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$\mathcal{PT}$ Symmetric, Hermitian and $\mathcal{P}$-Self-Adjoint Operators Related to Potentials in $\mathcal{PT}$ Quantum Mechanics

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Abstract

In the recent years a generalization $H = p^2 + x^2(ix)^\epsilon$ of the harmonic oscillator using a complex deformation was investigated, where ϵ is a real parameter. Here, we will consider the most simple case: ϵ even and x real. We will give a complete characterization of three different classes of operators associated with the differential expression H: The class of all self-adjoint (Hermitian) operators, the class of all $\mathcal{PT}$ symmetric operators and the class of all $\mathcal{P}$-self-adjoint operators. Surprisingly, some of the $\mathcal{PT}$ symmetric operators associated to this expression have no resolvent set.

1 Introduction

In the well-known paper [1] from 1998 C.M. Bender and S. Boettcher considered the following Hamiltonians τ_ϵ,

$$\tau_\epsilon(y)(x) := -y''(x) + x^2(ix)^\epsilon y(x), \quad \epsilon > 0. \tag{1.1}$$

This gave rise to a mathematically consistent complex extension of conventional quantum mechanics into $\mathcal{PT}$ quantum mechanics, see, e.g., the review paper [2]. During the past ten years these $\mathcal{PT}$ models have been analyzed intensively.
Starting from the pioneering work of C.M. Bender and S. Boettcher [1], the above Hamiltonian τ_ϵ was always understood as a complex extension of the

harmonic oscillator $H = \frac{d^2}{dx^2} + x^2$ defined along an appropriate complex contour within Stokes wedges. In [3] the problem was mapped back to the real axis using a real parametrization of a suitable contour within the Stokes wedges and in [4, 5, 6] this approach was extended to different parametrizations and contours.

Usually, see, e.g., [1, 2, 7, 8, 9], a closed densely defined operator H in the Hilbert space $L^2(\mathbb{R})$ is called $\mathcal{PT}$ symmetric if H commutes with $\mathcal{PT}$, where $\mathcal{P}$ represents parity reflection and the operator $\mathcal{T}$ represents time reversal, i.e.

$$(\mathcal{P}f)(x) = f(-x) \quad \text{and} \quad (\mathcal{T}f)(x) = \overline{f(x)}, \quad f \in L^2(\mathbb{R}). \tag{1.2}$$

Via the parity operator $\mathcal{P}$ an indefinite inner product is given by

$$[f, g] := \int_{\mathbb{R}} f(x)\overline{(\mathcal{P}g)(x)}\, dx = \int_{\mathbb{R}} f(x)\overline{g(-x)}\, dx, \quad f, g \in L^2(\mathbb{R}).$$

With respect to this inner product, $L^2(\mathbb{R})$ becomes a Krein space and, as usual, a closed densely defined operator H is called $\mathcal{P}$-self-adjoint if H coincides with its $[\cdot,\cdot]$-adjoint, see, e.g., [10, 11, 12, 13, 14].

For unbounded operators both notions, $\mathcal{PT}$ symmetry and $\mathcal{P}$-self-adjointness, are also conditions on the domains. These two notions will be of central interest in this paper, therefore we emphasize them in the following definition. We denote by $\operatorname{dom} H$ the domain of the operator H.

Definition 1.1. *A closed densely defined operator H in $L^2(\mathbb{R})$ is said to be $\mathcal{PT}$ symmetric if for all $f \in \operatorname{dom} H$ we have*

$$\mathcal{PT} f \in \operatorname{dom} H \quad \text{and} \quad \mathcal{PT} Hf = H\mathcal{PT} f.$$

It is called $\mathcal{P}$-self-adjoint if we have

$$\operatorname{dom} H = \operatorname{dom} H^*\mathcal{P} \quad \text{and} \quad Hf = \mathcal{P}H^*\mathcal{P}f \quad \text{for } f \in \operatorname{dom} H.$$

Clearly, a $\mathcal{P}$-self-adjoint operator H is also $\mathcal{P}$-symmetric, that is, we have

$$[Hf, g] = [f, Hg] \quad \text{for all } f, g \in \operatorname{dom} H.$$

Here we will restrict ourselves to the most simple case: We will consider the differential expression τ_ϵ in (1.1) only for real x. Moreover, if ϵ is even, we obtain a real-valued potential, i.e. if $\epsilon = 4n$ the above differential expression τ_{4n}, $n \in \mathbb{N}$, in (1.1) will be of the form

$$\tau_{4n}(y)(x) := -y''(x) + x^{4n+2}y(x), \quad x \in \mathbb{R}. \tag{1.3}$$

and it will be of the form

$$\tau_{4n+2}(y)(x) := -y''(x) - x^{4n+4}y(x), \quad x \in \mathbb{R}. \tag{1.4}$$

in case $\epsilon = 4n+2$. In this situation we can make use of the well-developed theory of Sturm-Liouville operators (see, e.g., [15, 16, 17, 18]). Namely, it turns out that the expression τ_{4n} is in the limit point case at ∞ and at $-\infty$, hence there is only one self adjoint operator connected to τ_{4n} which is also $\mathcal{PT}$ symmetric and $\mathcal{P}$-self-adjoint.
The more interesting case is $\epsilon = 4n+2$. The differential expression τ_{4n+2} is then in limit circle case at $+\infty$ and at $-\infty$ and it admits many different extensions. These extensions are described via restrictions of the maximal domain $\mathcal{D}_{\max}$ by "boundary conditions at $+\infty$ and $-\infty$". Therefore, we will consider the differential expression τ_ϵ only in the case of $\epsilon = 4n+2$, $n \in \mathbb{N}$. Actually, we will consider a slightly more general case which includes the case of τ_{4n+2}. For this, we will always assume that q is a real valued function from $L^1_{loc}(\mathbb{R})$ which is even, that is,

$$q(x) = q(-x) \quad \text{for all } x \in \mathbb{R},$$

such that the differential equation

$$\tau_q(y)(x) := -y''(x) - q(x)y(x), \quad x \in \mathbb{R}. \tag{1.5}$$

is in limit circle case at $+\infty$ and $-\infty$.
It is the aim of this paper to specify three classes of operators connected with the differential expression τ_q in (1.5): $\mathcal{PT}$ symmetric operators, $\mathcal{P}$-self-adjoint operators and self-adjoint (Hermitian) operators. The main result of this paper is a full characterization of these classes, which, in addition, enables one to precisely describe the intersection of these classes. In this sense, it is a continuation of [19], where all self-adjoint (Hermitian) and at the same time $\mathcal{PT}$ symmetric operators in $L^2(\mathbb{R})$ associated with τ_ϵ were described.
Surprisingly, it turns out that with the differential expression τ_q in (1.5) there are $\mathcal{PT}$ symmetric operators which correspond to one- and three-dimensional extensions of the minimal operator which are neither Hermitian nor $\mathcal{P}$-self-adjoint and which

possesses an empty resolvent set.

In a next step we will consider complex deformations, which are, from the mathematical point of view, less understood. These questions will be treated in a subsequent note. However, in our opinion even the most "simple" case (i.e. $\epsilon = 4n+2$, x real) contains enough unsolved questions and possesses a rich structure which one needs to understand first.
This paper is organized as follows: After introducing the basic notions like minimal/maximal operator associated with τ_q and bi-extensions in Section 2, we consider 2-dimensional extensions in Section 4, 3-dimensional extensions in Section 5 and 1-dimensional extensions in Section 6. In the case of 2-dimensional extensions in Section 4 we describe all bi-extensions which are $\mathcal{PT}$-symmetric or $\mathcal{P}$-self-adjoint. In the case of 3-dimensional extensions and 1-dimensional extensions there are no $\mathcal{P}$-self-adjoint nor Hermitian extensions, but there exists $\mathcal{PT}$-symmetric extensions with empty resolvent set, cf. Sections 5 and 6.

2 Preliminaries: Operators in Krein spaces and bi-extensions

Recall that a complex linear space $\mathcal{H}$ with a hermitian nondegenerate sesquilinear form $[\cdot,\cdot]$ is called a *Krein space* if there exists a so called *fundamental decomposition* (cf. [10, 11, 12])

$$\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_- \tag{2.1}$$

with subspaces $\mathcal{H}_\pm$ being orthogonal to each other with respect to $[\cdot,\cdot]$ such that $(\mathcal{H}_\pm, \pm[\cdot,\cdot])$ are Hilbert spaces. Then

$$(x,x) := [x_+,x_+] - [x_-,x_-], \quad x = x_+ + x_- \in \mathcal{H} \quad \text{with } x_\pm \in \mathcal{H}_\pm,$$

is an inner product and $(\mathcal{H},(\cdot,\cdot))$ is a Hilbert space. All topological notions are understood with respect to some Hilbert space norm $\|\cdot\|$ on $\mathcal{H}$ such that $[\cdot,\cdot]$ is $\|\cdot\|$-continuous. Any two such norms are equivalent, see [20, Proposition I.1.2]. Denote by P_+ and P_- the orthogonal projections onto $\mathcal{H}_+$ and $\mathcal{H}_-$, respectively. The operator $J := P_+ - P_-$ is called the *fundamental symmetry* corresponding to the decomposition (2.1) and we have

$$[f,g] = (Jf,g) \quad \text{for all } f,g \in \mathcal{H}.$$

For a detailed treatment of Krein spaces and operators therein we refer to the monographs [10] and [11]. If $\mathcal{L}$ is an arbitrary subset of a Krein space $(\mathcal{H}, [\cdot,\cdot])$ we set

$$\mathcal{L}^{[\perp]} := \{x \in \mathcal{H} : [x, y] = 0 \text{ for all } y \in \mathcal{L}\}.$$

In the sequel we will make use of the following proposition.

Proposition 2.1. *Let $\mathcal{L}$, $\mathcal{M}$ be closed subspaces of a Krein space $(\mathcal{H}, [\cdot,\cdot])$ and let $\mathcal{L} \subset \mathcal{M}$. Then $\dim \mathcal{L}^{[\perp]}/\mathcal{M}^{[\perp]} = \dim \mathcal{M}/\mathcal{L}$.*

Proof. Let J be a canonical symmetry in the Krein space $\mathcal{K}$. For subspaces X, Y, Z of $\mathcal{H}$ with $X + Z = Y$ and $X \cap Z = \{0\}$ we obtain $JX + JZ = JY$ and therefore

$$\dim Y/X = \dim Z = \dim JZ = \dim JY/JX.$$

Set $Y := \mathcal{L}^{[\perp]}$ and $X := \mathcal{M}^{[\perp]}$ we see

$$\dim \mathcal{L}^{[\perp]}/\mathcal{M}^{[\perp]} = \dim J\mathcal{L}^{[\perp]}/J\mathcal{M}^{[\perp]}.$$

As for each subspace $\mathcal{N}$ the equality $J\mathcal{N}^{[\perp]} = \mathcal{N}^{\perp}$ holds, we conclude

$$\dim \mathcal{L}^{[\perp]}/\mathcal{M}^{[\perp]} = \dim \mathcal{L}^{\perp}/\mathcal{M}^{\perp} = \dim \mathcal{M}/\mathcal{L}.$$

□

Let T be a densely defined linear operator in $\mathcal{H}$. The adjoint of T in the Krein space $(\mathcal{H}, [\cdot,\cdot])$ is defined by

$$T^+ := JT^*J, \tag{2.2}$$

where T^* denotes the adjoint of T in the Hilbert space $(\mathcal{H}, (\cdot,\cdot))$. We have

$$[Tf, g] = [f, T^+g] \quad \text{for all } f \in \operatorname{dom} T,\ g \in \operatorname{dom} T^+.$$

The operator T is called *selfadjoint* (in the Krein space $(\mathcal{H}, [\cdot,\cdot])$) if $T = T^+$.

In what follows, we will consider extensions of a closed densely defined symmetric operator in a Hilbert space $\mathcal{H}$. As we will consider also non-symmetric extensions, we will emphazise this in the following definition.

Definition 2.2. *A closed extension* $\widetilde{A}$ *of a closed densely defined symmetric operator* A *in a Hilbert space* $\mathcal{H}$ *is called a bi-extension if*

$$A \subset \widetilde{A} \subset A^*.$$

For $r \in \mathbb{N}$ *a bi-extension* $\widetilde{A}$ *is called a* r*-dimensional bi-extension, if*

$$\dim (\operatorname{dom} \widetilde{A} / \operatorname{dom} A) = r.$$

For a bi-extension $\widetilde{A}$ of A we have

$$A \subset \widetilde{A}^* \subset A^*.$$

Hence both $\widetilde{A}$ and $\widetilde{A}^*$ are extensions of A.

Proposition 2.3. *Let* A *be a closed densely defined symmetric operator in a Hilbert space* $\mathcal{H}$ *with the defect indices* (m, n) *and* $p = m+n < \infty$*. Then* $\widetilde{A}$ *is an* r*-dimensional bi-extension of* A *if and only if* $\widetilde{A}^*$ *is a* $(p-r)$*-dimensional bi-extension of* $\widetilde{A}$*.*

Proof. Let us consider the space $\mathcal{K} := \mathcal{H} \times \mathcal{H}$ as a Krein space with the indefinite metric

$$[x, y] = \frac{(x_2, y_1) - (x_1, y_2)}{2i}, \quad x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \ y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \in \mathcal{H} \times \mathcal{H}.$$

Hence the symmetry of A implies that the graph Γ_A of A is a neutral subspace in $\mathcal{K}$. Moreover $\Gamma_{A^*} = (\Gamma_A)^{[\perp]}$. The assumption that $\widetilde{A}$ is an r-dimensional bi-extension of A is equivalent to $\Gamma_A \subset \Gamma_{\widetilde{A}} \subset \Gamma_{A^*}$ and $\dim \Gamma_{\widetilde{A}} / \Gamma_A = r$. By Proposition 2.1 with $\mathcal{L} = \Gamma_A$ and $\mathcal{M} = \Gamma_{\widetilde{A}}$ we obtain that $\dim \Gamma_{A^*} / \Gamma_{\widetilde{A}^*} = r$ and therefore from $\Gamma_A \subset \Gamma_{\widetilde{A}^*} \subset \Gamma_{A^*}$ it follows that $\widetilde{A}^*$ is a $(p-r)$-dimensional bi-extension of A.

□

Remark 2.4. If A is a closed densely defined symmetric operator in a Hilbert space $\mathcal{H}$ with defect indices $(2, 2)$, then $\widetilde{A}$ is a 1-dimensional bi-extension of A if and only if $\widetilde{A}^*$ is a 3-dimensional bi-extension of A and $\widetilde{A}$ is a 2-dimensional extension of A if and only if $\widetilde{A}^*$ is also a 2-dimensional bi-extension of A .

3 The Hamiltonian τ_q

By $L^2(\mathbb{R})$ we denote the space of all equivalence classes of complex valued, measurable functions f defined on $\mathbb{R}$ for which $\int_{\mathbb{R}} |f(x)|^2 dx$ is finite. We equip $L^2(\mathbb{R})$ with the usual Hilbert scalar product

$$(f,g) := \int_{\mathbb{R}} f(x)\overline{g(x)}\,dx, \quad f,g \in L^2(\mathbb{R}).$$

Let $\mathcal{P}$ represents parity reflection and $\mathcal{T}$ represents time reversal as in (1.2). Then $\mathcal{P}^2 = \mathcal{T}^2 = (\mathcal{PT})^2 = I$ and $\mathcal{PT} = \mathcal{TP}$. Observe that the operator $\mathcal{T}$ is nonlinear. The operator $\mathcal{P}$ gives in a natural way rise to an indefinite inner product $[\cdot,\cdot]$ which will play an important role in the following. We equip $L^2(\mathbb{R})$ with the indefinite inner product

$$[f,g] := \int_{\mathbb{R}} f(x)\overline{(\mathcal{P}g)(x)}\,dx = \int_{\mathbb{R}} f(x)\overline{g(-x)}\,dx, \quad f,g \in L^2(\mathbb{R}). \tag{3.1}$$

With respect to this inner product, $L^2(\mathbb{R})$ becomes a Krein space. Observe that in this case the operator $\mathcal{P}$ serves as a fundamental symmetry in the Krein space $(L^2(\mathbb{R}),[\cdot,\cdot])$. In the situation where $[\cdot,\cdot]$ is given as in (3.1), it is easy to see that the set of all even functions can be chosen as the positive component $\mathcal{H}_+$ and the set of all odd functions can be chosen as the negative component $\mathcal{H}_-$ in a decomposition (2.1). We easily see that the $\mathcal{P}$-self-adjointness from Definition 1.1 coincides with self-adjointness in the Krein space $(L^2(\mathbb{R})[\cdot,\cdot])$, see (2.2).

Lemma 3.1. *Let $\widetilde{A}$ be a bi-extension of a closed densely defined symmetric operator A in $L^2(\mathbb{R})$ and let A^* be a $\mathcal{PT}$ symmetric operator. Then $\widetilde{A}$ is $\mathcal{PT}$-symmetric if and only if $\widetilde{A}^*$ is $\mathcal{PT}$ symmetric.*

Proof. Let $\widetilde{A}$ be $\mathcal{PT}$-symmetric. We will show that $\mathcal{PT}\,\mathrm{dom}\,\widetilde{A} = \mathrm{dom}\,\widetilde{A}$ implies $\mathcal{PT}\,\mathrm{dom}\,\widetilde{A}^* = \mathrm{dom}\,\widetilde{A}^*$ and $\mathcal{PT}\,\widetilde{A}^*f = \widetilde{A}^*\mathcal{PT}f$ for all $f \in \mathrm{dom}\,\widetilde{A}^*$. Let us note that $f \in \mathrm{dom}\,\widetilde{A}^*$ if and only if $(\widetilde{A}g,f) = (g,A^*f)$ for all $g \in \mathrm{dom}\,\widetilde{A}$. For $g \in \mathrm{dom}\,\widetilde{A}$ and $f \in \mathrm{dom}\,\widetilde{A}^*$ the $\mathcal{PT}$ symmetry of A^* implies

$$(\widetilde{A}g,\mathcal{PT}f) = (g,A^*\mathcal{PT}f) = (g,\mathcal{PT}A^*f) = (g,\mathcal{PT}\widetilde{A}^*f).$$

From this we conclude $\mathcal{PT}f \in \mathrm{dom}\,\widetilde{A}^*$ and $\mathcal{PT}\widetilde{A}^*f = A^*\mathcal{PT}f = \widetilde{A}^*\mathcal{PT}f$. Hence, $\mathcal{PT}\,\mathrm{dom}\,\widetilde{A}^* \subset \mathrm{dom}\,\widetilde{A}^*$ and from $(\mathcal{PT})^2 = I$ we derive $\mathcal{PT}\,\mathrm{dom}\,\widetilde{A}^* = \mathrm{dom}\,\widetilde{A}^*$ and the operator $\widetilde{A}^*$ is $\mathcal{PT}$ symmetric.

If $\widetilde{A}^*$ is $\mathcal{PT}$ symmetric, then, by the first part of the proof, $\widetilde{A}^{**} = \widetilde{A}$ is also $\mathcal{PT}$ symmetric. $\square$

Corollary 3.2. *Let $\widetilde{A}$ be a bi-extension of A and let A^* be a $\mathcal{PT}$ symmetric operator. Then $\widetilde{A}$ is $\mathcal{PT}$-symmetric if and only if $\widetilde{A}^+$ is $\mathcal{PT}$ symmetric.*

Proof. Assume $\widetilde{A}$ is a $\mathcal{PT}$ symmetry. Then Lemma 3.1 implies $\mathcal{PT}\,\mathrm{dom}\,\widetilde{A}^* = \mathrm{dom}\,\widetilde{A}^*$. Since $\mathcal{PT} = \mathcal{TP}$ and $\mathrm{dom}\,\widetilde{A}^+ = \mathcal{P}\,\mathrm{dom}\,\widetilde{A}^*$ we have

$$\begin{aligned}\mathcal{PT}\,\mathrm{dom}\,\widetilde{A}^+ &= \mathcal{PT}\,\mathcal{P}\,\mathrm{dom}\,\widetilde{A}^* = \mathcal{P}\,\mathcal{PT}\,\mathrm{dom}\,\widetilde{A}^* = \mathcal{P}\,\mathrm{dom}\,\widetilde{A}^* \\ &= \mathrm{dom}\,\widetilde{A}^+,\end{aligned}$$

what is equivalent to $\mathcal{PT}$ symmetry of $\widetilde{A}^+$.
If $\widetilde{A}^+$ is $\mathcal{PT}$ symmetric, then, by the first part of the proof, $\widetilde{A}^{++} = \widetilde{A}$ is also $\mathcal{PT}$ symmetric. $\square$

In the following, we consider the differential expression τ_q. We assume that q is a real valued function from $L^1_{loc}(\mathbb{R})$ which is even, that is,

$$q(x) = q(-x) \quad \text{for all } x \in \mathbb{R},$$

such that the differential equation

$$\tau_q(y)(x) := -y''(x) - q(x)y(x), \quad x \in \mathbb{R}. \tag{3.2}$$

is in limit circle case at $+\infty$ and $-\infty$.
From [18, Remark 7.4.2 (2)][1] we see that, e.g., τ_q is in limit circle case at $+\infty$ and $-\infty$ for all $\delta > 0$ and for

$$q(t) = t^{2+\delta}.$$

Hence, the differential expression τ_{4n+2} in (1.4) is in the limit circle case at ∞ and at $-\infty$.
Recall that τ_q is called in limit circle at ∞ (at $-\infty$) if all solutions of the equation $\tau_q(y) - \lambda y = 0$, $\lambda \in \mathbb{C}$, are in $L^2((a,\infty))$ (resp. $L^2((-\infty,a))$) for some $a \in \mathbb{R}$, cf. e.g. [18, Chapter 7], [16, Section 5] or [17, Section 13.3].
With the differential expression τ_q we will associate an operator $A_{\max}$ defined on the maximal domain $\mathcal{D}_{\max}$, i.e.,

$$\mathcal{D}_{\max} := \{y \in L^2(\mathbb{R}) : y, y' \in AC_{loc}(\mathbb{R}), \tau_q y \in L^2(\mathbb{R})\},$$

[1] In the formulation of [18, Example 7.4.1] and, hence, in [18, Remark 7.4.2 (2)] a minus sign is missing.

via

$$\operatorname{dom} A_{\max} := \mathcal{D}_{\max}, \quad A_{\max} y := \tau_q(y) \quad \text{for } y \in \mathcal{D}_{\max}.$$

Here and in the following $AC_{loc}(\mathbb{R})$ denotes the space of all complex valued functions which are absolutely continuous on all compact subsets of $\mathbb{R}$. As usual, with (3.2), there is also connected the so-called *pre-minimal* operator A_0 defined on the domain

$$\mathcal{D}_0 := \{y \in \mathcal{D}_{\max} : y \text{ has compact support}\}$$

and defined via

$$\operatorname{dom} A_0 := \mathcal{D}_0, \quad A_0 y := \tau_q(y) \quad \text{for } y \in \mathcal{D}_0.$$

The operator A_0 is symmetric and not closed but it is closable. Its closure $\overline{A_0}$ is called the *minimal* operator and we denote it by A,

$$A := \overline{A_0}.$$

It turns out that the maximal operator is precisely the adjoint of the minimal operator, see, e.g., [16, Theorem 3.9] or [18, Lemma 10.3.1],

$$A^* = (\overline{A_0})^* = A_{\max}.$$

Obviously, by the definition of the maximal and the minimal operator the following lemma holds true.

Lemma 3.3. *The operators A and A^* are $\mathcal{PT}$-symmetric.*

Moreover, by [18, Theorem 10.4.1] or [16, Theorem 5.7], we obtain a statement on the deficiency indices of A.

Lemma 3.4. *The closed symmetric operator A has deficiency indices $(2, 2)$, i.e. $\dim\ker(A^* - i) = 2 = \dim\ker(A^* + i)$. In particular, we have*

$$\dim\ \operatorname{dom} A^*/\operatorname{dom} A = 4.$$

Hence, by Lemma 3.4, bi-extensions $\widetilde{A}$ of A are either trivial, that is, they equal A or A^* or they fell into one of the following cases

- $\dim\operatorname{dom}\widetilde{A}/\operatorname{dom} A = 1$; this case is discussed in Section 6,

- $\dim \operatorname{dom} \widetilde{A}/\operatorname{dom} A = 2$; this case is discussed in Section 4,
- $\dim \operatorname{dom} \widetilde{A}/\operatorname{dom} A = 3$; this case is discussed in Section 5.

It is our aim to describe all bi-extensions $\widetilde{A}$ of A. For this we define for functions $g, f \in AC_{loc}(\mathbb{R})$ with continuous derivative, the expression $[f,g]_x$ for $x \in \mathbb{R}$ via

$$[f,g]_x := \overline{f(x)}g'(x) - \overline{f'(x)}g(x).$$

Note that if f and g are real valued, then $[f,g]_x$ is the Wronskian $W(f,g)$. It is well known (e.g. [18, Lemma 10.2.3], [16, Theorem 3.10]) that the limit of $[g,f]_x$ as $x \to \infty$ and $x \to -\infty$ exists for $f, g \in \mathcal{D}_{\max}$, We set

$$[f,g]_\infty := \lim_{x\to\infty}[f,g]_x, \quad [f,g]_{-\infty} := \lim_{x\to-\infty}[f,g]_x$$

and

$$[f,g]_{-\infty}^{\infty} = [f,g]_\infty - [f,g]_{-\infty}.$$

By [18, Section 10.4.4], [16, Theorem 3.10], we have for $f, g \in \mathcal{D}_{\max}$

$$(g, A^*f) - (A^*g, f) = [f,g]_{-\infty}^{\infty}. \tag{3.3}$$

The following Lemmas 3.5 and 3.7 are from [19], where they are proved for the differential expression τ_{4n+2}. However, it is easy to see that the proofs in [19] also applies to the differential expression τ_q due to the assumption that q is an even function.

Lemma 3.5. *There exist real valued solutions $w_1, w_2 \in \mathcal{D}_{\max}$ of the equation*

$$\tau_q(y) = 0$$

such that w_1 is an odd and w_2 an even function with

$$[w_1, w_2]_{-\infty} = [w_1, w_2]_\infty = 1$$

and

$$[w_1, w_1]_{-\infty} = [w_1, w_1]_\infty = [w_2, w_2]_{-\infty} = [w_2, w_2]_\infty = 0.$$

For simplicity we set for $f \in \mathcal{D}_{\max}$

$$\begin{aligned} \alpha_1(f) &:= [w_1, f]_{-\infty}, & \alpha_2(f) &:= [w_2, f]_{-\infty}, \\ \beta_1(f) &:= [w_1, f]_\infty, & \beta_2(f) &:= [w_2, f]_\infty. \end{aligned}$$

We obtain (see, e.g. [17, Satz 13.21])

$$\operatorname{dom} A = \{f \in \mathcal{D}_{\max} : \alpha_1(f) = \alpha_2(f) = \beta_1(f) = \beta_2(f) = 0\}. \tag{3.4}$$

Lemma 3.6. *To each vector* $z = (z_1, z_2, z_3, z_{,4})^\top$ *in* $\mathbb{C}^4$ *there exists a function* f_z *from the domain* $\mathcal{D}_{\max}$ *of the maximal operator* A^* *with*

$$\begin{aligned} \alpha_1(f_z) &= z_1, & \alpha_2(f_z) &= z_2, \\ \beta_1(f_z) &= z_3, & \beta_2(f_z) &= z_4. \end{aligned}$$

Proof. We consider functions u_1, u_2, v_1, v_2 from $\mathcal{D}_{\max}$ such that u_j, $j = 1, 2$ equal w_j on the interval $(1, \infty)$, equal zero on the interval $(-\infty, -1)$ and the functions v_j, $j = 1, 2$ equal w_j on the interval $(-\infty, -1)$ and equal zero on the interval $(1, \infty)$. Then

$$f_z := -z_4 u_1 + z_3 u_2 - z_2 v_1 + z_1 v_2.$$

is the function with the desired properties. □

The next lemma[2] describes the behaviour of the above numbers under the operators $\mathcal{P}$ and $\mathcal{T}$.

Lemma 3.7. *For* $f \in \mathcal{D}_{\max}$ *we have*

$$\begin{aligned} \alpha_1(\mathcal{P}f) &= \beta_1(f), & \alpha_2(\mathcal{P}f) &= -\beta_2(f), \\ \beta_1(\mathcal{P}f) &= \alpha_1(f), & \beta_2(\mathcal{P}f) &= -\alpha_2(f), \end{aligned} \tag{3.5}$$

$$\begin{aligned} \alpha_1(\mathcal{PT} f) &= \overline{\beta_1(f)}, & \alpha_2(\mathcal{PT} f) &= -\overline{\beta_2(f)}, \\ \beta_1(\mathcal{PT} f) &= \overline{\alpha_1(f)}, & \beta_2(\mathcal{PT} f) &= -\overline{\alpha_2(f)}. \end{aligned} \tag{3.6}$$

4 2-dimensional extensions

First we will consider 2-dimensional extensions $\widetilde{A}$. Their domain is given by

$$\operatorname{dom} \widetilde{A} = \left\{ f \in \mathcal{D}_{\max} \mid \begin{bmatrix} a_1 & b_1 \\ c_1 & d_1 \end{bmatrix} \begin{pmatrix} \alpha_1(f) \\ \alpha_2(f) \end{pmatrix} = \begin{bmatrix} e & f \\ g & h \end{bmatrix} \begin{pmatrix} \beta_1(f) \\ \beta_2(f) \end{pmatrix} \right\} \tag{4.1}$$

with

$$\operatorname{rank} \begin{bmatrix} a_1 & b_1 & e & f \\ c_1 & d_1 & g & h \end{bmatrix} = 2.$$

There are 3 possibilities:

[2]Here we mention that in the second part of the statement of [19, Lemma 4] $\mathcal{T}$ should be replaced by $\mathcal{PT}$.

(*i*) The matrix $\begin{bmatrix} a_1 & b_1 \\ c_1 & d_1 \end{bmatrix}$ is nondegenerate. Then we can express $\alpha_1(f),\ \alpha_2(f)$ via $\beta_1(f),\ \beta_2(f)$:

$$\begin{pmatrix} \alpha_1(f) \\ \alpha_2(f) \end{pmatrix} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{pmatrix} \beta_1(f) \\ \beta_2(f) \end{pmatrix}, \tag{4.2}$$

where

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} a_1 & b_1 \\ c_1 & d_1 \end{bmatrix}^{-1} \begin{bmatrix} e & f \\ g & h \end{bmatrix}.$$

Hence

$$\operatorname{dom} \widetilde{A} = \left\{ f \in \mathcal{D}_{\max} \mid \begin{pmatrix} \alpha_1(f) \\ \alpha_2(f) \end{pmatrix} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{pmatrix} \beta_1(f) \\ \beta_2(f) \end{pmatrix} \right\}. \tag{4.3}$$

(*ii*) The matrix $\begin{bmatrix} e & f \\ g & h \end{bmatrix}$ is nondegenerate. Then we can express $\beta_1(f),\ \beta_2(f)$ via $\alpha_1(f),\ \alpha_2(f)$ and rewrite (4.1) in the form:

$$\begin{pmatrix} \beta_1(f) \\ \beta_2(f) \end{pmatrix} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{pmatrix} \alpha_1(f) \\ \alpha_2(f) \end{pmatrix}, \tag{4.4}$$

where in this case

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} e & f \\ g & h \end{bmatrix}^{-1} \begin{bmatrix} a_1 & b_1 \\ c_1 & d_1 \end{bmatrix}.$$

Hence

$$\operatorname{dom} \widetilde{A} = \left\{ f \in \mathcal{D}_{\max} \mid \begin{pmatrix} \beta_1(f) \\ \beta_2(f) \end{pmatrix} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{pmatrix} \alpha_1(f) \\ \alpha_2(f) \end{pmatrix} \right\}. \tag{4.5}$$

(*iii*) Both matrices $\begin{bmatrix} a_1 & b_1 \\ c_1 & d_1 \end{bmatrix}$ and $\begin{bmatrix} e & f \\ g & h \end{bmatrix}$ are degenerate. Then they are both of rank $= 1$ and therefore there exist numbers a, b, c, d with $|a|+|b| \neq 0$ and $|c| + |d| \neq 0$ such that one can rewrite (4.1) as a system:

$$\begin{cases} a\,\alpha_1(f) + b\,\alpha_2(f) &= 0, \\ c\,\beta_1(f) + d\,\beta_2(f) &= 0. \end{cases} \tag{4.6}$$

Let us recall that (4.2) and (4.4) are called mixed boundary conditions and (4.6) is called separated boundary conditions. By our assumptions, cases (i) and (iii) can not occur simultaneously. Similarly, cases (ii) and (iii) can not occur simultaneously.
We normalize (4.6) and rewrite for this case (4.1) as

$$\operatorname{dom}\widetilde{A} = \left\{ f \in \mathcal{D}_{\max} \mid \begin{array}{rcl} \alpha_1(f)\,\xi\cos\alpha - \alpha_2(f)\,\sin\alpha & = & 0, \\ \beta_1(f)\,\eta\cos\beta - \beta_2(f)\,\sin\beta & = & 0. \end{array} \right\} \tag{4.7}$$

Here $|\xi| = |\eta| = 1$ and $\alpha,\ \beta\ \in [0, 2\pi)$.
Note that in the case of separated boundary conditions there exist vectors $f_1, f_2 \in \operatorname{dom}\widetilde{A}$ such that:

$$|\alpha_1(f_1)| + |\alpha_2(f_1)| \neq 0, \qquad |\beta_1(f_2)| + |\beta_2(f_2)| \neq 0. \tag{4.8}$$

which is due to the fact that $\widetilde{A}$ is a 2-dimensional extension of A.
In both cases, separated and mixed boundary conditions, extensions $\widetilde{A}$ are bi-extensions since $A \subset \widetilde{A} \subset A^*$. Our aim in this section is to describe adjoint and $\mathcal{P}$-adjoint operators to the extension $\widetilde{A}$ and give criteria when this extension is $\mathcal{PT}$ symmetry, selfadjoint and $\mathcal{P}$-selfadjoint.
For this we need the following result.

Lemma 4.1. *Let $f, g \in \mathcal{D}_{\max}$. Then*

$$[g, f]_{-\infty}^{\infty} = \overline{\beta_2(g)}\beta_1(f) - \overline{\alpha_2(g)}\alpha_1(f) - \overline{\beta_1(g)}\beta_2(f) + \overline{\alpha_1(g)}\alpha_2(f). \tag{4.9}$$

Proof. Consider the function

$$F(x; g, f, w_1, w_2) = [g, f]_x [w_1, w_2]_x. \tag{4.10}$$

A direct calculation shows that

$$F(x; g, f, w_1, w_2) = [g, w_2]_x [w_1, f]_x - [g, w_1]_x [w_2, f]_x. \tag{4.11}$$

Since $[w_1, w_2]_{-\infty} = [w_1, w_2]_{\infty} = 1$, on the one hand from (4.10) it follows that

$$\lim_{x\to\infty} F(x; g, f, w_1, w_2) - \lim_{x\to-\infty} F(x; g, f, w_1, w_2) = [g, f]_{-\infty}^{\infty},$$

and from the other hand side (4.11) implies

$$\lim_{x\to\infty} F(x; g, f, w_1, w_2) - \lim_{x\to-\infty} F(x; g, f, w_1, w_2) =$$

$$\overline{\beta_2(g)}\beta_1(f) - \overline{\alpha_2(g)}\alpha_1(f) - \overline{\beta_1(g)}\beta_2(f) + \overline{\alpha_1(g)}\alpha_2(f).$$

Therefore (4.9) holds. □

Corollary 4.2. *Let $\widetilde{A}$ be a bi-extension of A. Then $g \in \operatorname{dom} \widetilde{A}^*$ if and only if*

$$\overline{\beta_1(g)}\beta_2(f) - \overline{\beta_2(g)}\beta_1(f) = \overline{\alpha_1(g)}\alpha_2(f) - \overline{\alpha_2(g)}\alpha_1(f) \tag{4.12}$$

for all $f \in \operatorname{dom} \widetilde{A}$.

Proof. This follows immediately from Lemma 4.1 and the fact that $g \in \operatorname{dom} \widetilde{A}^*$ if and only if $[g, f]_{-\infty}^{\infty} = 0$ for all $f \in \operatorname{dom} \widetilde{A}$, see (3.3). □

Proposition 4.3. (1) *If $\widetilde{A}$ is given by* (4.7)*, then*

$$\operatorname{dom} \widetilde{A}^* = \left\{ g \in \mathcal{D}_{\max} \mid \begin{array}{lcl} \alpha_1(g)\cos\alpha - \alpha_2(g)\xi\sin\alpha & = & 0, \\ \beta_1(g)\cos\beta - \beta_2(g)\eta\sin\beta & = & 0, \end{array} \right\} \tag{4.13}$$

$$\operatorname{dom} \widetilde{A}^+ = \left\{ g \in \mathcal{D}_{\max} \mid \begin{array}{lcl} \alpha_1(g)\cos\beta + \alpha_2(g)\eta\sin\beta & = & 0, \\ \beta_1(g)\cos\alpha + \beta_2(g)\xi\sin\alpha & = & 0. \end{array} \right\} \tag{4.14}$$

(2) *If $\widetilde{A}$ is given by* (4.5)*, then*

$$\operatorname{dom} \widetilde{A}^* = \left\{ g \in \mathcal{D}_{\max} \mid \begin{pmatrix} \alpha_1(g) \\ \alpha_2(g) \end{pmatrix} = \begin{bmatrix} \bar{d} & -\bar{b} \\ -\bar{c} & \bar{a} \end{bmatrix} \begin{pmatrix} \beta_1(g) \\ \beta_2(g) \end{pmatrix} \right\}, \tag{4.15}$$

$$\operatorname{dom} \widetilde{A}^+ = \left\{ g \in \mathcal{D}_{\max} \mid \begin{pmatrix} \beta_1(g) \\ \beta_2(g) \end{pmatrix} = \begin{bmatrix} \bar{d} & \bar{b} \\ \bar{c} & \bar{a} \end{bmatrix} \begin{pmatrix} \alpha_1(g) \\ \alpha_2(g) \end{pmatrix} \right\}. \tag{4.16}$$

(3) *If $\widetilde{A}$ satisfy* (4.3) *then*

$$\operatorname{dom} \widetilde{A}^* = \left\{ g \in \mathcal{D}_{\max} \mid \begin{pmatrix} \beta_1(g) \\ \beta_2(g) \end{pmatrix} = \begin{bmatrix} \bar{d} & -\bar{b} \\ -\bar{c} & \bar{a} \end{bmatrix} \right\} \begin{pmatrix} \alpha_1(g) \\ \alpha_2(g) \end{pmatrix}, \tag{4.17}$$

$$\operatorname{dom} \widetilde{A}^+ = \left\{ g \in \mathcal{D}_{\max} \mid \begin{pmatrix} \alpha_1(g) \\ \alpha_2(g) \end{pmatrix} = \begin{bmatrix} \bar{d} & \bar{b} \\ \bar{c} & \bar{a} \end{bmatrix} \begin{pmatrix} \beta_1(g) \\ \beta_2(g) \end{pmatrix} \right\}. \tag{4.18}$$

Proof. Since $\widetilde{A}$ and operators with domains (4.13), (4.15), and (4.17) correspond to two dimensional extensions of A for a proof of the statement it is sufficient to check (4.12) for $f \in \operatorname{dom} \widetilde{A}$ and g from (4.13), (4.15), or (4.17), respectively. But this directly follows from (4.9).

Since $\operatorname{dom} \widetilde{A}^+ = \{g = \mathcal{P}f \mid f \in \operatorname{dom} \widetilde{A}^*\}$ a proof of (4.14), (4.16), and (4.18) taking in account Lemma 3.7, relations (3.5), follows immediately from (4.13) and (4.15), or (4.17), respectively. □

Corollary 4.4. (1) *Let $\widetilde{A}$ has the domain (4.7). Then $\widetilde{A} = \widetilde{A}^*$ if and only if $\xi = \eta = 1$.*

(2) *Let $\widetilde{A}$ has the domain (4.3) or (4.5). Set $\Delta = ad - bc$. Then $\widetilde{A} = \widetilde{A}^*$ if and only if for some $\varphi \in \mathbb{R}$ we have*

$$\Delta = e^{2i\varphi} \text{ and } \left\{e^{-i\varphi}a,\, e^{-i\varphi}b,\, e^{-i\varphi}c,\, e^{-i\varphi}d\right\} \subset \mathbb{R}. \tag{4.19}$$

Proof. Let us note that $\widetilde{A} = \widetilde{A}^*$ if and only if $\operatorname{dom} \widetilde{A} = \operatorname{dom} \widetilde{A}^*$. Assertion (1) follows immediately if one compares $\operatorname{dom} \widetilde{A}$ and $\operatorname{dom} \widetilde{A}^*$.

(2) Assume $\widetilde{A}$ has domain (4.3). Obviously, if (4.19) holds, then we have

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} \overline{d} & -\overline{b} \\ -\overline{c} & \overline{a} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

and $\widetilde{A} = \widetilde{A}^*$, see (4.17).
For the contrary, we assume $\operatorname{dom} \widetilde{A} = \operatorname{dom} \widetilde{A}^*$. First, we will show that in this case the matrix

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} \tag{4.20}$$

has full rank. Indeed, assume that there exists $\eta \in \mathbb{C}$ with $c = \eta a$ and $d = \eta b$. From (4.3), (4.17) we obtain for $f \in \operatorname{dom} \widetilde{A}$

$$\alpha_2(f) = \eta\alpha_1(f), \quad \beta_1(f) = \overline{b}(\overline{\eta} - \eta)\alpha_1(f) \quad \text{and} \quad \beta_2(f) = \overline{a}(\overline{\eta} - \eta)\alpha_1(f).$$

But this implies that $\widetilde{A}$ is a 1-dimensional extension of A, a contradiction. Hence, the matrix in (4.20) has full rank.
There are two vectors $f, g \in \operatorname{dom} \widetilde{A}$ such that the vectors

$$\begin{pmatrix} \alpha_1(f) \\ \alpha_2(f) \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \alpha_1(g) \\ \alpha_2(g) \end{pmatrix} \quad \text{are linearly independent.} \tag{4.21}$$

Indeed, assume that all such vectors are linearly dependent. Since $\operatorname{dom} \widetilde{A} \neq \operatorname{dom} A$ and by (3.4) there is a vector $f_0 \in \operatorname{dom} \widetilde{A}$ such that $|\alpha_1(f_0)| + |\alpha_2(f_0)| \neq 0$. Then for each $f \in \operatorname{dom} \widetilde{A}$ there exists a number $\lambda(f) \in \mathbb{C}$ with

$$\begin{pmatrix} \alpha_1(f) \\ \alpha_2(f) \end{pmatrix} = \lambda(f) \begin{pmatrix} \alpha_1(f_0) \\ \alpha_2(f_0) \end{pmatrix}. \tag{4.22}$$

and, from (4.3) and the fact that the matrix in (4.20) has full rank, we deduce

$$\begin{pmatrix} \beta_1(f) \\ \beta_2(f) \end{pmatrix} = \lambda(f) \begin{pmatrix} \beta_1(f_0) \\ \beta_2(f_0) \end{pmatrix}. \tag{4.23}$$

Using (4.23) and (4.22) one can conclude that the functions f from the domain of $\widetilde{A}$ satisfy the following system

$$\begin{cases} \alpha_1(f)\alpha_2(f_0) - \alpha_2(f)\alpha_1(f_0) = 0, \\ \beta_1(f)\beta_2(f_0) - \beta_2(f)\beta_1(f_0) = 0, \end{cases}$$

that is, the boundary conditions are separated, a contradiction. Hence there are two vectors f and g in $\operatorname{dom} \widetilde{A}$ such that (4.21) holds. As $\operatorname{dom} \widetilde{A} = \operatorname{dom} \widetilde{A}^*$, both boundary conditions (4.3) and (4.17) hold, that is, for $f \in \operatorname{dom} \widetilde{A}$ we have

$$\begin{pmatrix} \alpha_1(f) \\ \alpha_2(f) \end{pmatrix} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{pmatrix} \beta_1(f) \\ \beta_2(f) \end{pmatrix} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} \overline{d} & -\overline{b} \\ -\overline{c} & \overline{a} \end{bmatrix} \begin{pmatrix} \alpha_1(f) \\ \alpha_2(f) \end{pmatrix}.$$

The matrix in (4.20) has full rank and from (4.21) we obtain $|\Delta| = 1$. That is $\Delta = e^{2i\varphi}$, $\varphi = \frac{1}{2} \arg \Delta$. In particular it follows

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} = \frac{1}{\overline{\Delta}} \begin{bmatrix} \overline{a} & \overline{b} \\ \overline{c} & \overline{d} \end{bmatrix}.$$

Hence,

$$e^{-i\varphi}\, a = e^{-i\varphi} \frac{\overline{a}}{\overline{\Delta}} = \frac{\overline{a}}{e^{-i\varphi}} = \overline{e^{-i\varphi}\, a}$$

and $e^{-i\varphi}\, a$ is real. By similar arguments, one conclude $e^{-i\varphi}\, b \in \mathbb{R}$, $e^{-i\varphi}\, c \in \mathbb{R}$ and $e^{-i\varphi}\, d \in \mathbb{R}$ and (4.19) holds. The case when $\operatorname{dom} \widetilde{A}$ is defined by (4.5) can be proved by the same arguments. □

Corollary 4.5. (1) *Let $\widetilde{A}$ has the domain* (4.7). *Then*

- *(i) for $\alpha \in \{0, \pi/2, \pi, 3\pi/2\}$ or $\beta \in \{0, \pi/2, \pi, 3\pi/2\}$ the operator $\widetilde{A}$ is $\mathcal{P}$-selfadjoint if and only if*

$$\alpha + \beta = 0 \;(\bmod \pi).$$

(*ii*) *For* $\alpha, \beta \notin \{0,\, \pi/2,\, \pi,\, 3\pi/2\}$ *the operator* $\widetilde{A}$ *is* $\mathcal{P}$*-selfadjoint if and only if one of the following conditions holds:*

$$\alpha + \beta = 0 \ (\bmod \pi),\ \xi\,\eta = 1 \ \textit{or} \tag{4.24}$$

$$|\alpha - \beta| = 0 \ (\bmod \pi),\ \xi\eta = -1. \tag{4.25}$$

(2) *Let* $\widetilde{A}$ *has the domain given by* (4.3) *or* (4.5)*. Then the operator* $\widetilde{A}$ *is* $\mathcal{P}$*-selfadjoint if and only if*

$$d = \overline{a}, \quad b,\, c \in \mathbb{R}. \tag{4.26}$$

Proof. Since both $\widetilde{A}$ and $\widetilde{A}^{+}$ are restrictions of the same maximal operator we have

$$\widetilde{A} = \widetilde{A}^{+} \quad \Longleftrightarrow \quad \operatorname{dom} \widetilde{A} = \operatorname{dom} \widetilde{A}^{+}. \tag{4.27}$$

(1) Assume $\widetilde{A}$ has the domain (4.7). We prove the statement (*i*) for $\alpha = 0$. For a proof of the other cases, i.e., $\alpha \in \{\pi/2,\, \pi,\, 3\pi/2\}$, $\beta \in \{0,\, \pi/2,\, \pi,\, 3\pi/2\}$ one can use similar arguments.
Let $\alpha = 0$. We will show $A = A^{+}$ if and only if $\beta = 0$ or $\beta = \pi$.
If $\beta = 0$ or $\beta = \pi$ then, by (4.7) and (4.14) we see immediately $\operatorname{dom} \widetilde{A} = \operatorname{dom} \widetilde{A}^{+}$ and according to (4.27) $\widetilde{A}$ is $\mathcal{P}$-selfadjoint.
Conversely, assume $\widetilde{A} = \widetilde{A}^{+}$. Then $\alpha = 0$ implies $\alpha_1(f) = \beta_1(f) = 0$ for all $f \in \operatorname{dom} \widetilde{A} = \operatorname{dom} \widetilde{A}^{+}$. Hence from (4.8) it follows that $\sin \beta = 0$, that is, either $\beta = 0$ or $\beta = \pi$ and statement (*i*) is proved.
In order to show (*ii*) let $\alpha, \beta \notin \{0,\, \pi/2,\, \pi,\, 3\pi/2\}$ and assume $\widetilde{A}$ is $\mathcal{P}$-selfadjoint. Then for $f \in \operatorname{dom} \widetilde{A} = \operatorname{dom} \widetilde{A}^{+}$ the boundary conditions (4.7) and (4.14) give

$$\begin{cases} \alpha_1(f)\, \xi \cos \alpha - \alpha_2(f)\, \sin \alpha = 0, \\ \alpha_1(f)\, \overline{\eta} \cos \beta + \alpha_2(f)\, \sin \beta = 0, \end{cases}$$

$$\begin{cases} \beta_1(f)\, \eta \cos \beta - \beta_2(f)\, \sin \beta = 0. \\ \beta_1(f)\, \overline{\xi} \cos \alpha + \beta_2(f)\, \sin \alpha = 0. \end{cases}$$

Taking into account (4.8) we obtain

$$\eta \cos \beta \sin \alpha + \overline{\xi} \sin \beta \cos \alpha = 0,$$

or, since $|\xi| = |\eta| = 1$,

$$\xi\eta \cos\beta \sin\alpha + \sin\beta \cos\alpha = 0.$$

By the conditions $\alpha, \beta \notin \{0,\, \pi/2,\, \pi,\, 3\pi/2\}$ and therefore all the numbers $\sin\alpha$, $\cos\alpha$, $\sin\beta$, $\cos\beta$ are nonzero. Therefore $\xi\eta \in \mathbb{R}$, that is, $\xi\eta = \pm 1$. Hence we have two possibilities:

$$\sin(\alpha - \beta) = 0, \quad \text{or} \quad \sin(\alpha + \beta) = 0.$$

The latter is equivalent to (4.24), (4.25).
The converse can be checked directly.

(2) Let $\widetilde{A}$ has the domain (4.3). Then it is $\mathcal{P}$-selfadjoint if and only if functions f from $\operatorname{dom} \widetilde{A}$ satisfy also conditions (4.18). Therefore

$$\begin{bmatrix} \overline{d} - a & \overline{b} - b \\ \overline{c} - c & \overline{a} - d \end{bmatrix} \begin{pmatrix} \beta_1(f) \\ \beta_2(f) \end{pmatrix} = 0.$$

Since $\widetilde{A}$ is a 2-dimensional extension of A (4.26) holds.
The converse statement can be checked by direct calculations. A proof for $\widetilde{A}$ with domain (4.5) is similar. □

Proposition 4.6. (1) *Let $\widetilde{A}$ has the domain* (4.7). *Then $\widetilde{A}$ is $\mathcal{PT}$ symmetric if and only if it is $\mathcal{P}$-selfadjoint.*

(2) *Let $\widetilde{A}$ has the domain given by* (4.3) *or* (4.5). *Then $\widetilde{A}$ is $\mathcal{PT}$ symmetric if and only if for some $\varphi \in \mathbb{R}$*

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} = e^{i\varphi} \begin{bmatrix} \alpha & \beta \\ \gamma & \overline{\alpha} \end{bmatrix}, \quad \beta, \gamma \in \mathbb{R}, \quad |\alpha|^2 - \beta\gamma = 1. \tag{4.28}$$

Proof. Taking into account that A^* is a $\mathcal{PT}$ symmetry we conclude that $\widetilde{A}$ is a $\mathcal{PT}$ symmetry if and only if

$$\mathcal{PT} \operatorname{dom} \widetilde{A} = \operatorname{dom} \widetilde{A}. \tag{4.29}$$

(1) According to (3.6) the latter means that $f \in \operatorname{dom} \widetilde{A}$ also satisfies the conditions

$$\begin{aligned} \beta_1(f)\, \overline{\xi} \cos\alpha + \beta_2(f)\, \sin\alpha &= 0, \\ \alpha_1(f)\, \overline{\eta} \cos\beta + \alpha_2(f)\, \sin\beta &= 0 \end{aligned}$$

which coincide with boundary conditions (4.14) for $\widetilde{A}^+$. Hence statement (1) follows.
(2) Let boundary conditions of $\widetilde{A}$ be not separated, for instance, let the domain of $\widetilde{A}$ satisfies (4.3). According to (3.6) the equality $\mathcal{PT}\,\mathrm{dom}\,\widetilde{A} = \mathrm{dom}\,\widetilde{A}$ is equivalent to (4.3) with an additionally condition:

$$\begin{pmatrix}\beta_1(f)\\ \beta_2(f)\end{pmatrix} = \begin{bmatrix}\overline{a} & -\overline{b}\\ -\overline{c} & \overline{d}\end{bmatrix}\begin{pmatrix}\alpha_1(f)\\ \alpha_2(f)\end{pmatrix} \quad \text{for all } f \in \mathrm{dom}\,\widetilde{A}. \tag{4.30}$$

Assume that the matrix

$$\begin{bmatrix}a & b\\ c & d\end{bmatrix} \tag{4.31}$$

has a rank less than two. Then there exists $\eta \in \mathbb{C}$ with $c = \eta a$ and $d = \eta b$ and from (4.3), (4.30) we obtain for $f \in \mathrm{dom}\,\widetilde{A}$

$$\alpha_2(f) = \eta\alpha_1(f), \quad \beta_1(f) = (\overline{a} - \overline{b}\eta)\alpha_1(f) \quad \text{and} \quad \beta_2(f) = -\overline{\eta}\beta_1(f).$$

But this implies that $\widetilde{A}$ is a 1-dimensional extension of A, a contradiction. Hence, the matrix in (4.31) has full rank. Together with (4.3) it follows that for $f \in \mathrm{dom}\,\widetilde{A}$ we have

$$\begin{pmatrix}\beta_1(f)\\ \beta_2(f)\end{pmatrix} = \begin{bmatrix}\overline{a} & -\overline{b}\\ -\overline{c} & \overline{d}\end{bmatrix}\begin{bmatrix}a & b\\ c & d\end{bmatrix}\begin{pmatrix}\beta_1(f)\\ \beta_2(f)\end{pmatrix}, \tag{4.32}$$

There are two vectors $f, g \in \mathrm{dom}\,\widetilde{A}$ such that the vectors

$$\begin{pmatrix}\beta_1(f)\\ \beta_2(f)\end{pmatrix} \quad \text{and} \quad \begin{pmatrix}\beta_1(g)\\ \beta_2(g)\end{pmatrix} \quad \text{are linearly independent.} \tag{4.33}$$

Indeed, assume that all such vectors are linearly dependent. Since $\mathrm{dom}\,\widetilde{A} \neq \mathrm{dom}\,A$ and by (3.4) there is a vector $f_0 \in \mathrm{dom}\,\widetilde{A}$ such that $|\beta_1(f_0)|+|\beta_2(f_0)| \neq 0$. Then for each $f \in \mathrm{dom}\,\widetilde{A}$ there exists a number $\lambda(f) \in \mathbb{C}$ with

$$\begin{pmatrix}\beta_1(f)\\ \beta_2(f)\end{pmatrix} = \lambda(f)\begin{pmatrix}\beta_1(f_0)\\ \beta_2(f_0)\end{pmatrix}. \tag{4.34}$$

and, from (4.3) and the fact that the matrix in (4.31) has full rank, we deduce

$$\begin{pmatrix}\alpha_1(f)\\ \alpha_2(f)\end{pmatrix} = \lambda(f)\begin{pmatrix}\alpha_1(f_0)\\ \alpha_2(f_0)\end{pmatrix}. \tag{4.35}$$

Using (4.35) and (4.34) one can conclude that the functions f from the domain of $\widetilde{A}$ satisfy the following system:

$$\begin{cases} \alpha_1(f)\alpha_2(f_0) - \alpha_2(f)\alpha_1(f_0) = 0, \\ \beta_1(f)\beta_2(f_0) - \beta_2(f)\beta_1(f_0) = 0, \end{cases}$$

that is, the boundary conditions are separated, a contradiction. Hence there are two vectors f and g in $\operatorname{dom}\widetilde{A}$ such that (4.33) holds. Then from (4.32) it follows that

$$\begin{bmatrix} \overline{a} & -\overline{b} \\ -\overline{c} & \overline{d} \end{bmatrix} \begin{bmatrix} a & b \\ c & d \end{bmatrix} = I.$$

Therefore the matrix

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

is nondegenerate and we have $\Delta := ad - bc \neq 0$ with $|\Delta| = 1$. If we set $\varphi := \frac{1}{2}\arg\Delta$ then $\Delta = e^{2i\varphi}$ and we obtain

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} \overline{a} & -\overline{b} \\ -\overline{c} & \overline{d} \end{bmatrix}^{-1} = \begin{bmatrix} \overline{d}/\overline{\Delta} & \overline{b}/\overline{\Delta} \\ \overline{c}/\overline{\Delta} & \overline{a}/\overline{\Delta} \end{bmatrix}.$$

This implies that $e^{-i\varphi}a = \overline{e^{-i\varphi}d}$, and the numbers $e^{-i\varphi}b$ and $e^{-i\varphi}c$ are real. Set

$$\alpha := e^{-i\varphi}a, \quad \beta := e^{-i\varphi}b \quad \text{and} \quad \gamma := e^{-i\varphi}c.$$

Then we have $|\alpha|^2 - \beta\gamma = 1$ and one can rewrite boundary conditions (4.3) for the $\mathcal{PT}$ symmetric operator $\widetilde{A}$ in the form (4.28).

For the converse statement assume that for some $\alpha \in \mathbb{C}$, $\beta, \gamma \in \mathbb{R}$ with $|\alpha|^2 - \beta\gamma = 1$ (4.28) is satisfied. Then, according to (3.6), we obtain for $f \in \operatorname{dom}\widetilde{A}$

$$\begin{aligned} \begin{bmatrix} \alpha & \beta \\ \gamma & \overline{\alpha} \end{bmatrix} \begin{pmatrix} \beta_1(\mathcal{PT} f) \\ \beta_2(\mathcal{PT} f) \end{pmatrix} &= \begin{bmatrix} \alpha & \beta \\ \gamma & \overline{\alpha} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \overline{\begin{pmatrix} \alpha_1(f) \\ \alpha_2(f) \end{pmatrix}} \\ &= \begin{bmatrix} \alpha & \beta \\ \gamma & \overline{\alpha} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} e^{-i\varphi} \begin{bmatrix} \overline{\alpha} & \beta \\ \gamma & \alpha \end{bmatrix} \overline{\begin{pmatrix} \beta_1(f) \\ \beta_2(f) \end{pmatrix}} \\ &= e^{-i\varphi} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \overline{\begin{pmatrix} \beta_1(f) \\ \beta_2(f) \end{pmatrix}} = e^{-i\varphi} \begin{pmatrix} \alpha_1(\mathcal{PT} f) \\ \alpha_2(\mathcal{PT} f) \end{pmatrix} \end{aligned}$$

and, hence, $\mathcal{PT}\,\mathrm{dom}\,\widetilde{A} \subset \mathrm{dom}\,\widetilde{A}$. Then, by $\mathcal{PT}^{\,2} = I$, (4.29) holds.

The case of a domain given by (4.5) can be proved in a similar way. In the reasoning one just has to changes the roles of α_1, α_2 and β_1, β_2. □

In the following corollaries we will describe the situations when two out of the three properties $\mathcal{PT}$ symmetry, selfadjointness and $\mathcal{P}$-selfadjointness are satisfied. Due to the fact that for an extension $\widetilde{A}$ with domain (4.7) $\mathcal{PT}$ symmetry is equivalent to $\mathcal{P}$-selfadjointness by Proposition 4.6, there is only one case to consider for separated boundary conditions.

Corollary 4.7. *Let $\widetilde{A}$ has the domain* (4.7). *Then $\widetilde{A}$ is $\mathcal{PT}$ symmetric, selfadjoint and $\mathcal{P}$-selfadjoint if and only if*

$$\xi = \eta = 1 \quad \textit{and} \quad \alpha + \beta = 0 \ (\bmod \pi).$$

In the case of mixed boundary conditions, there are more cases.

Corollary 4.8. *Let $\widetilde{A}$ has the domain given by* (4.3) *or* (4.5). *Then*

(1) *$\widetilde{A}$ is $\mathcal{PT}$ symmetric, selfadjoint and $\mathcal{P}$-selfadjoint if and only if*

$$a, b, c, d \in \mathbb{R}, \quad a = d \quad \textit{and} \quad a^2 - bc = 1. \tag{4.36}$$

(2) *$\widetilde{A}$ is selfadjoint and $\mathcal{P}$-selfadjoint if and only if* (4.36) *holds. In this case $\widetilde{A}$ is also $\mathcal{PT}$ symmetric.*

(3) *$\widetilde{A}$ is selfadjoint and $\mathcal{PT}$ symmetric if and only if for some $\varphi \in \mathbb{R}$*

$$e^{-i\varphi}a, e^{-i\varphi}b, e^{-i\varphi}c, e^{-i\varphi}d \in \mathbb{R}, \quad d = e^{2i\varphi}\overline{a} \quad \textit{and} \quad ad - bc = e^{2i\varphi}.$$

(4) *$\widetilde{A}$ is $\mathcal{P}$-selfadjoint and $\mathcal{PT}$ symmetric if and only if*

$$b, c \in \mathbb{R}, \quad d = \overline{a} \quad \textit{and} \quad |a|^2 - bc = 1.$$

Remark 4.9. *Corollary 4.7 and Corollary 4.8, item (2), are already contained in [19, Theorem 4 and Theorem 5]. Here we use the opportunity to point out that the statement in [19, Theorem 5] is slightly incorrect. Obviously,* (4.36) *implies that the corresponding extension $\widetilde{A}$ is $\mathcal{PT}$ symmetric and selfadjoint (and at the same time $\mathcal{P}$-selfadjoint), but the converse is not true: There are $\mathcal{PT}$ symmetric and selfadjoint extensions $\widetilde{A}$ which do not satisfy* (4.36), *cf. Corollary 4.8, item (3). Hence, the correct version of [19, Theorem 5] is Corollary 4.8, item (2).*

5 3-dimensional extensions

Let $\widetilde{A}$ be a 3-dimensional extension of A. Then there are numbers a, b, c, d, $|a| + |b| + |c| + |d| \neq 0$ such that

$$\operatorname{dom} \widetilde{A} = \{f \in \operatorname{dom} \mathcal{D}_{\max} \mid a\,\alpha_1(f) + b\,\alpha_2(f) = c\,\beta_1(f) + d\,\beta_2(f)\}\,. \tag{5.1}$$

Proposition 5.1. *Let $\widetilde{A}$ be a 3-dimensional extension of A with domain* (5.1)*. Then the following statements hold.*

(1) *Let $a \neq 0$. Then*

$$\operatorname{dom} \widetilde{A}^* = \left\{ g \in \mathcal{D}_{\max} \;\middle|\; \begin{array}{rcl} \overline{a}\,\alpha_1(g) + \overline{b}\,\alpha_2(g) & = & 0, \\ \begin{bmatrix} 0 & -\overline{d}/\overline{a} \\ 0 & \overline{c}/\overline{a} \end{bmatrix} \begin{pmatrix} \alpha_1(g) \\ \alpha_2(g) \end{pmatrix} & = & \begin{pmatrix} \beta_1(g) \\ \beta_2(g) \end{pmatrix} \end{array} \right\}. \tag{5.2}$$

$$\operatorname{dom} \widetilde{A}^+ = \left\{ h \in \mathcal{D}_{\max} \;\middle|\; \begin{array}{rcl} \overline{a}\,\beta_1(h) - \overline{b}\,\beta_2(h) & = & 0, \\ \begin{bmatrix} 0 & \overline{d}/\overline{a} \\ 0 & \overline{c}/\overline{a} \end{bmatrix} \begin{pmatrix} \beta_1(h) \\ \beta_2(h) \end{pmatrix} & = & \begin{pmatrix} \alpha_1(h) \\ \alpha_2(h) \end{pmatrix} \end{array} \right\}. \tag{5.3}$$

(2) *Let $b \neq 0$. Then*

$$\operatorname{dom} \widetilde{A}^* = \left\{ g \in \mathcal{D}_{\max} \;\middle|\; \begin{array}{rcl} \overline{a}\,\alpha_1(g) + \overline{b}\,\alpha_2(g) & = & 0, \\ \begin{bmatrix} \overline{d}/\overline{b} & 0 \\ -\overline{c}/\overline{b} & 0 \end{bmatrix} \begin{pmatrix} \alpha_1(g) \\ \alpha_2(g) \end{pmatrix} & = & \begin{pmatrix} \beta_1(g) \\ \beta_2(g) \end{pmatrix} \end{array} \right\}. \tag{5.4}$$

$$\operatorname{dom} \widetilde{A}^+ = \left\{ h \in \mathcal{D}_{\max} \;\middle|\; \begin{array}{rcl} \overline{a}\,\beta_1(h) - \overline{b}\,\beta_2(h) & = & 0, \\ \begin{bmatrix} \overline{d}/\overline{b} & 0 \\ \overline{c}/\overline{b} & 0 \end{bmatrix} \begin{pmatrix} \beta_1(g) \\ \beta_2(g) \end{pmatrix} & = & \begin{pmatrix} \alpha_1(g) \\ \alpha_2(g) \end{pmatrix} \end{array} \right\}. \tag{5.5}$$

(3) *Let $c \neq 0$. Then*

$$\operatorname{dom} \widetilde{A}^* = \left\{ g \in \mathcal{D}_{\max} \;\middle|\; \begin{array}{rcl} \overline{c}\,\beta_1(g) + \overline{d}\,\beta_2(g) & = & 0, \\ \begin{bmatrix} 0 & -\overline{b}/\overline{c} \\ 0 & \overline{a}/\overline{c} \end{bmatrix} \begin{pmatrix} \beta_1(g) \\ \beta_2(g) \end{pmatrix} & = & \begin{pmatrix} \alpha_1(g) \\ \alpha_2(g) \end{pmatrix} \end{array} \right\}. \tag{5.6}$$

$$\operatorname{dom} \widetilde{A}^{+} = \left\{ h \in \mathcal{D}_{\max} \;\middle|\; \begin{array}{rcl} \overline{c}\,\alpha_1(h) - \overline{d}\,\alpha_2(h) & = & 0, \\ \begin{bmatrix} 0 & \overline{b}/\overline{c} \\ 0 & \overline{a}/\overline{c} \end{bmatrix} \begin{pmatrix} \alpha_1(h) \\ \alpha_2(h) \end{pmatrix} & = & \begin{pmatrix} \beta_1(h) \\ \beta_2(h) \end{pmatrix} \end{array} \right\}. \tag{5.7}$$

(4) *Let* $d \neq 0$. *Then*

$$\operatorname{dom} \widetilde{A}^{*} = \left\{ g \in \mathcal{D}_{\max} \;\middle|\; \begin{array}{rcl} \overline{c}\,\beta_1(g) + \overline{d}\,\beta_2(g) & = & 0, \\ \begin{bmatrix} \overline{b}/\overline{d} & 0 \\ -\overline{a}/\overline{d} & 0 \end{bmatrix} \begin{pmatrix} \beta_1(g) \\ \beta_2(g) \end{pmatrix} & = & \begin{pmatrix} \alpha_1(g) \\ \alpha_2(g) \end{pmatrix} \end{array} \right\}. \tag{5.8}$$

$$\operatorname{dom} \widetilde{A}^{+} = \left\{ h \in \mathcal{D}_{\max} \;\middle|\; \begin{array}{rcl} \overline{c}\,\alpha_1(h) - \overline{h}\,\alpha_2(h) & = & 0, \\ \begin{bmatrix} \overline{b}/\overline{d} & 0 \\ -\overline{a}/\overline{d} & 0 \end{bmatrix} \begin{pmatrix} \alpha_1(h) \\ \alpha_2(h) \end{pmatrix} & = & \begin{pmatrix} \beta_1(h) \\ \beta_2(h) \end{pmatrix} \end{array} \right\}. \tag{5.9}$$

Proof. Let us prove (1). The others one can be shown in a similar manner. Since $a \neq 0$ we can express $\alpha_1(f)$ for $f \in \operatorname{dom} \widetilde{A}$:

$$\alpha_1(f) = -\frac{b}{a}\,\alpha_2(f) + \frac{c}{a}\,\beta_1(f) + \frac{d}{a}\,\beta_2(f).$$

Then, by (4.12), $g \in \operatorname{dom} \widetilde{A}^{*}$ if and only if

$$\beta_2(f)\left(\overline{\beta_1(g)} + \frac{d}{a}\,\overline{\alpha_2(g)}\right) - \beta_1(f)\left(\overline{\beta_2(g)} - \frac{c}{a}\,\overline{\alpha_2(g)}\right) = \alpha_2(f)\left(\overline{\alpha_1(g)} + \frac{b}{a}\,\overline{\alpha_2(g)}\right)$$

for all $f \in \operatorname{dom} \widetilde{A}$. Then by Lemma 3.6, there exists $f \in \operatorname{dom} \widetilde{A}$ such that

$$\begin{array}{ll} \alpha_1(f) = -\dfrac{b}{a}, & \alpha_2(f) = 1, \\ \beta_1(f) = 0, & \beta_2(f) = 0 \end{array}$$

and, hence, $g \in \operatorname{dom} \widetilde{A}^{*}$ has to satisfy

$$\overline{\alpha_1(g)} + \frac{b}{a}\,\overline{\alpha_2(g)} = 0.$$

In a similar way, we obtain

$$\overline{\beta_1(g)} + \frac{d}{a}\,\overline{\alpha_2(g)} = 0 \quad \text{and} \quad \overline{\beta_2(g)} - \frac{c}{a}\,\overline{\alpha_2(g)} = 0$$

and (5.2) is proved. For a proof of (5.3) we use the relation $\operatorname{dom} \widetilde{A}^{+} = \mathcal{P} \operatorname{dom} \widetilde{A}^{*}$ and Lemma 3.7. □

Proposition 5.2. *The* 3*-dimensional extension* $\widetilde{A}$ *with domain* (5.1) *is a* $\mathcal{PT}$ *symmetry if and only if*

$$|a| = |c|, \quad |b| = |d|, \quad \text{and} \quad a\overline{d} + b\overline{c} = 0. \tag{5.10}$$

Proof. We assume that the relation (5.10) holds and show that $\widetilde{A}$ is a $\mathcal{PT}$-symmetry, or, what is equivalent (see Lemma 3.3), $\mathcal{PT} \operatorname{dom} \widetilde{A} = \operatorname{dom} \widetilde{A}$. Since $(\mathcal{PT})^2 = I$ it is sufficient to show that $\mathcal{PT} \operatorname{dom} \widetilde{A} \subset \operatorname{dom} \widetilde{A}$, that is, (5.1) implies for $f \in \operatorname{dom} \widetilde{A}$

$$a\,\alpha_1(\mathcal{PT} f) + b\,\alpha_2(\mathcal{PT} f) = c\,\beta_1(\mathcal{PT} f) + d\,\beta_2(\mathcal{PT} f),$$

or, equivalently (see Lemma 3.7)

$$\overline{c}\,\alpha_1(f) - \overline{d}\,\alpha_2(f) = \overline{a}\,\beta_1(f) - \overline{b}\,\beta_2(f). \tag{5.11}$$

Consider 3 cases:

(i) $a = c = 0$. Then from $|b| = |d|$ it follows directly that (5.10) implies (5.11).

(ii) $b = d = 0$. Analogously to (i), from $|a| = |c|$ it follows directly that (5.10) implies (5.11).

(iii) $abcd \neq 0$. In this case one can rewrite (5.10) and (5.11) in forms (5.12) and (5.13) respectively:

$$-\frac{a}{b}\,(\alpha_1(f) - \frac{c}{a}\,\beta_1(f)) \;=\; \alpha_2(f) - \frac{d}{b}\,\beta_2(f), \tag{5.12}$$

$$\frac{\overline{c}}{\overline{d}}\,(\alpha_1(f) - \frac{\overline{a}}{\overline{c}}\,\beta_1(f)) \;=\; \alpha_2(f) - \frac{\overline{b}}{\overline{d}}\,\beta_2(f). \tag{5.13}$$

Now from (5.10) it follows that (5.12) implies (5.13). Therefore $\widetilde{A}$ is a $\mathcal{PT}$ symmetry.

To prove the converse assume that both (5.1) and (5.11) hold. Then (cf. Lemma 3.3) there exists a function $f_1 \in \operatorname{dom} \widetilde{A}$ with $\alpha_1(f_1) = \beta_1(f_1) = 0$ and $|\alpha_2(f_1)| + |\beta_2(f_1)| \neq 0$ and we have

$$
\begin{aligned}
b\,\alpha_2(f_1) - d\,\beta_2(f_1) &= 0, \\
\overline{d}\,\alpha_2(f_1) - \overline{b}\,\beta_2(f_1) &= 0.
\end{aligned}
$$

Since at least one of the numbers $\alpha_2(f_1)$, $\beta_2(f_1)$ is nonzero we have $|b| = |d|$. Analogously using a function $f_2 \in \operatorname{dom} \widetilde{A}$ such that $\alpha_2(f_2) = \beta_2(f_2) = 0$ and $|\alpha_1(f_2)| + |\beta_1(f_2)| \neq 0$ we obtain $|a| = |c|$.

If $abcd = 0$ the equality $a\overline{d} + b\overline{c} = 0$ is trivial.

Let $abcd \neq 0$. Consider a vector $f_3 \in \operatorname{dom} \widetilde{A}$ such that $\alpha_1(f_3) - \frac{c}{a}\,\beta_1(f_3) \neq 0$ and $\alpha_2(f_3) - \frac{d}{b}\,\beta_2(f_3) \neq 0$. Then from (5.12) and (5.13) it follows that $a\overline{d} + b\overline{c} = 0$. □

The operator $\widetilde{A}$ is a 3-dimensional extension of A but the kernel of $A^* - \lambda$ for non-real λ equals 2, see Lemma 3.4, and we obtain $\mathbb{C} \setminus \mathbb{R} \subset \sigma_p(\widetilde{A})$. Hence the resolvent set of $\widetilde{A}$ is empty and the following theorem is shown.

Theorem 5.3. *Let $\widetilde{A}$ be a 3-dimensional extension of A with domain* (5.1)*. Then*

$$\sigma(\widetilde{A}) = \mathbb{C}.$$

In particular (cf. Proposition 5.2), there are $\mathcal{PT}$ symmetric 3-dimensional extensions of A with empty resolvent set.

6 1-dimensional extensions

The domain of a 1-dimensional extension $\widetilde{A}$ is defined by 3 independent relations between $\alpha_1(f)$, $\alpha_2(f)$, $\beta_1(f)$, $\alpha_1(f)$ for $f \in \operatorname{dom} \widetilde{A}$. From Proposition 2.3 it follows that $\widetilde{A}$ is 1-dimensional extension of A if and only if its adjoint is 3-dimensional extension of A; it remains to apply Proposition 5.1. Hence we have two different cases.

$$(I) \quad \operatorname{dom} \widetilde{A} = \left\{ f \in \mathcal{D}_{\max} \;\middle|\; \begin{array}{rcl} a_1\, \alpha_1(f) + b_1\, \alpha_2(f) & = & 0, \quad |a_1| + |b_1| \neq 0, \\ \begin{bmatrix} \alpha & \beta \\ \gamma & \delta \end{bmatrix} \begin{pmatrix} \alpha_1(f) \\ \alpha_2(f) \end{pmatrix} & = & \begin{pmatrix} \beta_1(f) \\ \beta_2(f) \end{pmatrix} \end{array} \right\}. \tag{6.1}$$

$$(II) \quad \operatorname{dom} \widetilde{A} = \left\{ f \in \mathcal{D}_{\max} \;\middle|\; \begin{array}{rcl} c_1\, \beta_1(g) + d_1\, \beta_2(g) & = & 0, \quad |c_1| + |d_1| \neq 0, \\ \begin{bmatrix} \alpha & \beta \\ \gamma & \delta \end{bmatrix} \begin{pmatrix} \beta_1(f) \\ \beta_2(f) \end{pmatrix} & = & \begin{pmatrix} \alpha_1(g) \\ \alpha_2(g) \end{pmatrix} \end{array} \right\}. \tag{6.2}$$

One can check directly using (4.12) that the following proposition is true.

Proposition 6.1. *(i) Let $\widetilde{A}$ has domain (6.1). Then*

$$\operatorname{dom} \widetilde{A}^* = \{ g \in \mathcal{D}_{\max} \mid a\, \alpha_1(g) + b\, \alpha_2(g) + c\, \beta_1(g) + d\, \beta_2(g) = 0, \}$$

with

$$a = \overline{a_1}, \quad b = \overline{b_1}, \quad \text{and} \quad \begin{pmatrix} c \\ d \end{pmatrix} = \begin{bmatrix} \overline{\delta} & -\overline{\gamma} \\ -\overline{\beta} & \overline{\alpha} \end{bmatrix} \begin{pmatrix} \overline{a_1} \\ \overline{b_1} \end{pmatrix}. \tag{6.3}$$

$$\operatorname{dom} \widetilde{A}^+ = \mathcal{P} \operatorname{dom} \widetilde{A}^* = \{ h \in \mathcal{D}_{\max} \mid a\, \beta_1(h) - b\, \beta_2(h) + c\, \alpha_1(h) - d\, \alpha_2(h) = 0, \}$$

where a, b, c, d are the same as above.

(ii) Let $\widetilde{A}$ has domain (6.2). Then

$$\operatorname{dom} \widetilde{A}^* = \{ g \in \mathcal{D}_{\max} \mid a\, \alpha_1(g) + b\, \alpha_2(g) + c\, \beta_1(g) + d\, \beta_2(g) = 0, \}$$

with

$$c = \overline{c_1}, \quad d = \overline{d_1}, \quad \text{and} \quad \begin{pmatrix} a \\ b \end{pmatrix} = \begin{bmatrix} \overline{\delta} & -\overline{\gamma} \\ -\overline{\beta} & \overline{\alpha} \end{bmatrix} \begin{pmatrix} \overline{c_1} \\ \overline{d_1} \end{pmatrix}. \tag{6.4}$$

$$\operatorname{dom} \widetilde{A}^+ = \mathcal{P} \operatorname{dom} \widetilde{A}^* = \{ h \in \mathcal{D}_{\max} \mid a\, \beta_1(h) - b\, \beta_2(g) + c\, \alpha_1(g) - d\, \alpha_2(g) = 0, \}$$

where a, b, c, d the same as above. □

Remark 6.2. *From Lemma 3.1 and Proposition 5.2 follow that a* 1-*dimensional extension* $\widetilde{A}$ *is* $\mathcal{PT}$ *-symmetry if and only if the numbers* a, b, c, d *defined in Proposition 6.1* (6.3) *and* (6.4)*, respectively, satisfy* (5.10).

If $\widetilde{A}$ is a 1-dimensional extension of A, then $\widetilde{A}^*$ is a 3-dimensional extension of A with empty resolvent set, see Theorem 5.3 and we obtain the following.

Theorem 6.3. *Let* $\widetilde{A}$ *be a* 1*-dimensional extension of* A*. Then*

$$\sigma(\widetilde{A}) = \mathbb{C}.$$

In particular, there are $\mathcal{PT}$ *symmetric* 1*-dimensional extensions of* A *with empty resolvent set.*

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