}. \tag{2.9}$$

Set $(\cdot, \cdot)_\mathcal{C} \equiv [\mathcal{C}\cdot, \cdot]_J$. Due to (2.9), $(\cdot, \cdot)_\mathcal{C} = (e^{-Q/2}\cdot, e^{-Q/2}\cdot)$. The sesquilinear form $(\cdot, \cdot)_\mathcal{C}$ determines a new inner product in \mathfrak{H} that is equivalent to the initial one. Since $\mathcal{C} = P_{\mathfrak{L}_+} - P_{\mathfrak{L}_-}$ (by (2.8)), the J -orthogonal decomposition (2.3) is transformed into the orthogonal sum $\mathfrak{H} = \mathfrak{L}_+ \oplus_\mathcal{C} \mathfrak{L}_-$ with respect to the inner product $(\cdot, \cdot)_\mathcal{C}$, and the decomposition (2.7) takes the form $A = A_+ \oplus_\mathcal{C} A_-$.

Corollary 2.1. *Let A be a J -self-adjoint operator. The following statements are equivalent:*

- (i) A has the property of \mathcal{C} -symmetry;
- (ii) the operators A_+ and A_- in the decomposition $A = A_+ \oplus_\mathcal{C} A_-$ are self-adjoint in the Hilbert spaces \mathfrak{L}_+ and \mathfrak{L}_- with the inner product $(\cdot, \cdot)_\mathcal{C}$;
- (iii) the operator $H = e^{-Q/2} A e^{Q/2}$ is self-adjoint in \mathfrak{H} .

Proof. By (2.8) the restriction of $(\cdot, \cdot)_C$ on the subspaces \mathfrak{L}_+ and \mathfrak{L}_- coincides with $[\cdot, \cdot]_J$ and $-[\cdot, \cdot]_J$, respectively. This means that the assumption of J -self-adjointness of A is equivalent to the property of self-adjointness of $A_\pm = A \upharpoonright \mathfrak{L}_\pm$ with respect to $(\cdot, \cdot)_C$. Hence, (i) \iff (ii).

By virtue of (ii), A is self-adjoint in \mathfrak{H} with respect to the inner product $(\cdot, \cdot)_C$. Therefore, $(e^{-Q/2}Ax, e^{-Q/2}y) = (Ax, y)_C = (x, Ay)_C = (e^{-Q/2}x, e^{-Q/2}Ay)$, $\forall x, y \in \mathfrak{H}$.

This means that the operator $H = e^{-Q/2}Ae^{Q/2}$ is self-adjoint in \mathfrak{H} with respect to the initial product (\cdot, \cdot) if and only if A is self-adjoint with respect to $(\cdot, \cdot)_C$. Thus (ii) \iff (iii). \square

Corollary 2.2. *If a J -self-adjoint operator A has the property of \mathcal{C} -symmetry then its spectrum $\sigma(A)$ is real, and the adjoint operator C^* provides the property of \mathcal{C} -symmetry for A^* .*

Proof. The reality of $\sigma(A)$ follows from the assertion (ii) of Corollary 2.1. If A has \mathcal{C} -symmetry, the adjoint C^* satisfies all conditions of definition 1.1 for A^* . So, C^* provides the property of \mathcal{C} -symmetry for A^* . \square

Remark 2.2. In the context of PTQM, the existence of an equivalence mapping (similarity transformation) $e^{Q/2}$ between a pseudo-Hermitian operator A and a Hermitian operator H was first demonstrated by Mostafazadeh in [51]. Operators A which are similarity mapped onto Hermitian operators H by the positive definite Hermitian $e^{Q/2}$ have been earlier studied in [52] and are also known as quasi-Hermitian operators. The \mathcal{C} operator was introduced in PTQM by Bender, Brody and Jones in [39]. As it is obvious from (2.9), \mathcal{C} as a dynamically adapted (A -dependent) involution is a similarity transformed version of the original involution J .

3. Extension theory approach

3.1. Preliminaries to extension theory. General case

Let A_{sym} be a closed symmetric densely defined operator in \mathfrak{H} with the equal deficiency indices (n, n) ($n \in \mathbb{N} \cup \{\infty\}$). Denote by $\mathfrak{N}_i = \mathfrak{H} \ominus \mathcal{R}(A_{\text{sym}} + iI)$ and $\mathfrak{N}_{-i} = \mathfrak{H} \ominus \mathcal{R}(A_{\text{sym}} - iI)$ the defect subspaces of A_{sym} and consider the Hilbert space $\mathfrak{M} = \mathfrak{N}_{-i} \dot{+} \mathfrak{N}_i$ with the inner product

$$(x, y)_{\mathfrak{M}} = 2[(x_i, y_i) + (x_{-i}, y_{-i})] \quad x = x_i + x_{-i}, \quad y = y_i + y_{-i} \quad \{x_{\pm i}, y_{\pm i}\} \subset \mathfrak{N}_{\pm i}. \tag{3.1}$$

Obviously, the operator $Z(x_i + x_{-i}) = x_i - x_{-i}$ is a fundamental symmetry in the Hilbert space \mathfrak{M} and it acts as an identity operator on \mathfrak{N}_i and as a minus identity operator on \mathfrak{N}_{-i} .

In what follows we assume that

$$A_{\text{sym}}J = JA_{\text{sym}}, \tag{3.2}$$

where J is a fundamental symmetry in \mathfrak{H} . Then the subspaces $\mathfrak{N}_{\pm i}$ reduce J and the restriction $J \upharpoonright \mathfrak{M}$ gives rise to the fundamental symmetry in the Hilbert space \mathfrak{M} . Moreover, according to the properties of Z mentioned above, $JZ = ZJ$ and JZ is a fundamental symmetry in \mathfrak{M} . Therefore, the sesquilinear form

$$[x, y]_{JZ} = (JZx, y)_{\mathfrak{M}} = 2[(Jx_i, y_i) - (Jx_{-i}, y_{-i})] \tag{3.3}$$

defines an indefinite metric on \mathfrak{M} .

According to von-Neumann formulae any closed intermediate extension A of A_{sym} (i.e., $A_{\text{sym}} \subset A \subset A_{\text{sym}}^*$) is uniquely determined by the choice of a subspace $M \subset \mathfrak{M}$. This means

that $\mathcal{D}(A) = \mathcal{D}(A_{\text{sym}}) \dot{+} M$ and

$$Af = A_{\text{sym}}^*(u + x) = A_{\text{sym}}u + iZx, \quad \forall u \in \mathcal{D}(A_{\text{sym}}), \quad \forall x \in M. \quad (3.4)$$

Taking (3.2)–(3.4) into account we immediately derive

$$[A_1 f_1, f_2]_J - [f_1, A_2 f_2]_J = i[x_1, x_2]_{JZ}, \quad \forall f_j = u_j + x_j \in \mathcal{D}(A_j), \quad x_j \in M_j \quad (3.5)$$

for the arbitrary intermediate extensions A_1 and A_2 of A_{sym} which are defined by the subspaces M_1 and M_2 , respectively (see, e.g., [53, lemma 9.6]).

It follows from (3.5) that an extension $A \supset A_{\text{sym}}$ defined by M is a J -self-adjoint operator if and only if

$$M = M^{\perp_{JZ}} = \{y \in \mathfrak{M} : [x, y]_{JZ} = 0, \forall x \in M\}, \quad (3.6)$$

i.e., if M is a hypermaximal neutral subspace of the Krein space $(\mathfrak{M}, [\cdot, \cdot]_{JZ})$.

The following statement is a ‘folklore’ result of extension theory.

Proposition 3.1. *Let $A_{\text{sym}}J = JA_{\text{sym}}$. Then the correspondence $A \leftrightarrow M$ determined by (3.4) is a bijection between the set of all J -self-adjoint extensions A of A_{sym} and the set of all hypermaximal neutral subspaces M of $(\mathfrak{M}, [\cdot, \cdot]_{JZ})$.*

We note that the choice of J would via the J -induced Krein-space metric $[\cdot, \cdot]_{JZ}$ define the concrete parametrization of the hypermaximal neutral subspaces⁶.

To underline the relationship $A \leftrightarrow M$ in (3.6) we will use the notation A_M for J -self-adjoint extensions A of A_{sym} determined by (3.4).

Theorem 3.1. *Let $A_{\text{sym}}J = JA_{\text{sym}}$ and let $A_{\text{sym}}\mathcal{C} = \mathcal{C}A_{\text{sym}}$, where \mathcal{C} is a bounded linear operator in \mathfrak{H} such that $\mathcal{C}^2 = I$ and $J\mathcal{C} > 0$. Then a J -self-adjoint extension A_M of A_{sym} has \mathcal{C} -symmetry if and only if $\mathcal{C}M = M$.*

Proof. Since A_{sym} commutes with J and \mathcal{C} one gets $A_{\text{sym}}e^{\mathcal{Q}} = e^{\mathcal{Q}}A_{\text{sym}}$, where the self-adjoint operator $e^{\mathcal{Q}}$ is defined in (2.9). But then $A_{\text{sym}}\mathcal{C}^* = A_{\text{sym}}Je^{\mathcal{Q}} = Je^{\mathcal{Q}}A_{\text{sym}} = \mathcal{C}^*A_{\text{sym}}$. The relations $\mathcal{C}^*A_{\text{sym}} = A_{\text{sym}}\mathcal{C}^*$ and $\mathcal{C}^2 = I$ imply $\mathcal{C}\mathfrak{N}_{\pm} = \mathfrak{N}_{\pm}$ and hence, $\mathcal{C}\mathfrak{M} = \mathfrak{M}$.

Using the identity $\mathcal{C}A_{\text{sym}}^* = A_{\text{sym}}^*\mathcal{C}$ which immediately follows from $\mathcal{C}^*A_{\text{sym}} = A_{\text{sym}}\mathcal{C}^*$ one concludes that $\mathcal{C}A_M = A_M\mathcal{C} \iff \mathcal{C}\mathcal{D}(A_M) = \mathcal{D}(A_M)$. Taking the relations $\mathcal{D}(A_M) = \mathcal{D}(A_{\text{sym}}) \dot{+} M$, $\mathcal{C}\mathcal{D}(A_{\text{sym}}) = \mathcal{D}(A_{\text{sym}})$ and $\mathcal{C}\mathfrak{M} = \mathfrak{M}$ into account one gets $\mathcal{C}A_M = A_M\mathcal{C} \iff \mathcal{C}M = M$. Theorem 3.1 is proved. \square

Remark 3.1. The commutation relation $A_{\text{sym}}J = JA_{\text{sym}}$ in theorem 3.1 is a natural condition in the present approach because the complex-potential properties of the J -self-adjoint operators A are induced only by the boundary-condition-related extension families (see below). A weaker J -symmetric condition $A \subset JA^*J$ would allow for a consideration of \mathcal{PT} -symmetric Hamiltonians with regular \mathcal{PT} -symmetric potentials. But such models would require for extension techniques which should be well adapted to the specifics of the concrete potentials. Here, we focus on purely boundary induced \mathcal{PT} -symmetric (J -symmetric) set-ups.

3.2. The case of deficiency indices $\langle 2, 2 \rangle$

In what follows we assume that the symmetric operator A_{sym} has the deficiency indices $\langle 2, 2 \rangle$, and there exists at least one J -self-adjoint extension A_M of A_{sym} . In that case $\dim \mathfrak{M} = 4$ and

⁶ The physically relevant parametrization freedom of the pseudo-Hermitian metric η is via $J = \eta|\eta|^{-1}$ naturally encoded in J .

each of the orthogonal subspaces of \mathfrak{M} :

$$\begin{aligned} \mathfrak{M}_{++} &= (I + Z)(I + J)\mathfrak{M}; & \mathfrak{M}_{--} &= (I - Z)(I - J)\mathfrak{M}; \\ \mathfrak{M}_{+-} &= (I + Z)(I - J)\mathfrak{M}; & \mathfrak{M}_{-+} &= (I - Z)(I + J)\mathfrak{M} \end{aligned}$$

is one dimensional. (Otherwise, $Z = J$ or $Z = -J$ and there exist no J -self-adjoint extensions of A_{sym} —in contradiction to the above assumption.)

Let $\{e_{\pm\pm}\}$ be an orthonormal basis of \mathfrak{M} such that $\mathfrak{M}_{\pm\pm} = \langle e_{\pm\pm} \rangle$. It follows from the definition of $\mathfrak{M}_{\pm\pm}$ that

$$\begin{aligned} J e_{++} &= e_{++}, & J e_{-+} &= e_{-+}, & J e_{+-} &= -e_{+-}, & J e_{--} &= -e_{--}; \\ Z e_{++} &= e_{++}, & Z e_{-+} &= -e_{-+}, & Z e_{+-} &= e_{+-}, & Z e_{--} &= -e_{--}. \end{aligned} \tag{3.7}$$

This means that the fundamental decomposition of the Krein space $(\mathfrak{M}, [\cdot, \cdot]_{JZ})$ has the form

$$\mathfrak{M} = \mathfrak{M}_- \oplus \mathfrak{M}_+, \quad \mathfrak{M}_- = \langle e_{+-}, e_{-+} \rangle, \quad \mathfrak{M}_+ = \langle e_{++}, e_{--} \rangle. \tag{3.8}$$

According to general theory [27], an arbitrary hypermaximal neutral subspace M of $(\mathfrak{M}, [\cdot, \cdot]_{JZ})$ can be uniquely determined by a unitary mapping of \mathfrak{M}_- onto \mathfrak{M}_+ . Since $\dim \mathfrak{M}_+ = \dim \mathfrak{M}_- = 2$ the set of unitary mappings $\mathfrak{M}_- \rightarrow \mathfrak{M}_+$ is determined by the set of unitary matrices

$$U = e^{i\phi} \begin{pmatrix} q e^{i\gamma} & r e^{i\xi} \\ -r e^{-i\xi} & q e^{-i\gamma} \end{pmatrix}, \quad q^2 + r^2 = 1, \quad \phi, \gamma, \xi \in [0, 2\pi). \tag{3.9}$$

(We have used the standard representation $U(2) \cong U(1) \times SU(2)$ for the reducible $U(2)$ group elements [54].)

In other words, the decomposition (3.8) and representation (3.9) allow one to describe a hypermaximal neutral subspace M of $(\mathfrak{M}, [\cdot, \cdot]_{JZ})$ as a linear span

$$M = M(U) = \langle d_1, d_2 \rangle \tag{3.10}$$

of elements

$$\begin{aligned} d_1 &= e_{++} + q e^{i(\phi+\gamma)} e_{+-} + r e^{i(\phi+\xi)} e_{-+}; \\ d_2 &= e_{--} - r e^{i(\phi-\xi)} e_{+-} + q e^{i(\phi-\gamma)} e_{-+}. \end{aligned} \tag{3.11}$$

By proposition 3.1, formula (3.10) provides a one-to-one correspondence between the domains $\mathcal{D}(A_{M(U)}) = \mathcal{D}(A_{\text{sym}}) + M(U)$ of J -self-adjoint extensions $A_{M(U)}$ of A_{sym} and the unitary matrices U .

Lemma 3.1. *A J -self-adjoint extension $A_{M(U)}$ defined by (3.4) and (3.10) is self-adjoint if and only if $q = 0$.*

Proof. According to proposition 3.1, a J -self-adjoint operator $A_{M(U)}$ is self-adjoint if and only if $M(U)$ is also a hypermaximal neutral subspace in the Krein space $(\mathfrak{M}, [\cdot, \cdot]_Z)$.

By (3.7) the fundamental decomposition of $(\mathfrak{M}, [\cdot, \cdot]_Z)$ has the form

$$\mathfrak{M} = \mathfrak{N}_{-i} \oplus \mathfrak{N}_i, \quad \mathfrak{N}_{-i} = \langle e_{-+}, e_{--} \rangle, \quad \mathfrak{N}_i = \langle e_{++}, e_{+-} \rangle, \tag{3.12}$$

where \mathfrak{N}_{-i} and \mathfrak{N}_i are, respectively, negative and positive subspaces. Taking (3.12) into account, we derive from (3.10) that $M(U)$ is a hypermaximal neutral subspace of $(\mathfrak{M}, [\cdot, \cdot]_Z)$ if and only if $q = 0$. \square

Lemma 3.2. *A J -self-adjoint extension $A_{M(U)}$ does not have the property of \mathcal{C} -symmetry if $r = 0$.*

Proof. If $r = 0$, then $d_1 = e_{++} + e^{i(\phi+\gamma)}e_{+-} \in M(U) \cap \mathfrak{N}_i$ (on the basis of (3.12)). In that case $A_{M(U)}d_1 = id_1$ by (3.4). Therefore, $A_{M(U)}$ has a non-real spectrum and there are no \mathcal{C} -symmetries for $A_{M(U)}$ (see corollary 2.2). \square

Remark 3.2. Lemmas 3.1, 3.2 and the constraint $q^2 + r^2 = 1$ in (3.9) show that there should exist a critical angle $\sigma_c \in (0, 2\pi)$ in $q = \sin(\sigma)$, $r = \cos(\sigma)$ where the \mathcal{C} -symmetry relation $A_{M(U)}\mathcal{C} = \mathcal{C}A_{M(U)}$ breaks down⁷.

Remark 3.3. In the case of deficiency indices $\langle n, n \rangle$ a natural parametrization for all J -self-adjoint extensions is given by a matrix $U(n) \cong U(1) \times SU(n) : \mathfrak{M}_- \rightarrow \mathfrak{M}_+$.

3.3. Family of $\mathcal{C}_{\theta,\omega}$ -symmetries

Let R be a fundamental symmetry in \mathfrak{H} (i.e., $R^2 = I$ and $R = R^*$) such that

$$A_{\text{sym}}R = RA_{\text{sym}}, \quad \text{and} \quad JR = -RJ. \quad (3.13)$$

The first identity in (3.13) means that the subspaces $\mathfrak{N}_{\pm i}$ reduce R and the restriction $R|_{\mathfrak{M}}$ is a fundamental symmetry in the Hilbert space \mathfrak{M} . The second identity and the definition of the elements $\{e_{\pm\pm}\}$ imply

$$Re_{++} = e_{+-}, \quad Re_{+-} = e_{++}, \quad Re_{--} = e_{-+}, \quad Re_{-+} = e_{--}. \quad (3.14)$$

Furthermore, the relation $JR = -RJ$ enables one to state that the operator

$$R_\omega = R e^{i\omega J} = e^{-i\omega J/2} R e^{i\omega J/2}, \quad \omega \in [0, 2\pi) \quad (3.15)$$

is an involution ($R_\omega^2 = I$, $R_\omega = R_\omega^*$) in \mathfrak{H} and $JR_\omega = -R_\omega J$. It follows from (3.7), (3.14) and (3.15) that

$$\begin{aligned} R_\omega e_{++} &= e^{i\omega} e_{+-}, & R_\omega e_{+-} &= e^{-i\omega} e_{++}, \\ R_\omega e_{--} &= e^{-i\omega} e_{-+}, & R_\omega e_{-+} &= e^{i\omega} e_{--}. \end{aligned} \quad (3.16)$$

Let us consider the collection of the operators

$$T_{\theta,\omega} = \frac{1-\theta}{1+\theta} R_\omega, \quad \theta > 0, \quad \omega \in [0, 2\pi).$$

Obviously, $T_{\theta,\omega}$ is self-adjoint in \mathfrak{H} , $JT_{\theta,\omega} = -T_{\theta,\omega}J$ and $\|T_{\theta,\omega}\| < 1$. By (2.4) and (2.6), $T_{\theta,\omega}$ is the operator of transition from (2.1) to the decomposition

$$\mathfrak{H} = \mathfrak{L}_+^{\theta,\omega} \oplus_J \mathfrak{L}_-^{\theta,\omega}, \quad \mathfrak{L}_+^{\theta,\omega} = (I + T_{\theta,\omega})\mathfrak{H}_+, \quad \mathfrak{L}_-^{\theta,\omega} = (I + T_{\theta,\omega})\mathfrak{H}_-. \quad (3.17)$$

Let us introduce the notation

$$\alpha_\theta = \frac{1}{2}(\theta + \theta^{-1}) = \cosh(\chi) \quad \text{and} \quad \beta_\theta = \frac{1}{2}(\theta - \theta^{-1}) = \sinh(\chi), \quad \theta = e^\chi$$

so that $\alpha_\theta^2 - \beta_\theta^2 = 1$. Due to (2.8) the operator $\mathcal{C}_{\theta,\omega}$ associated with (3.17) has the form

$$\mathcal{C}_{\theta,\omega} = (I + T_{\theta,\omega})(I - T_{\theta,\omega})^{-1}J = [\alpha_\theta I - \beta_\theta R_\omega]J = e^{-\chi R_\omega} J. \quad (3.18)$$

In particular $\mathcal{C}_{1,\omega} = J$, $\forall \omega \in [0, 2\pi)$. Moreover, due to (2.9) one has $Q = -\chi R_\omega$.

By theorem 2.1 and (3.18) the decomposition (3.17) can be rewritten as

$$\mathfrak{H} = \mathfrak{L}_+^{\theta,\omega} \oplus_{\mathcal{C}} \mathfrak{L}_-^{\theta,\omega}, \quad \mathfrak{L}_+^{\theta,\omega} = \frac{1}{2}(I + \mathcal{C}_{\theta,\omega})\mathfrak{H}, \quad \mathfrak{L}_-^{\theta,\omega} = \frac{1}{2}(I - \mathcal{C}_{\theta,\omega})\mathfrak{H}. \quad (3.19)$$

(The formulae (3.17) and (3.19) determine the same decomposition of \mathfrak{H} ; the first formula emphasizes the J -orthogonality of $\mathfrak{L}_\pm^{\theta,\omega}$, the second formula illustrates the orthogonality of $\mathfrak{L}_\pm^{\theta,\omega}$ with respect to the inner product $(\cdot, \cdot)_{\mathcal{C}}$.)

⁷ These critical configurations will be analyzed in a separate paper.

Lemma 3.3. *The following relations hold:*

$$C_{\theta,\omega}^2 = I, \quad C_{\theta,\omega}^* = C_{1/\theta,\omega} \quad JC_{\theta_1,\omega}C_{\theta_2,\omega} = C_{\theta_2/\theta_1,\omega}. \quad (3.20)$$

Furthermore, $\|C_{\theta,\omega}\| = \theta$ if $\theta \geq 1$ and $\|C_{\theta,\omega}\| = 1/\theta$ if $\theta < 1$.

Proof. Relations (3.20) immediately follow from (3.15) and (3.18). By virtue of (2.9), $C_{\theta,\omega}J = e^{-\chi R_\omega}$ with R_ω a bounded self-adjoint operator. According to (3.18),

$$(e^{-\chi R_\omega} x, x) = \alpha_\theta \|x\|^2 - \beta_\theta (R_\omega x, x) \leq (\alpha_\theta + |\beta_\theta|) \|x\|^2, \quad \forall x \in \mathfrak{H}. \quad (3.21)$$

Obviously, (3.21) turns out to be identity for any $x \in \ker(R_\omega + \text{sign}(\beta_\theta)I)$. Therefore, $\|C_{\theta,\omega}\| = \|e^{-\chi R_\omega}\| = \alpha_\theta + |\beta_\theta|$ since $e^{-\chi R_\omega}$ is a positive self-adjoint operator. Recalling the definition of α_θ and β_θ we complete the proof of the lemma. \square

3.4. The description of J -self-adjoint extensions with $C_{\theta,\omega}$ -symmetries.

Let $A_{M(U)}$ be a J -self-adjoint extension of A_{sym} defined by (3.4) and (3.10).

Lemma 3.4. *A J -self-adjoint extension $A_{M(U)}$ has $C_{1,\omega}$ -symmetry if and only if $q = 0$ (or, equivalently, $A_{M(U)}$ is self-adjoint).*

Proof. A J -self-adjoint extension $A_{M(U)}$ has $C_{1,\omega}$ -symmetry $\iff A_{M(U)}J = JA_{M(U)}$. Comparing this with the relation $A_{M(U)}^*J = JA_{M(U)}$ (since $A_{M(U)}$ is J -self-adjoint) one derives that $A_{M(U)}^* = A_{M(U)}$. Applying now lemma 3.1 we complete the proof. \square

Definition 3.1. *Let Υ denote the collection of all J -self-adjoint extensions $A_{M(U)}$ having $C_{\theta,\omega}$ -symmetry for any choice of θ and ω :*

$$\Upsilon = \{A_{M(U)} : A_{M(U)}C = CA_{M(U)}, \forall \theta \in (0, \infty) \cup \forall \omega \in [0, 2\pi)\}.$$

In analogy with Lie algebra theory [55] it appears natural to call Υ the *extension center*.

Obviously, an operator $A_{M(U)} \in \Upsilon$ is self-adjoint (since $A_{M(U)}$ has $C_{1,\omega}$ -symmetry) and it has a special structure closely related to the properties of A_{sym} . One of the possible ways to describe this structure deals with the concept of supersymmetry (SUSY).

Let H and Q be self-adjoint operators in \mathfrak{H} . Following [56] we will say that the system (H, J, Q) possesses *supersymmetry* if $H = Q^2 \geq 0$ and $JQ = -QJ$.

Proposition 3.2. *Let $A_{M(U)}$ be a J -self-adjoint extension of A_{sym} . The following statements are equivalent:*

- (i) $A_{M(U)}$ belongs to Υ ;
- (ii) $A_{M(U)}J = JA_{M(U)}$ and $A_{M(U)}R = RA_{M(U)}$;
- (iii) The system $(A_{M(U)}^2, J, RA_{M(U)})$ has supersymmetry.

Proof. It follows from (3.15) and (3.18) that $A_{M(U)} \in \Upsilon$ if and only if $JA_{M(U)} = A_{M(U)}J$ and $RA_{M(U)} = A_{M(U)}R$. So, (i) \iff (ii). The latter relation and $JR = -RJ$ mean that $Q = RA_{M(U)}$ is self-adjoint and $JQ = -QJ$. Since $H = (RA_{M(U)})^2 = A_{M(U)}^2 \geq 0$ the system $(A_{M(U)}^2, J, RA_{M(U)})$ has supersymmetry.

Conversely, if $(A_{M(U)}^2, J, RA_{M(U)})$ has supersymmetry, $JRA_{M(U)} = -RA_{M(U)}J$ or $JA_{M(U)} = A_{M(U)}J$. Therefore, the J -self-adjoint operator $A_{M(U)}$ is also self-adjoint. In that case the self-adjointness of $RA_{M(U)}$ gives $RA_{M(U)} = (RA_{M(U)})^* = A_{M(U)}R$. So, $A_{M(U)}$ commutes with J and R . Hence, (ii) \iff (iii). \square

The following statement gives the description of extension center elements $A_{M(U)} \in \Upsilon$ in terms of entries of U (see (3.9)).

Proposition 3.3. $A_{M(U)} \in \Upsilon \iff q = 0$ and $\phi \in \{\frac{\pi}{2}, \frac{3\pi}{2}\}$.

Proof. Let $A_{M(U)} \in \Upsilon$. Since A_{sym} commutes with J and R , the assertion (ii) of proposition 3.2 can be rewritten as $JM(U) = M(U)$ and $RM(U) = M(U)$.

It follows from (3.7) and the description (3.10) of $M(U)$ that $JM(U) = M(U)$ if and only if

$$\begin{aligned} Jd_1 &= e_{++} - q e^{i(\phi+\gamma)} e_{+-} + r e^{i(\phi+\xi)} e_{-+} \in M(U), \\ Jd_2 &= -e_{--} + r e^{i(\phi-\xi)} e_{+-} + q e^{i(\phi-\gamma)} e_{-+} \in M(U). \end{aligned}$$

This is possible if and only if $q = 0$ (since $\{e_{\pm\pm}\}$ are orthonormal and d_i have the form (3.11)).

A similar reasoning for $RM(U) = M(U)$ with the use of (3.14) gives

$$\begin{aligned} Rd_1 &= R(e_{++} + r e^{i(\phi+\xi)} e_{-+}) = r e^{i(\phi+\xi)} (e_{--} + r e^{-i(\phi+\xi)} e_{+-}) \in M(U) \\ Rd_2 &= R(e_{--} - r e^{i(\phi-\xi)} e_{+-}) = -r e^{i(\phi-\xi)} (e_{++} - r e^{-i(\phi-\xi)} e_{-+}) \in M(U), \end{aligned}$$

where $r^2 = 1$. Obviously the latter relations are satisfied if and only if $e^{-i\phi} = -e^{i\phi}$. This is possible when $\phi = \frac{\pi}{2}$ or $\phi = \frac{3\pi}{2}$. Proposition 3.3 is proved. \square

Theorem 3.2. Let $A_{M(U)}$ be a J -self-adjoint extension of A_{sym} and $A_{M(U)} \neq A_{M(U)}^*$ (i.e. $A_{M(U)}$ is not a self-adjoint operator). Then $A_{M(U)}$ has $\mathcal{C}_{\theta,\omega}$ -symmetry if and only if

$$0 < |q| < |\cos \phi|. \tag{3.22}$$

In that case $\omega = \gamma$ and θ is determined by the relation $q = \frac{\theta^{-1}-\theta}{\theta^{-1}+\theta} \cos \phi$.

Proof. Since A_{sym} commutes with J and R , it commutes with R_ω defined by (3.15). This gives $A_{\text{sym}}\mathcal{C}_{\theta,\omega} = \mathcal{C}_{\theta,\omega}A_{\text{sym}}$ (since $\mathcal{C}_{\theta,\omega}$ has the form (3.18)). Employing theorem 3.1 one concludes that the property of $\mathcal{C}_{\theta,\omega}$ -symmetry for $A_{M(U)}$ is equivalent to the relation $\mathcal{C}_{\theta,\omega}M(U) = M(U)$. By (3.10), $\mathcal{C}_{\theta,\omega}M(U) = M(U) \iff \mathcal{C}_{\theta,\omega}d_1 \in M(U)$ and $\mathcal{C}_{\theta,\omega}d_2 \in M(U)$, where d_i have the form (3.11).

It follows from (3.7), (3.16) and (3.18) that

$$\begin{aligned} \mathcal{C}_{\theta,\omega}d_1 &= (\alpha_\theta + \beta_\theta q e^{i(\gamma+\phi-\omega)})e_{++} - (\beta_\theta e^{i\omega} + \alpha_\theta q e^{i(\gamma+\phi-\omega)})e_{+-} \\ &\quad + \alpha_\theta r e^{i(\xi+\phi)} e_{-+} - \beta_\theta r e^{i(\xi+\phi+\omega)} e_{--}. \end{aligned} \tag{3.23}$$

Taking the definition of d_1 and the first and last terms in (3.23) into account one concludes that $\mathcal{C}_{\theta,\omega}d_1 \in M(U) \iff \mathcal{C}_{\theta,\omega}d_1 = k_1d_1 + k_2d_2$, where $k_1 = \alpha_\theta + \beta_\theta q e^{i(\gamma+\phi-\omega)}$ and $k_2 = -\beta_\theta r e^{i(\xi+\phi+\omega)}$. This is possible if and only if the following equalities are satisfied:

$$\begin{aligned} \beta_\theta q r e^{i(\gamma+\xi+2\phi-\omega)} &= \beta_\theta q r e^{i(-\gamma+\xi+2\phi+\omega)} \\ \beta_\theta q^2 e^{i(2\gamma+2\phi-\omega)} + 2\alpha_\theta q e^{i(\gamma+\phi)} + \beta_\theta e^{i\omega} (r^2 e^{2i\phi} + 1) &= 0. \end{aligned} \tag{3.24}$$

A similar reasoning for $\mathcal{C}_{\theta,\omega}d_2 = \tilde{k}_1d_1 + \tilde{k}_2d_2$ with $\tilde{k}_1 = -\beta_\theta r e^{i(-\xi+\phi-\omega)}$ and $\tilde{k}_2 = -\alpha_\theta - \beta_\theta q e^{i(-\gamma+\phi+\omega)}$ implies

$$\begin{aligned} -\beta_\theta q r e^{i(\gamma-\xi+2\phi-\omega)} &= -\beta_\theta q r e^{i(-\gamma-\xi+2\phi+\omega)} \\ \beta_\theta q^2 e^{i(-2\gamma+2\phi+\omega)} + 2\alpha_\theta q e^{i(-\gamma+\phi)} + \beta_\theta e^{-i\omega} (r^2 e^{2i\phi} + 1) &= 0. \end{aligned} \tag{3.25}$$

Therefore, $A_{M(U)}$ has $\mathcal{C}_{\theta,\omega}$ -symmetry if and only if relations (3.24) and (3.25) hold.

Let $A_{M(U)}$ have $\mathcal{C}_{\theta,\omega}$ -symmetry and $A_{M(U)} \neq A_{M(U)}^*$. Then $\theta \neq 1$ (otherwise, $A_{M(U)}$ turns out to be self-adjoint). Further, $q \neq 0$ (by lemma 3.1), $r \neq 0$ (by lemma 3.2) and

$\beta_\theta \neq 0$ (since $\theta \neq 1$). Taking these facts into account we derive from (3.24) and (3.25) that $\mathcal{C}_{\theta \neq 1, \omega} M(U) = M(U)$ if and only if

$$\omega = \gamma \quad \text{and} \quad \beta_\theta q^2 e^{i(2\phi+\omega)} + 2\alpha_\theta q e^{i(\omega+\phi)} + \beta_\theta e^{i\omega} (r^2 e^{2i\phi} + 1) = 0. \quad (3.26)$$

Since $q^2 + r^2 = 1$ (by (3.9)) the second relation in (3.26) can be rewritten as

$$q = -\frac{\beta_\theta}{\alpha_\theta} \left[\frac{e^{i\phi} + e^{-i\phi}}{2} \right] = \frac{\theta^{-1} - \theta}{\theta^{-1} + \theta} \cos \phi. \quad (3.27)$$

Since $\theta \neq 1$, the relation (3.27) implies inequality (3.22).

Conversely, let the parameters ϕ and q of the unitary matrix U (see (3.9)) satisfy (3.22). Then the corresponding J -self-adjoint extension $A_{M(U)}$ does not have $\mathcal{C}_{1, \omega}$ -symmetry and hence $A_{M(U)}$ is not a self-adjoint operator.

The condition (3.22) allows one to choose a parameter θ ($\theta \neq 1$) in such a way that (3.27) holds. Finally setting $\omega = \gamma$, we satisfy relations (3.26). This means that $A_{M(U)}$ has $\mathcal{C}_{\theta, \omega}$ -symmetry for such a choice of ω and θ . Theorem 3.2 is proved. \square

Theorem 3.3. *A J -self-adjoint extension $A_{M(U)}$ of A_{sym} has $\mathcal{C}_{\theta, \omega}$ -symmetry if and only if the matrix U takes the form*

$$U = U(\theta, \omega, \psi, \xi) = \frac{e^{i\phi}}{\alpha_\theta} \begin{pmatrix} -\beta_\theta \cos \phi e^{i\omega} & \sqrt{1 + \beta_\theta^2 \sin^2 \phi} e^{i\xi} \\ -\sqrt{1 + \beta_\theta^2 \sin^2 \phi} e^{-i\xi} & -\beta_\theta \cos \phi e^{-i\omega} \end{pmatrix}, \quad (3.28)$$

where $\phi, \xi \in [0, 2\pi)$.

Proof. Let us consider the case $\theta \neq 1$ and $\phi \notin \{\frac{\pi}{2}, \frac{3\pi}{2}\}$. Then (3.28) is a particular case of the general representation of unitary matrices (3.9) with $q = -\frac{\beta_\theta}{\alpha_\theta} \cos \phi$ that satisfies (3.22). This means that the J -self-adjoint operator $A_{M(U)}$ has $\mathcal{C}_{\theta, \omega}$ -symmetry (by theorem 3.2).

Conversely, let $U = \|u_{ij}\|$ be determined by (3.9) with $\phi \notin \{\frac{\pi}{2}, \frac{3\pi}{2}\}$ and let the corresponding J -self-adjoint extension $A_{M(U)}$ have $\mathcal{C}_{\theta \neq 1, \omega}$ -symmetry. Due to (3.26) and (3.27), $u_{11} = q e^{i(\phi+\gamma)} = -\frac{\beta_\theta}{\alpha_\theta} \cos \phi e^{i(\phi+\omega)}$. But then $u_{22} = -\frac{\beta_\theta}{\alpha_\theta} \cos \phi e^{i(\phi-\omega)}$ by (3.9). Similarly,

$$\begin{aligned} u_{12} &= r e^{i(\phi+\xi)} = \sqrt{1 - q^2} e^{i(\phi+\xi)} = \frac{1}{\alpha_\theta} \sqrt{\alpha_\theta^2 - \beta_\theta^2 \cos^2 \phi} e^{i(\phi+\xi)} \\ &= \frac{1}{\alpha_\theta} \sqrt{1 + \beta_\theta^2 \sin^2 \phi} e^{i(\phi+\xi)}, \end{aligned}$$

and

$$u_{22} = -r e^{i(\phi-\xi)} = -\frac{1}{\alpha_\theta} \sqrt{1 + \beta_\theta^2 \sin^2 \phi} e^{i(\phi-\xi)}.$$

Hence, the matrix U is determined by (3.28).

Let $\theta = 1$ and let ϕ be arbitrary. By lemma 3.4 the J -self-adjoint extension $A_{M(U)}$ with $\mathcal{C}_{1, \omega}$ -symmetry is self-adjoint and $q = 0$. In that case the representation (3.9) of U coincides with (3.28).

Let $\theta \neq 1$ and $\phi \in \{\frac{\pi}{2}, \frac{3\pi}{2}\}$. It follows from theorem 3.2 that $A_{M(U)}$ has to be self-adjoint (otherwise, the inequality (3.22) must be satisfied, which is impossible since $\phi \in \{\frac{\pi}{2}, \frac{3\pi}{2}\}$). Hence, $q = 0$ (by lemma 3.1) and the representation (3.9) of U coincides with (3.28). Theorem 3.3 is proved. \square

3.5. Completeness of the $\mathcal{C}_{\theta,\omega}$ -symmetry family

As was mentioned above (see the proof of theorem 3.2), an arbitrary operator $\mathcal{C}_{\theta,\omega}$ from the two-parameter set $\{\mathcal{C}_{\theta,\omega}\}$ commutes with A_{sym} . We are going to show that, in a certain sense, this family is complete in the set of \mathcal{C} -symmetries commuting with A_{sym} . Precisely, we show that an arbitrary J -self-adjoint extension $A_{M(U)} \supset A_{\text{sym}}$ with the property of \mathcal{C} -symmetry, where \mathcal{C} commutes with A_{sym} , possesses $\mathcal{C}_{\theta,\omega}$ -symmetry for some choice of θ and ω . From this point of view, the family $\mathcal{C}_{\theta,\omega}$ allows for an adequate description of the set of \mathcal{C} -symmetries commuting with A_{sym} .

Our proof below requires the existence of at least one real point λ of regular type for the initial symmetric operator A_{sym} , which is defined in the standard manner as: $\lambda \in \mathbb{R}$ is a point of regular type of A_{sym} if there exists a number $k = k(\lambda) > 0$ such that $\|(A_{\text{sym}} - \lambda I)u\| \geq k\|u\|$, $\forall u \in \mathcal{D}(A_{\text{sym}})$. This condition is not restrictive because it is satisfied for any symmetric operator A_{sym} having at least one self-adjoint extension A with spectrum $\sigma(A)$ which does not cover the whole real line \mathbb{R} (i.e., $\sigma(A) \neq \mathbb{R}$).

Theorem 3.4. *Let a symmetric operator A_{sym} with deficiency indices $\langle 2, 2 \rangle$ have at least one real point λ of regular type and let a J -self-adjoint extension $A_{M(U)} \supset A_{\text{sym}}$ have the property of \mathcal{C} -symmetry, where \mathcal{C} commutes with A_{sym} . Then $A_{M(U)}$ also has the property of $\mathcal{C}_{\theta,\omega}$ -symmetry for a certain choice of θ and ω .*

The proof of theorem 3.4 is based on the following auxiliary result.

Lemma 3.5. *Let A_{sym} satisfy the conditions of theorem 3.4 and let $A_{\text{sym}}\mathcal{C} = \mathcal{C}A_{\text{sym}}$, where \mathcal{C} is a bounded linear operator in \mathfrak{H} with the properties: $\mathcal{C}^2 = I$ and $J\mathcal{C} > 0$. Then the restrictions of \mathcal{C} on $\mathfrak{M} = \mathfrak{N}_i + \mathfrak{N}_{-i}$ coincide with the restrictions of $\mathcal{C}_{\theta,\omega}$ for a certain choice of θ and ω , i.e., $\mathcal{C} \upharpoonright \mathfrak{M} = \mathcal{C}_{\theta,\omega} \upharpoonright \mathfrak{M}$.*

Proof of theorem 3.4. Let the J -self-adjoint extension $A_{M(U)} \supset A_{\text{sym}}$ have the property of \mathcal{C} -symmetry, where \mathcal{C} commutes with A_{sym} . Then $\mathcal{C}M(U) = M(U)$ by theorem 3.1. Since $M(U) \subset \mathfrak{M}$, the last equality is equivalent to $\mathcal{C}_{\theta,\omega}M(U) = M(U)$ for a certain choice of θ and ω by lemma 3.5. Using theorem 3.1 again one derives the property of $\mathcal{C}_{\theta,\omega}$ -symmetry for $A_{M(U)}$. \square

Proof of lemma 3.5. It follows from the proof of theorem 3.1 that $\mathcal{C}\mathfrak{N}_{\pm i} = \mathfrak{N}_{\pm i}$. Therefore, \mathcal{C} has the block structure $\mathcal{C} = \begin{pmatrix} \mathcal{C}_+ & 0 \\ 0 & \mathcal{C}_- \end{pmatrix} (\mathcal{C}_{\pm} := \mathcal{C} \upharpoonright \mathfrak{N}_{\pm i})$ with respect to the decomposition $\mathfrak{M} = \mathfrak{N}_i + \mathfrak{N}_{-i}$.

Let us fix \mathfrak{N}_i and consider the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (3.29)$$

Since $\mathfrak{N}_i = \langle e_{++}, e_{+-} \rangle$, formulae (3.7) and (3.14) imply that $J = \sigma_3$ and $R = \sigma_1$ with respect to the basis $\{e_{++}, e_{+-}\}$.

The conditions $\mathcal{C}^2 = I$ and $J\mathcal{C} > 0$ imposed on \mathcal{C} in lemma 3.5 together with (3.18) enable one to represent \mathcal{C} as follows: $\mathcal{C} = e^{-\chi R_{\omega}} J$, where due to (3.15) $R_{\omega}J = -JR_{\omega}$, $R_{\omega} = R_{\omega}^*$ and $R_{\omega}^2 = I$. Obviously, the same relation must hold for the 2×2 matrix \mathcal{C}_+ , i.e. $\mathcal{C}_+ = e^{-\chi_+ R_{\omega_1}} \sigma_3$ with

$$R_{\omega_1} = R e^{i\omega_1 J} = \cos(\omega_1)\sigma_1 + \sin(\omega_1)\sigma_2. \quad (3.30)$$

From the relation $R_{\omega_1}^2 = I_2$ it follows

$$e^{-\chi_+ R_{\omega_1}} = \cosh(\chi_+)I_2 - \sinh(\chi_+)R_{\omega_1}. \quad (3.31)$$

Identifying $\alpha_{\theta_1} = \cosh(\chi_+)$, $\beta_{\theta_1} = \sinh(\chi_+)$ and using (3.30) we get for $\mathcal{C}_+ = e^{-\chi_+ R_{\omega_1}} \sigma_3$ the explicit representation

$$\mathcal{C}_+ = \begin{pmatrix} \alpha_{\theta_1} & \beta_{\theta_1} e^{-i\omega_1} \\ -\beta_{\theta_1} e^{i\omega_1} & -\alpha_{\theta_1} \end{pmatrix} \tag{3.32}$$

with respect to the basis $\{e_{++}, e_{+-}\}$.

On the other hand, relations (3.7), (3.16) and (3.18) mean that the operator $\mathcal{C}_{\theta_1, \omega_1} \upharpoonright \mathfrak{N}_i$ has the same matrix representation (3.32) with respect to $\{e_{++}, e_{+-}\}$. Therefore, $\mathcal{C}_+ = \mathcal{C} \upharpoonright \mathfrak{N}_i = \mathcal{C}_{\theta_1, \omega_1} \upharpoonright \mathfrak{N}_i$.

It should be noted that the parameters θ_1, ω_1 in (3.32) are not determined uniquely and that the pairs θ_1, ω_1 and $1/\theta_1, \omega_1 - \pi$ define the same matrix \mathcal{C}_+ . In what follows, without loss of generality we will suppose $\theta_1 \geq 1$.

Arguing similarly one derives

$$\mathcal{C}_- = \begin{pmatrix} \alpha_{\theta_2} & \beta_{\theta_2} e^{-i\omega_2} \\ -\beta_{\theta_2} e^{i\omega_2} & -\alpha_{\theta_2} \end{pmatrix}, \quad \theta_2 \geq 1 \tag{3.33}$$

with respect to the basis $\{e_{-+}, e_{--}\}$ of \mathfrak{N}_{-i} and $\mathcal{C}_- = \mathcal{C}_{\theta_2, \omega_2} \upharpoonright \mathfrak{N}_{-i}$.

Let us show that $\theta_1 = \theta_2$ and $\omega_1 = \omega_2$. To prove this we fix a real point λ of regular type of A_{sym} and consider an operator

$$A(u + x_\lambda) = A_{\text{sym}}u + \lambda x_\lambda, \quad \mathcal{D}(A) = \mathcal{D}(A_{\text{sym}}) \dot{+} \mathfrak{N}_{-\lambda} \quad (\mathfrak{N}_{-\lambda} = \mathfrak{H} \ominus \mathcal{R}(A_{\text{sym}} - \lambda I)).$$

Since the real point λ is of regular type, the operator A is a self-adjoint extension of A_{sym} . Furthermore, the commutativity of A_{sym} with the family $\{\mathcal{C}_{\theta, \omega}\}$ gives $\mathcal{C}_{\theta, \omega} \mathfrak{N}_{-\lambda} = \mathfrak{N}_{-\lambda}$. Therefore, $A \mathcal{C}_{\theta, \omega} = \mathcal{C}_{\theta, \omega} A$ for any choice of ω and θ . Thus $A = A_{M(U)} \in \Upsilon$. In that case proposition 3.3 allows one to simplify the general description $M(U)$ given by (3.10) and (3.11) as follows:

$$M(U) = \langle d_1, d_2 \rangle, \quad d_1 = e_{++} + i e^{i\xi} e_{-+}, \quad d_2 = e_{--} - i e^{-i\xi} e_{+-}. \tag{3.34}$$

Turning to the original operator \mathcal{C} we deduce from the proof of theorem 3.1 that $\mathcal{C}^* A_{\text{sym}} = A_{\text{sym}} \mathcal{C}^*$. This gives $\mathcal{C} \mathfrak{N}_{-\lambda} = \mathfrak{N}_{-\lambda}$ and hence, the operator $A = A_{M(U)}$ commutes with \mathcal{C} . Employing theorem 3.1 one derives $\mathcal{C} M(U) = M(U)$, where $M(U)$ is defined by (3.34). Taking relations (3.32) and (3.33) into account and arguing as in the proof of theorem 3.2 we conclude that the equality $\mathcal{C} M(U) = M(U)$ is equivalent to the relations

$$\alpha_{\theta_1} = \alpha_{\theta_2}, \quad \beta_{\theta_1} e^{i\omega_1} = \beta_{\theta_2} e^{i\omega_2}. \tag{3.35}$$

The first relation in (3.35) gives $\theta := \theta_1 = \theta_2$. If $\theta = 1$, then the second relation in (3.35) vanishes. In that case $\mathcal{C}_{1, \omega_1} = \mathcal{C}_{1, \omega_2} = J$ and the restriction $\mathcal{C} \upharpoonright \mathfrak{M}$ coincides with J . If $\theta > 1$ then $\beta_\theta \neq 0$ and the second relation in (3.35) gives $\omega := \omega_1 = \omega_2$. Hence, $\mathcal{C} \upharpoonright \mathfrak{M} = \mathcal{C}_{\theta, \omega}$. Lemma 3.5 is proved. \square

Remark 3.4. Physically, $\mathcal{C}_\pm = \exp[-\chi_\pm R_{\omega_{1,2}}/2](J \upharpoonright \mathfrak{N}_{\pm i}) \exp[\chi_\pm R_{\omega_{1,2}}/2]$ in (3.32) and (3.33) are just the hyperbolically rotated (boosted) versions of the involution $J \upharpoonright \mathfrak{N}_{\pm i}$. The transformation matrices $\exp[\chi_\pm R_{\omega_{1,2}}/2]$ are the elements of the pseudounitary group $SU(1, 1) \cong SO(1, 2) \cong SL(2, \mathbb{R})$ [57] with $R_\omega = e^{-i\omega J/2} R e^{i\omega J/2}$ in (3.30) as Lie algebra elements conjugate to R under the transformations of the compact subgroup $U(1) \cong SO(2) \ni e^{i\omega J/2}$.

3.6. The resolvent formula

As was stated above, the operator A_{sym} commutes with the family $\{\mathcal{C}_{\theta,\omega}\}$. Therefore, with respect to the decomposition (3.19), A_{sym} can be presented as the direct sum: $A_{\text{sym}} = A_{\text{sym}}^+ \dot{+} A_{\text{sym}}^-$ of the symmetric operators $A_{\text{sym}}^\pm = A_{\text{sym}} \upharpoonright_{\mathfrak{L}_\pm^{\theta,\omega}}$ acting in the subspaces $\mathfrak{L}_\pm^{\theta,\omega}$ of \mathfrak{H} .

Obviously, the defect subspaces $\mathfrak{N}_{\pm i}(A_{\text{sym}}^+) = \mathfrak{L}_+^{\theta,\omega} \ominus \mathcal{R}(A_{\text{sym}}^+ \pm iI)$ of A_{sym}^+ coincide with $\mathfrak{N}_{\pm i} \cap \mathfrak{L}_+^{\theta,\omega}$, where $\mathfrak{N}_{\pm i}$ are the defect subspaces of A_{sym} in \mathfrak{H} . Taking this fact and formulae (3.16) into account it is easy to verify that $\mathfrak{N}_i(A_{\text{sym}}^+) = \langle g_i^+(\theta) \rangle$ and $\mathfrak{N}_{-i}(A_{\text{sym}}^+) = \langle g_{-i}^+(\theta) \rangle$, where

$$g_i^+(\theta) = \left(I + \frac{1 - \alpha_\theta}{\beta_\theta} R_\omega \right) e_{++}, \quad g_{-i}^+(\theta) = \left(I + \frac{1 - \alpha_\theta}{\beta_\theta} R_\omega \right) e_{-+}. \quad (3.36)$$

Arguing similarly for A_{sym}^- one derives $\mathfrak{N}_i(A_{\text{sym}}^-) = \langle g_i^-(\theta) \rangle$ and $\mathfrak{N}_{-i}(A_{\text{sym}}^-) = \langle g_{-i}^-(\theta) \rangle$, where the defect elements

$$g_i^-(\theta) = \left(I + \frac{1 - \alpha_\theta}{\beta_\theta} R_\omega \right) e_{+-}, \quad g_{-i}^-(\theta) = \left(I + \frac{1 - \alpha_\theta}{\beta_\theta} R_\omega \right) e_{--} \quad (3.37)$$

belong to $\mathfrak{L}_-^{\theta,\omega}$.

Formulae (3.36) and (3.37) were obtained for $\theta \neq 1$. If $\theta = 1$, then: $g_i^+(1) = e_{++}$, $g_{-i}^+(1) = e_{-+}$, $g_i^-(1) = e_{+-}$, $g_{-i}^-(1) = e_{--}$.

Note that the norms of $g_{\pm i}^\pm(\theta)$ are equal to $\sqrt{\alpha_\theta/(\alpha_\theta + 1)}$. Indeed, the orthonormality of $\{e_{\pm\pm}\}$ in \mathfrak{M} and relations (3.1) and (3.12) imply $\|e_{\pm\pm}\|^2 = 1/2$. Taking (3.16) into account we deduce from (3.36)

$$\|g_i^+(\theta)\|^2 = \|e_{++}\|^2 + \left(\frac{1 - \alpha_\theta}{\beta_\theta} \right)^2 \|e_{+-}\|^2 = \frac{\alpha_\theta}{\alpha_\theta + 1}.$$

The other elements $g_{\pm i}^\pm(\theta)$ are considered by analogy.

Let us fix an arbitrary extension center element $A = A_{M(U)} \in \Upsilon$. According to the definition of Υ (subsection 3.4), A is a self-adjoint extension of A_{sym} and A is reduced by the decomposition (3.19) for an arbitrary choice of θ and ω . The collection of unitary matrices U corresponding to the operators $A_{M(U)} \in \Upsilon$ is described by (3.28) with $\phi \in \{\frac{\pi}{2}, \frac{3\pi}{2}\}$. This means that, without loss of generality (multiplying e_{+-} and e_{-+} by suitable unimodular constants if it is necessary), one can assume that the operator $A = A_{M(U)}$ is defined by the matrix $U = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$.

Obviously, A is decomposed into $A = A^+ \dot{+} A^-$ with respect to (3.19), where A^\pm are the self-adjoint extensions of the symmetric operators A_{sym}^\pm acting in the spaces $\mathfrak{L}_\pm^{\theta,\omega}$ and having the deficiency index $\langle 1, 1 \rangle$ (due to (3.36) and (3.37)). It is easy to see that for arbitrary θ and ω

$$\mathcal{D}(A^+) = \mathcal{D}(A_{\text{sym}}^+) \dot{+} \langle g_i^+(\theta) - g_{-i}^+(\theta) \rangle, \quad \mathcal{D}(A^-) = \mathcal{D}(A_{\text{sym}}^-) \dot{+} \langle g_i^-(\theta) - g_{-i}^-(\theta) \rangle.$$

Let $A_{M(U)}$ be an arbitrary J -self-adjoint extension of A_{sym} with $\mathcal{C}_{\theta,\omega}$ -symmetry. Then the matrix U has the form (3.28) (by theorem 3.3) and the operator $A_{M(U)}$ is reduced by the decomposition (3.19) (for fixed θ and ω). Therefore, $A_{M(U)} = A_{M(U)}^+ \dot{+} A_{M(U)}^-$, where $A_{M(U)}^\pm$ are intermediate extensions of A_{sym}^\pm in $\mathfrak{L}_\pm^{\theta,\omega}$. A direct calculation shows

$$\mathcal{D}(A_{M(U)}^\pm) = \mathcal{D}(A_{\text{sym}}^\pm) \dot{+} \langle g_i^\pm(\theta) + p_\pm g_{-i}^\pm(\theta) \rangle,$$

where

$$p_+ = e^{i(\xi+\mu)}, \quad p_- = -e^{i(\xi-\mu)} \quad \left(e^{i\mu} := \frac{\cos \phi + i\alpha_\theta \sin \phi}{|\cos \phi + i\alpha_\theta \sin \phi|} \right). \quad (3.38)$$

Theorem 3.5. Let $A \in \Upsilon$ and let $A_{M(U)}$ be an arbitrary J -self-adjoint extension of A_{sym} with $C_{\theta,\omega}$ -symmetry (i.e., the matrix U is determined by (3.28)). Then, for any $z \in \mathbb{C} \setminus \mathbb{R}$,

$$\frac{1}{A_{M(U)} - z} = \frac{1}{A - z} + \frac{\alpha_\theta(\alpha_\theta + 1)}{\alpha_\theta \tan \frac{\xi + \mu}{2} - Q(z)} \left(\frac{A + i}{A - z}, g_i^+(1/\theta) \right) \frac{A - i}{A - z} g_i^+(\theta) - \frac{\alpha_\theta(\alpha_\theta + 1)}{\alpha_\theta \cot \frac{\xi - \mu}{2} + Q(z)} \left(\frac{A + i}{A - z}, g_i^-(1/\theta) \right) \frac{A - i}{A - z} g_i^-(\theta),$$

where $\mu = \mu(\phi, \theta)$ is determined in (3.38) and $Q(z) = 2\left(\frac{1+zA}{A-z}e_{++}, (\alpha_\theta I - \beta_\theta R_\omega)e_{++}\right)$.

Proof. Let $z \in \mathbb{C} \setminus \mathbb{R}$ be fixed. Considering A^+ and $A_{M(U)}^+$ as one-dimensional perturbations of the symmetric operator A_{sym}^+ in the space $\mathfrak{L}_+^{\theta,\omega}$ and repeating the standard arguments (see, e.g., [[48], pp 23–28]), one derives the Krein-type resolvent formula:

$$\frac{1}{A_{M(U)}^+ - z} = \frac{1}{A^+ - z} + \frac{1}{i \frac{1-p_+}{1+p_+} \frac{\alpha_\theta}{\alpha_\theta+1} - \tilde{Q}(z)} \left(\frac{A + i}{A - z}, g_i^+(\theta) \right) \frac{A - i}{A - z} g_i^+(\theta). \tag{3.39}$$

Here, the notation $\frac{1}{B-zI}$ is used and $\tilde{Q}(z) = \left(\frac{1+zA}{A-z}g_i^+(\theta), g_i^+(\theta)\right)$ is Krein's Q function [48]. Similarly, the formula

$$\frac{1}{A_{M(U)}^- - z} = \frac{1}{A^- - z} + \frac{1}{i \frac{1-p_-}{1+p_-} \frac{\alpha_\theta}{\alpha_\theta+1} - Q'(z)} \left(\frac{A + i}{A - z}, g_i^-(\theta) \right) \frac{A - i}{A - z} g_i^-(\theta) \tag{3.40}$$

relates the resolvents of A^- and $A_{M(U)}^-$ in $\mathfrak{L}_-^{\theta,\omega}$. Here $\tilde{Q}'(z) = \left(\frac{1+zA}{A-z}g_i^-(\theta), g_i^-(\theta)\right)$.

Let us slightly simplify these formulae. First,

$$i \frac{1 - p_+}{1 + p_+} = \tan \frac{\xi + \mu}{2} \quad \text{and} \quad i \frac{1 - p_-}{1 + p_-} = -\cot \frac{\xi - \mu}{2}$$

due to (3.38). Further, it follows from (3.36), (3.37) and (3.16) that

$$R_\omega g_i^-(\theta) = \left(I + \frac{1 - \alpha_\theta}{\beta_\theta} R_\omega \right) R_\omega e_{+-} = e^{-i\omega} g_i^+(\theta).$$

Since $A \in \Upsilon$ and therefore, A commutes with R_ω (see the proof of proposition 3.2) one concludes

$$\tilde{Q}'(z) = \left(R_\omega \frac{1+zA}{A-z} g_i^-(\theta), R_\omega g_i^-(\theta) \right) = \left(\frac{1+zA}{A-z} R_\omega g_i^-(\theta), R_\omega g_i^-(\theta) \right) = \tilde{Q}(z).$$

Furthermore, employing (3.36), one derives

$$\tilde{Q}(z) = \left(\frac{1+zA}{A-z} e_{++}, \left(I + \frac{1 - \alpha_\theta}{\beta_\theta} R_\omega \right)^2 e_{++} \right) = \frac{\alpha_\theta - 1}{\beta_\theta^2} Q(z),$$

where $Q(z) = 2\left(\frac{1+zA}{A-z}e_{++}, (\alpha_\theta I - \beta_\theta R_\omega)e_{++}\right)$.

Combining (3.39) and (3.40) with the expressions above and taking into account that the formula $f = \frac{(I+C_{\theta,\omega})}{2} f + \frac{(I-C_{\theta,\omega})}{2} f$ gives the decomposition of an arbitrary element $f \in \mathfrak{H}$ into its $\mathfrak{L}_\pm^{\theta,\omega}$ -parts, one gets (after trivial calculations) the following resolvent formula in \mathfrak{H} :

$$\frac{1}{A_{M(U)} - z} = \frac{1}{A - z} + \frac{\beta_\theta^2}{(\alpha_\theta - 1)[\alpha_\theta \tan \frac{\xi + \mu}{2} - Q(z)]} \left(\frac{A + i}{A - z} \frac{I + C_{\theta,\omega}}{2}, g_i^+(\theta) \right) \frac{A - i}{A - z} g_i^+(\theta) - \frac{\beta_\theta^2}{(\alpha_\theta - 1)[\alpha_\theta \cot \frac{\xi - \mu}{2} + Q(z)]} \left(\frac{A + i}{A - z} \frac{I - C_{\theta,\omega}}{2}, g_i^-(\theta) \right) \frac{A - i}{A - z} g_i^-(\theta).$$

It follows from (3.7), (3.16), (3.18), (3.20) and (3.36) that

$$(I + C_{\theta,\omega}^*)g_i^+(\theta) = (I + C_{1/\theta,\omega})g_i^+(\theta) = 2\alpha_\theta \left(e_{++} - \frac{1 - \alpha_\theta}{\beta_\theta} e^{i\omega} e_{+-} \right) = 2\alpha_\theta g_i^+(1/\theta).$$

Therefore, for any $f \in \mathfrak{H}$,

$$\left(\frac{A + i}{A - z} \frac{I + C_{\theta,\omega}}{2} f, g_i^+(\theta) \right) = \left(\frac{I + C_{\theta,\omega}}{2} \frac{A + i}{A - z} f, g_i^+(\theta) \right) = \alpha_\theta \left(\frac{A + i}{A - z} f, g_i^+(1/\theta) \right).$$

Similarly, $(I - C_{\theta,\omega}^*)g_i^-(\theta) = 2\alpha_\theta g_i^-(1/\theta)$ and

$$\left(\frac{A + i}{A - z} \frac{I - C_{\theta,\omega}}{2} f, g_i^-(\theta) \right) = \alpha_\theta \left(\frac{A + i}{A - z} f, g_i^-(1/\theta) \right).$$

Substituting the obtained expressions into the above resolvent formula and taking the evident relation $\frac{\alpha_\theta \beta_\theta^2}{\alpha_\theta - 1} = \frac{\alpha_\theta (\alpha_\theta + 1) \beta_\theta^2}{\alpha_\theta^2 - 1} = \alpha_\theta (\alpha_\theta + 1)$ into account, we complete the proof of theorem 3.5. \square

Let A_M be an arbitrary J -self-adjoint operator with \mathcal{C} -symmetry. This means that A_M is similar to a self-adjoint operator (see corollary 2.1) and, hence, one can define the essential spectrum $\sigma_{\text{ess}}(A_M)$ in analogy with that of self-adjoint operators⁸.

Corollary 3.1. *Let the spectrum of $A \in \Upsilon$ be purely essential (i.e., $\sigma(A) = \sigma_{\text{ess}}(A)$) and let $A_{M(U)}$ be an arbitrary J -self-adjoint extension of A_{sym} with $\mathcal{C}_{\theta,\omega}$ -symmetry. Then the essential spectrum of $A_{M(U)}$ coincides with $\sigma_{\text{ess}}(A)$ and the discrete spectrum $\sigma_{\text{disc}}(A_{M(U)})$ is determined as the solutions of the equation*

$$\left[\alpha_\theta \tan \frac{\xi + \mu}{2} - Q(z) \right] \cdot \left[\alpha_\theta \cot \frac{\xi - \mu}{2} + Q(z) \right] = 0, \quad z \in \mathbb{R} \setminus \sigma_{\text{ess}}(A), \quad (3.41)$$

where $Q(z) = 2 \left(\frac{1+zA}{A-z} e_{++}, (\alpha_\theta I - \beta_\theta R_\omega) e_{++} \right)$.

The proof of corollary 3.1 immediately follows from the resolvent formula in theorem 3.5 if one takes into account the following arguments: (1) A and $A_{M(U)}$ are self-adjoint in \mathfrak{H} with respect to the inner product $(\cdot, \cdot)_\mathcal{C}$ (subsection 2.2) and they are reduced by the decomposition $\mathfrak{H} = \mathfrak{L}_+^{\theta,\omega} \oplus_\mathcal{C} \mathfrak{L}_-^{\theta,\omega}$ (see (3.19)); (2) the second and third parts on the right-hand side of the resolvent formula belong to $\mathfrak{L}_+^{\theta,\omega}$ and $\mathfrak{L}_-^{\theta,\omega}$, respectively (since $g_i^\pm(\theta) \in \mathfrak{L}_\pm^{\theta,\omega}$).

4. Examples

4.1. The Schrödinger operator with a general zero-range potential

A one-dimensional Schrödinger operator corresponding to a general zero-range potential at the point $x = 0$ can be given by the expression

$$-\frac{d^2}{dx^2} + t_{11} \langle \delta, \cdot \rangle \delta + t_{12} \langle \delta', \cdot \rangle \delta + t_{21} \langle \delta, \cdot \rangle \delta' + t_{22} \langle \delta', \cdot \rangle \delta', \quad (4.1)$$

where δ and δ' are, respectively, the Dirac δ -function and its derivative (with support at 0) and t_{ij} are complex numbers.

⁸ For a self-adjoint operator A the essential spectrum $\sigma_{\text{ess}}(A)$ is obtained by removing from $\sigma(A)$ all isolated eigenvalues of finite multiplicity.

The standard approach [48] enables one to consider an operator realization A_T ($T = \|t_{ij}\|$) of (4.1) in $L_2(\mathbb{R})$ by setting

$$A_T = A_{\text{reg}} \upharpoonright \mathcal{D}(A_T), \quad \mathcal{D}(A_T) = \{f \in W_2^2(\mathbb{R} \setminus \{0\}) : A_{\text{reg}} f \in L_2(\mathbb{R})\}, \quad (4.2)$$

where the regularization of (4.1) onto $W_2^2(\mathbb{R} \setminus \{0\})$ has the form

$$A_{\text{reg}} = -\frac{d^2}{dx^2} + t_{11} \langle \delta_{ex}, \cdot \rangle \delta + t_{12} \langle \delta'_{ex}, \cdot \rangle \delta + t_{21} \langle \delta_{ex}, \cdot \rangle \delta' + t_{22} \langle \delta'_{ex}, \cdot \rangle \delta'.$$

Here, $-\frac{d^2}{dx^2}$ acts on $W_2^2(\mathbb{R} \setminus \{0\})$ in the distributional sense and

$$\langle \delta_{ex}, f \rangle = \frac{f(+0) + f(-0)}{2}, \quad \langle \delta'_{ex}, f \rangle = -\frac{f'(+0) + f'(-0)}{2}$$

for all $f \in W_2^2(\mathbb{R} \setminus \{0\})$.

An operator realization A_T of (4.1) is an intermediate extension (i.e., $A_{\text{sym}} \subset A_T \subset A_{\text{sym}}^*$) of the symmetric operator

$$A_{\text{sym}} = -\frac{d^2}{dx^2} \upharpoonright \{u \in W_2^2(\mathbb{R}) : u(0) = u'(0) = 0\} \quad (4.3)$$

associated with (4.1).

Let \mathcal{P} be the space parity operator ($\mathcal{P}f(x) = f(-x)$) in $L_2(\mathbb{R})$. The family of \mathcal{P} -self-adjoint operator realizations A_T of (4.1) is distinguished by the conditions $t_{11}, t_{22} \in \mathbb{R}, t_{21} = -\overline{t_{12}}$ imposed on the entries t_{ij} of T [50]. Another description of \mathcal{P} -self-adjoint extensions of A_{sym} can be found in [49].

Let us consider the fundamental symmetry $Rf(x) = \text{sign}(x)f(x)$ in $L_2(\mathbb{R})$. Obviously, $\mathcal{P}R = -R\mathcal{P}$. Since the operator A_{sym} in (4.3) has the deficiency indices $(2, 2)$ and commutes with $J \equiv \mathcal{P}$ and R , one can define the family of $\mathcal{C}_{\theta, \omega}$ -symmetries by (3.15) and (3.18).

Theorem 4.1. *A \mathcal{P} -self-adjoint operator realization A_T of (4.1) has the property of \mathcal{C} -symmetry, where \mathcal{C} commutes with A_{sym} if and only if there exist $\theta > 0, \omega, \phi, \xi \in [0, 2\pi)$ such that the matrix T has the form*

$$T = \frac{2}{\Delta} \begin{pmatrix} \sqrt{2}(\alpha_\theta \sin \phi - \sqrt{1 + \beta_\theta^2 \sin^2 \phi} \cos \xi) & -\beta_\theta \cos \phi e^{-i\omega} \\ \beta_\theta \cos \phi e^{i\omega} & -\sqrt{2}(\alpha_\theta \sin \phi - \sqrt{1 + \beta_\theta^2 \sin^2 \phi} \sin \xi) \end{pmatrix},$$

where $\Delta = \alpha_\theta(\cos \phi - \sin \phi) + \sqrt{1 + \beta_\theta^2 \sin^2 \phi}(\cos \xi + \sin \xi)$. In that case A_T has $\mathcal{C}_{\theta, \omega}$ -symmetry.

Proof. Since A_{sym} is non-negative, the existence of \mathcal{C} -symmetry for A_T , where $\mathcal{C}A_{\text{sym}} = A_{\text{sym}}\mathcal{C}$, is equivalent to the $\mathcal{C}_{\theta, \omega}$ -symmetry of A_T for some choice of $\theta > 0$ and $\omega \in [0, 2\pi)$ (see theorem 3.4).

The family of \mathcal{P} -self-adjoint extensions $A_{M(U)}$ of A_{sym} having the property of $\mathcal{C}_{\theta, \omega}$ -symmetry is described in theorem 3.3. Therefore, the proof of theorem 4.1 consists of finding direct connections between the parameters of matrices U in (3.28) and the entries t_{ij} of T providing the equality $A_T = A_{M(U)}$. To do this, we note that the defect subspaces \mathfrak{N}_{+i} and \mathfrak{N}_{-i} of A_{sym} coincide, respectively, with the linear spans of the functions $\langle h_{1+}, h_{2+} \rangle$ and $\langle h_{1-}, h_{2-} \rangle$, where

$$h_{1\pm}(x) = \begin{cases} e^{i\tau_\pm x}, & x > 0 \\ e^{-i\tau_\pm x}, & x < 0 \end{cases} \quad h_{2\pm}(x) = \begin{cases} -e^{i\tau_\pm x}, & x > 0 \\ e^{-i\tau_\pm x}, & x < 0 \end{cases} \quad (4.4)$$

and $\tau_\pm = \pm \frac{1}{\sqrt{2}} + i \frac{1}{\sqrt{2}} \quad (\tau_\pm^2 = \pm i)$.

Since $\mathcal{P}h_{1\pm} = h_{1\pm}$ and $\mathcal{P}h_{2\pm} = -h_{2\pm}$, the orthonormal basis $\{e_{\pm\pm}\}$ of the Hilbert space $\mathfrak{H} = \mathfrak{H}_{-i} \dot{+} \mathfrak{H}_i$ (see (3.1)) takes the form:

$$e_{++} = \alpha h_{1+}, \quad e_{+-} = \alpha h_{2+}, \quad e_{-+} = \alpha h_{1-}, \quad e_{--} = \alpha h_{2-}, \quad (4.5)$$

where $\alpha = 2^{-3/4}$ is a normalizing constant.

Let a \mathcal{P} -self-adjoint operator A_T be determined by (4.2). It is known [50] that A_T can be described as the restriction of A_{sym}^* on

$$\mathcal{D}(A_T) = \{f \in W_2^2(\mathbb{R} \setminus \{0\}) : T\Gamma_0 f = \Gamma_1 f\}, \quad (4.6)$$

where

$$\Gamma_0 f = \frac{1}{2} \begin{pmatrix} f(+0) + f(-0) \\ -f'(+0) - f'(-0) \end{pmatrix} \quad \text{and} \quad \Gamma_1 f = \begin{pmatrix} f'(+0) - f'(-0) \\ f(+0) - f(-0) \end{pmatrix}.$$

It follows from (3.10) and theorem 3.3 that A_T has $\mathcal{C}_{\theta,\omega}$ -symmetry if and only if $\mathcal{D}(A_T) = \mathcal{D}(A_{M(U)}) = \mathcal{D}(A_{\text{sym}}) \dot{+} M(U)$, where $M(U)$ is the linear span of

$$\begin{aligned} d_1 &= e_{++} - \frac{\beta_\theta}{\alpha_\theta} \cos \phi e^{i(\phi+\omega)} e_{+-} + \frac{1}{\alpha_\theta} \sqrt{1 + \beta_\theta^2 \sin^2 \phi} e^{i(\phi+\xi)} e_{-+}, \\ d_2 &= e_{--} - \frac{1}{\alpha_\theta} \sqrt{1 + \beta_\theta^2 \sin^2 \phi} e^{i(\phi-\xi)} e_{+-} - \frac{\beta_\theta}{\alpha_\theta} \cos \phi e^{i(\phi-\omega)} e_{-+}. \end{aligned} \quad (4.7)$$

The boundary values $\Gamma_i d_1$ and $\Gamma_i d_2$ ($i = 0, 1$) can easily be calculated with the help of (4.5). Substituting these values into (4.6) instead of $\Gamma_i f$ one derives a system of linear equations with respect to t_{ij} . Its solution (the matrix T in theorem 4.1) gives the general form of all T such that $A_T = A_{M(U)}$. Only in this case the operator A_T has $\mathcal{C}_{\theta,\omega}$ -symmetry. Theorem 4.1 is proved. \square

Combining the description of Υ given in proposition 3.3 with formulae (4.5) and (4.7) leads to the conclusion that a \mathcal{P} -self-adjoint extension $A_{M(U)}$ of A_{sym} belongs to Υ if and only if

$$\mathcal{D}(A_{M(U)}) = \{f \in W_2^2(\mathbb{R} \setminus \{0\}) : f(+0) = cf'(+0); f(-0) = -cf'(-0)\},$$

where $c \in \mathbb{R} \cup \{\infty\}$. So, operators from Υ are characterized by separated boundary conditions and they are just the second derivative self-adjoint operators on the half-lines. In particular, the operator $A \in \Upsilon$ which has been used in theorem 3.5 corresponds to the case $c = 0$, i.e.,

$$\mathcal{D}(A) = \{f \in W_2^2(\mathbb{R} \setminus \{0\}) : f(+0) = 0; f(-0) = 0\}.$$

This operator is the Friedrichs extension of A_{sym} and the spectrum of A is purely absolutely continuous and it coincides with $[0, \infty)$. According to corollary 3.1, the discrete spectrum of an arbitrary \mathcal{P} -self-adjoint extension $A_{M(U)}$ is determined by (3.41), where $Q(z)$ can be calculated in an explicit form with the use of (4.4) and (4.5): $Q(z) = k(z)\alpha_\theta$, where

$$k(z) = \frac{4\sqrt{2}}{\pi} \int_0^\infty \frac{y^2(1+zy^2)}{(y^2-z)(y^4+1)} dy.$$

Therefore, $A_{M(U)}$ has a negative eigenvalue z if and only if

$$\left[\tan \frac{\xi + \mu}{2} - k(z) \right] \cdot \left[\cot \frac{\xi - \mu}{2} + k(z) \right] = 0, \quad (4.8)$$

where $\mu = \mu(\theta, \phi)$ is determined by (3.38). The formula (4.8) does not depend on ω in (3.28). This means that the discrete spectrum of $A_{M(U)}(U = U(\theta, \omega, \psi, \xi))$ does not depend on the choice of ω .

4.2. One-dimensional Dirac operator with point perturbation

Let us consider the free Dirac operator D in the space $L_2(\mathbb{R}) \otimes \mathbb{C}^2$:

$$D = -ic \frac{d}{dx} \otimes \sigma_1 + \frac{c^2}{2} \otimes \sigma_3, \quad \mathcal{D}(D) = W_2^1(\mathbb{R}) \otimes \mathbb{C}^2,$$

where σ_1, σ_3 are Pauli matrices (see (3.29)) and $c > 0$ denotes the velocity of light.

The symmetric Dirac operator $A_{\text{sym}} = D \upharpoonright \{u \in W_2^1(\mathbb{R}) \otimes \mathbb{C}^2 : u(0) = 0\}$ has the deficiency indices $\langle 2, 2 \rangle$ [47, 58] and it commutes with the fundamental symmetry $J = \mathcal{P} \otimes \sigma_3$ in $L_2(\mathbb{R}) \otimes \mathbb{C}^2$. Here $u(\cdot) = \begin{pmatrix} u_1(\cdot) \\ u_2(\cdot) \end{pmatrix} \in W_2^1(\mathbb{R}) \otimes \mathbb{C}^2$.

The defect subspaces \mathfrak{N}_i and \mathfrak{N}_{-i} of A_{sym} coincide, respectively, with the linear spans of the functions $\langle h_{1+}, h_{2+} \rangle$ and $\langle h_{1-}, h_{2-} \rangle$, where

$$h_{1\pm}(x) = \begin{pmatrix} -i e^{\mp i\tau} \\ \text{sign}(x) \end{pmatrix} e^{i\tau|x|}, \quad h_{2\pm}(x) = \text{sign}(x)h_{1\pm}(x), \quad x \in \mathbb{R}, \quad (4.9)$$

$$\tau = \frac{i}{c} \sqrt{\frac{c^4}{4} + 1}, \text{ and } e^{i\tau} := \left(\frac{c^2}{2} - i\right) \left(\sqrt{\frac{c^4}{4} + 1}\right)^{-1}.$$

Since $Jh_{1\pm} = h_{1\pm}$ and $Jh_{2\pm} = -h_{2\pm}$, the orthonormal basis $\{e_{\pm\pm}\}$ of the Hilbert space $\mathfrak{M} = \mathfrak{N}_{-i} \dot{+} \mathfrak{N}_i$ (see (3.1)) takes the form:

$$e_{++} = \alpha h_{1+}, \quad e_{+-} = \alpha h_{2+}, \quad e_{-+} = \alpha h_{1-}, \quad e_{--} = \alpha h_{2-}, \quad (4.10)$$

where α is a normalizing constant providing $\|e_{\pm\pm}\|_{\mathfrak{M}} = 1$.

The adjoint operator $A_{\text{sym}}^* = -i \frac{d}{dx} \otimes \sigma_1 + m \otimes \sigma_3$ is defined in the domain $\mathcal{D}(A_{\text{sym}}^*) = W_2^1(\mathbb{R} \setminus \{0\}) \otimes \mathbb{C}^2$, and an arbitrary J -self-adjoint extension $A_{M(U)}$ of A_{sym} is the restriction of A_{sym}^* on $\mathcal{D}(A_{M(U)}) = \mathcal{D}(A_{\text{sym}}) \dot{+} M(U)$, where $M(U)$ is defined by (3.10) and (3.11) with $e_{\pm\pm}$ determined by (4.10). Other descriptions of J -self-adjoint extensions of A_{sym} can be found in [47, 59, 58].

To construct the family of $\mathcal{C}_{\theta,\omega}$ -symmetries for J -self-adjoint extensions $A_{M(U)}$ one needs to find a fundamental symmetry R in $L_2(\mathbb{R}) \otimes \mathbb{C}^2$ such that

$$JR = -RJ \quad \text{and} \quad A_{\text{sym}}R = RA_{\text{sym}}.$$

Obviously, these relations are satisfied for $R = \text{sign}(x)I$. In that case one can define the collection of $\mathcal{C}_{\theta,\omega}$ -symmetries by (3.18). According to theorem 3.3, a family of J -self-adjoint extensions $\{A_{M(U)}\}$ having at least one $\mathcal{C}_{\theta,\omega}$ -symmetry is described by subspaces $M(U) = \langle d_1, d_2 \rangle$, where d_i are determined by (4.7) and (4.10). In the particular case $A_{M(U)} \in \Upsilon$ (i.e., $A_{M(U)}$ commutes with any $\mathcal{C}_{\theta,\omega}$), relation (3.34) must be used instead of (4.7). A routine calculation gives $A_{M(U)} \in \Upsilon$ if and only if

$$\mathcal{D}(A_{M(U)}) = \left\{ f \in W_2^1(\mathbb{R} \setminus \{0\}) \otimes \mathbb{C}^2 : \begin{array}{l} i \cos\left(\frac{\xi}{2} + \frac{\pi}{4}\right) f_1(+0) = \cos\left(t + \frac{\xi}{2} + \frac{\pi}{4}\right) f_2(+0) \\ -i \cos\left(\frac{\xi}{2} + \frac{\pi}{4}\right) f_1(-0) = \cos\left(t + \frac{\xi}{2} + \frac{\pi}{4}\right) f_2(-0) \end{array} \right\},$$

where t is determined in (4.9) and $\xi \in [0, 2\pi)$. Hence, as in the case of a Schrödinger operator, the elements of Υ are characterized by separated boundary conditions. The operator $A \in \Upsilon$ in the resolvent formula (see theorem 3.5) corresponds to the case $\xi = \frac{\pi}{2}$, i.e.,

$$\mathcal{D}(A) = \{f \in W_2^1(\mathbb{R} \setminus \{0\}) \otimes \mathbb{C}^2 : f_2(+0) = f_2(-0) = 0\}$$

($\cos(t + \frac{\pi}{2}) \neq 0$ by the definition of t). Since

$$A^2 = \left(-c^2 \frac{d^2}{dx^2} + \frac{c^4}{4} \right) \otimes I, \quad \mathcal{D}(A^2) = \left\{ f \in W_2^2(\mathbb{R} \setminus \{0\}) \otimes \mathbb{C}^2: \begin{array}{l} f_1'(+0) = f_1'(-0) = 0 \\ f_2(+0) = f_2(-0) = 0 \end{array} \right\}$$

the spectrum of A is purely absolutely continuous and coincides with $(-\infty, -c^2/2] \cup [c^2/2, \infty)$.

Let $A_{M(U)}$ be a J -self-adjoint extension of A_{sym} with $\mathcal{C}_{\theta, \omega}$ -symmetry. Then $A_{M(U)}$ turns out to be self-adjoint in $L_2(\mathbb{R}) \otimes \mathbb{C}^2$ with respect to the inner product $(\cdot, \cdot)_{\mathcal{C}_{\theta, \omega}}$. The corresponding resolvent formula is given in theorem 3.5; the essential spectrum of $A_{M(U)}$ coincides with $(-\infty, -c^2/2] \cup [c^2/2, \infty)$ and its bound states $z \in (-c^2/2, c^2/2)$ can be found as solutions of (3.41).

5. Conclusions

In this paper von Neumann's self-adjoint extension technique for symmetric operators has been reshaped to provide *J-self-adjoint extensions* of symmetric operators with arbitrary but equal deficiency indices $\langle n, n \rangle$, $n \in \mathbb{N} \cup \infty$. The crucial role is played by a bijection between the resulting family of J -self-adjoint operators and the hypermaximal neutral subspaces of the defect Krein space. It is proven that the \mathcal{C} operators of the resulting Hamiltonians leave the defect Krein spaces invariant. For J -self-adjoint extensions of symmetric operators with deficiency indices $\langle 2, 2 \rangle$ the parametrization of the \mathcal{C} -operator family is worked out in detail and Krein-type resolvent formulae are constructed. The technique is exemplified on 1D pseudo-Hermitian Schrödinger and Dirac Hamiltonians with complex point-interaction potentials.

Due to their specific structure, Hamiltonians obtained as J -self-adjoint extensions of symmetric operators provide an excellent playing ground for studies on the Krein-space related features of pseudo-Hermitian and \mathcal{PT} -symmetric operators. The advantages of such model Hamiltonians have their origin in the following properties. For sufficiently simple symmetric differential operators the models remain exactly solvable. They have rich parameter spaces which are bijectively related to the hypermaximal neutral subspaces of the defect Krein spaces of the symmetric operators. As differential operators the resulting pseudo-Hermitian Hamiltonians possess, in general, much richer spectra than simple matrix Hamiltonians, i.e., apart from discrete spectra they will have continuous and, possibly, residual spectra. Corresponding resolvent studies can be carried out in full detail with exact results. In this way, these Hamiltonians have the capability to provide some deeper insights into the structural subtleties of pseudo-Hermitian and \mathcal{PT} -symmetric quantum theories.

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