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$$-y''(x) + (-1)nx2ny(x)$$

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On Domains of $\mathcal{PT}$ Symmetric Operators Related to $-y''(x) + (-1)^n x^{2n} y(x)$

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Abstract. In the recent years a generalization of Hermiticity was investigated using a complex deformation $H = p^2 + x^2(ix)^\epsilon$ of the harmonic oscillator Hamiltonian, where ϵ is a real parameter. These complex Hamiltonians, possessing $\mathcal{PT}$ symmetry (the product of parity and time reversal), can have real spectrum. We will consider the most simple case: ϵ even. In this paper we describe all self-adjoint (Hermitian) and at the same time $\mathcal{PT}$ symmetric operators associated to $H = p^2 + x^2(ix)^\epsilon$. Surprisingly it turns out that there are a large class of self-adjoint operators associated to $H = p^2 + x^2(ix)^\epsilon$ which are not $\mathcal{PT}$ symmetric.

1. Introduction

In the well-known paper from 1998 [11] C.M. Bender and S. Boettcher considered the following Hamiltonians τ_ϵ,

$$\tau_\epsilon(y)(x) := -y''(x) + x^2 (ix)^\epsilon y(x), \quad \epsilon > 0, \quad x \in \mathbb{R}. \tag{1}$$

These complex Hamiltonians, possessing $\mathcal{PT}$ symmetry (the product of parity and time reversal), can have real spectrum. This gave rise to a mathematically consistent complex extension of conventional quantum mechanics into $\mathcal{PT}$ quantum mechanics, see e.g. the review paper [10] and references therein. During the past ten years $\mathcal{PT}$ models have been analyzed intensively, e.g., Bethe Ansatz techniques were considered in [21], various global approaches based on the extension of the above operators into the complex plane are presented in [12, 15, 39, 48], $\mathcal{PT}$ symmetric perturbations of Hermitian operators can be found in [4, 17, 18, 19], extension theory for singular perturbations of $\mathcal{PT}$ symmetric operators in [1, 3] and considerations on spectral degeneracies in [20, 22, 24, 47]. In [38] $\mathcal{PT}$ symmetry was embedded in a general mathematical context: pseudo-Hermiticity or, what is the same, the study of self-adjoint operators in a Krein space, see also [2, 26, 25, 36, 40, 41].

Usually, see, e.g., [10, 11, 12], a closed densely defined operator H in the Hilbert space $L^2(\mathbb{R})$ is called $\mathcal{PT}$ symmetric if H commutes with $\mathcal{PT}$. For unbounded operators this is also a condition on the domains. It is the aim of this paper to specify $\mathcal{PT}$ symmetric operators connected with the differential expression τ_ϵ in (1).

Here we will restrict ourselves to the most simple case: We will consider the differential τ_ϵ only in the case of ϵ even. Hence, the above differential expression τ_ϵ in (1) will be either of the form

$$\tau_{4n}(y)(x) := -y''(x) + x^{4n+2} y(x), \quad \epsilon > 0, \quad x \in \mathbb{R}.$$

if $\epsilon = 4n$, $n \in \mathbb{N}$, or it will be of the form

$$\tau_{4n+2}(y)(x) := -y''(x) - x^{4n+4} y(x), \quad \epsilon > 0, \quad x \in \mathbb{R}.$$

in case $\epsilon = 4n + 2$.

We will describe all domains giving rise to a self-adjoint (Hermitian) operator in $L^2(\mathbb{R})$ associated to τ_ϵ which is at the same time $\mathcal{PT}$ symmetric. This seems to be a natural question. To our knowledge it is not addressed in earlier publications.

Obviously, different domains have dramatic influence on the spectrum of the corresponding operators. As an example, let us consider as a possible domain the set $\widetilde{D}$ of all locally absolutely continuous functions f on the real line with a locally absolutely continuous derivative f' such that f decays exponentially as $|x| \to \infty$. Define for $k \in \mathbb{N}$ the numbers $\alpha_k := (4n + 5 - k) k^{-4n-6} e^k$ and $\beta_k := (4n + 6 - k) k^{-4n-5} e^k$ and a function

c, twice continuously differentiable on $[-1, 1]$, such that the function y_k,

$$y_k(x) := \begin{cases} (-\alpha_k x + \beta_k)e^x & \text{if } x \leq -k, \\ (-x)^{-4n-5} & \text{if } -k < x < -1, \\ c(x) & \text{if } -1 \leq x \leq 1, \\ x^{-4n-5} & \text{if } 1 < x < k, \\ (\alpha_k x + \beta_k)e^{-x} & \text{if } x \geq k, \end{cases}$$

is in $\widetilde{D}$. Obviously (y_k) converges in $L^2(\mathbb{R})$ to the function y,

$$y(x) := \begin{cases} (-x)^{-4n-5} & \text{if } x < -1, \\ c(x) & \text{if } -1 \leq x \leq 1, \\ x^{-4n-5} & \text{if } 1 < x, \end{cases}$$

which is not in $\widetilde{D}$. Moreover, $\tau_{4n+2}(y)$ is in $L^2(\mathbb{R})$ and $(\tau_{4n+2}(y_k))$ converges in $L^2(\mathbb{R})$ to $\tau_{4n+2}(y)$. This shows the following.

Remark 1 *The densely defined operator H defined via $\operatorname{dom} H := \widetilde{D}$, $Hy := \tau_{4n+2}(y)$ for $f \in \operatorname{dom} H$, is not a closed operator in $L^2(\mathbb{R})$. Hence, its spectrum covers the complex plane, $\sigma(H) = \mathbb{C}$.*

The domain which is naturally associated to τ_{4n} is the maximal domain $\mathcal{D}_{\max}$. This is the set of all locally absolutely continuous functions $f \in L^2(\mathbb{R})$ with a locally absolutely continuous derivative f' such that $\tau_{4n}(f) \in L^2(\mathbb{R})$. As τ_{4n} is in limit point case at $+\infty$ and $-\infty$, it turns out, that there is only one self adjoint operator connected to τ_{4n} which is also $\mathcal{PT}$ symmetric.

The more interesting case is $\epsilon = 4n + 2$. The differential expression τ_{4n+2} is in limit circle case at $+\infty$ and $-\infty$ and it admits many different self-adjoint extensions. These self-adjoint extensions are described via restrictions of the maximal domain $\mathcal{D}_{\max}$ by "boundary conditions at $+\infty$ and $-\infty$" which determines the set of all domains of self-adjoint extensions associated to $\epsilon = 4n + 2$. However, as a main result of this paper we characterize precisely which of these "boundary conditions at $+\infty$ and $-\infty$" give rise to $\mathcal{PT}$ symmetric extensions. It turns out, see Section 4 below, that surprisingly only a rather small class of boundary conditions gives rise to $\mathcal{PT}$ symmetric extensions. Hence, in order to obtain a $\mathcal{PT}$ symmetric operator associated with τ_{4n+2} special attention has to be given to the right boundary conditions.

Limit point/limit circle classifications are a standard tool in Sturm-Liouville theory, we mention here only [37, 44, 45, 46]. Different boundary conditions at $+\infty$ and $-\infty$ change the point spectra, a fact, which has to be taken into account for numerical simulations.

All self-adjoint operators associated to τ_{4n} and τ_{4n+2} share one common property: They commute also with the parity operator $\mathcal{P}$, hence they are also self-adjoint in a Krein space where the inner product is given by

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

We describe the sign type properties of all extensions. This will serve as a basis for the application of the perturbation theory in Krein spaces which will be used in the study of the cases ϵ not even in a subsequent paper. A short introduction to self-adjoint operators in Krein spaces is given in the next section.

2. $\mathcal{PT}$ symmetric operators as self-adjoint operators in Krein spaces

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. [6, 16, 31])

$$\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_- \tag{2}$$

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

$$(x,x) := [x_+, x_+] - [x_-, x_-], \quad x = x_+ + x_- \in \mathcal{H} \quad \text{with } x_\pm \in \mathcal{H}_\pm, \tag{3}$$

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 [34, 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).

An element x in a Krein space $(\mathcal{H}, [\cdot,\cdot])$ is called *positive* (*negative, neutral,* respectively) if $[x,x] > 0$ ($[x,x] < 0$, $[x,x] = 0$, respectively). For the basic theory of Krein space and operators acting therein we refer to [6, 16] and, in the context of $\mathcal{PT}$ symmetry, we refer to [36].

Let A be a closed, densely defined operator in the Krein space $(\mathcal{H}, [\cdot,\cdot])$. The adjoint A^+ of A in the Krein space $(\mathcal{H}, [\cdot,\cdot])$ is defined with respect to the indefinite inner product $[\cdot,\cdot]$, that is, its domain dom A^+ is the set of all $x \in \mathcal{H}$ for which there exists a $z \in \mathcal{H}$ with

$$[Ay, x] = [y, z] \quad \text{for all } y \in \text{dom } A$$

and for these x we put $A^+ x := z$. It is easily seen that (see, e.g., [33, 34])

$$A^+ = JA^*J, \tag{4}$$

where A^* denotes the adjoint with respect to the Hilbert space inner product (3) and J is the fundamental symmetry corresponding to the decomposition (2). The operator A is called self-adjoint in the Krein space $(\mathcal{H}, [\cdot,\cdot])$ if $A = A^+$.

The indefiniteness of the scalar product $[\cdot,\cdot]$ on $\mathcal{H}$ induces a natural classification of isolated real eigenvalues: A real isolated eigenvalue λ_0 of A is called of *positive* (*negative*) *type* if all the corresponding eigenvectors are positive (negative, respectively). It is usual to call such points of positive type (negative type, respectively), see [7, 5, 9, 32, 34, 35] and in this case we write

$$\lambda_0 \in \sigma_{++}(A) \quad (\text{resp. } \lambda_0 \in \sigma_{--}(A)).$$

Observe that there is no Jordan chain of length greater than one which corresponds to a eigenvalue of A of positive type (or of negative type). This classification of real isolated eigenvalues is used frequently, we mention here only [13, 14, 19, 23, 25, 36].

By $L^2(\mathbb{R})$ we denote the space of all equivalence classes of 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

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

and we define

$$(\mathcal{P}f)(x) = f(-x) \quad \text{and} \quad (\mathcal{T}f)(x) = \overline{f(x)}, \quad f \in L^2(\mathbb{R}). \tag{5}$$

Then $\mathcal{P}^2 = \mathcal{T}^2 = (\mathcal{PT})^2 = I$ and $\mathcal{PT} = \mathcal{TP}$. The operator $\mathcal{P}$ represents parity reflection and the operator $\mathcal{T}$ represents time reversal. Observe that the operator $\mathcal{T}$ is nonlinear.

Usually, see, e.g., [10, 11, 12], a closed operator H is called $\mathcal{PT}$ symmetric if H commutes with $\mathcal{PT}$. For unbounded operators this is also a condition on the domains. Therefore we will repeat the notion of $\mathcal{PT}$ symmetry in the following definition (see, e.g., [10, 19, 17]). We denote by $\operatorname{dom} H$ the domain of the operator H.

Definition 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*

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

Obviously, it follows from Definition 1

$$\operatorname{dom} H = \operatorname{dom} H\mathcal{PT}.$$

To investigate the property of $\mathcal{PT}$ symmetric operators we will need in the following the next lemma.

Lemma 1 *Let H be a closed densely defined operator H in $L^2(\mathbb{R})$ and assume $\mathcal{T}\operatorname{dom} H \subset \operatorname{dom} H$. The operator H is $\mathcal{PT}$ symmetric if and only if*

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

Proof.
Let $f \in \operatorname{dom} H$. Let H be $\mathcal{PT}$ symmetric. By assumption we have $\mathcal{T}f \in \operatorname{dom} H$ and, from the $\mathcal{PT}$ symmetry we conclude $\mathcal{PTT}f = \mathcal{P}f$ is in $\operatorname{dom} H$.

Contrary, for $f \in \operatorname{dom} H$ we have by assumption $\mathcal{T}f \in \operatorname{dom} H$ and, hence, $\mathcal{PT}f \in \operatorname{dom} H$, that is, H is $\mathcal{PT}$ symmetric. $\qquad\square$

The operator $\mathcal{P}$ introduced in (5) 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

$$[f, g] := \int_{\mathbb{R}} f(x)\overline{(\mathcal{P}g)(x)}\, dx = \int_{\mathbb{R}} f(x)\overline{g(-x)}\, dx, \quad f, g \in L^2(\mathbb{R}). \tag{6}$$

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 (6), it is easy to see that as the positive component $\mathcal{H}_+$ in a decomposition (2) the set of even functions, and as the negative component $\mathcal{H}_-$ the set of all odd functions of $L^2(\mathbb{R})$ can be chosen.

Lemma 2 *Let H be a self-adjoint operator H in the Hilbert space $L^2(\mathbb{R})$, $H = H^*$, and assume that H commutes with $\mathcal{P}$. Then H is selfadjoint in the Krein space $(L^2(\mathbb{R}), [\cdot, \cdot])$.*

The proof of this lemma follows immediately from (4) and $H\mathcal{P} = \mathcal{P}H$. We mention that such operators are called *fundamental reducible*, see, e.g., [28] and that they possess a well developed spectral and perturbation theory, cf. [5, 8, 28, 29, 30, 31, 35, 42, 43].

3. Domains of $\mathcal{PT}$ symmetric operators in the case $\epsilon = 4n$

We discuss first the more easy case $\epsilon = 4n$ for some $n \in \mathbb{N}$, that is, we consider τ_{4n} defined according to (1) via

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

To this differential expression we will associate an operator H defined on the maximal domain, i.e.,

$$\mathcal{D}_{\max} := \{y \in L^2(\mathbb{R}) : y, y' \in AC_{loc}(\mathbb{R}), \tau_{4n}y \in L^2(\mathbb{R})\},$$

via

$$\operatorname{dom} H := \mathcal{D}_{\max}, \quad Hy := \tau_{4n}(y) \quad \text{for } f \in \operatorname{dom} H.$$

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 $\mathbb{R}$.

In the following theorem we collect some of the properties of H. Recall that the differential expression τ_{4n} is called in limit circle at ∞ (at $-\infty$) if all solutions of the equation $\tau_{4n}(y) - \lambda y = 0$, $\lambda \in \mathbb{C}$, are in $L^2((a, \infty))$ (resp. $L^2((-\infty, a)))$ for some, and, hence, for all $a \in \mathbb{R}$. The differential expression τ_{4n} is called in limit point at ∞ (resp. at $-\infty$), if it is not in limit circle at ∞ (resp. at $-\infty$), cf. [45, Section 13.3] or [46, Chapter 7]. In this case there exists one solution of $\tau_{4n}(y) - \lambda y = 0$ which is not in $L^2((a, \infty))$ (resp. $L^2((-\infty, a)))$.

Theorem 1 *The differential expression τ_{4n} is in the limit point case at ∞ and at $-\infty$. The operator H with domain $\operatorname{dom} H = \mathcal{D}_{\max}$ is self-adjoint in the Hilbert space $L^2(\mathbb{R})$ and the spectrum of H consists of isolated simple eigenvalues which are non negative, real and accumulating to infinity,*

$$\sigma(H) = \sigma_p(H) = \{\lambda_1, \lambda_2, \ldots\} \subset \mathbb{R}^+.$$

Proof.

By [46, Example 7.4.2 (1)] we have limit point case at ∞ and at $-\infty$ and the operator H with the domain $\operatorname{dom} H = \mathcal{D}_{\max}$ is self-adjoint in the Hilbert space $L^2(\mathbb{R})$. Denote by $\tau_{4n,+}$ and $\tau_{4n,-}$ the restriction of the differential expression τ_{4n} to $\mathbb{R}^+$ and $\mathbb{R}^-$, respectively. Obviously, $\tau_{4n,+}$ is in limit point case at ∞, $\tau_{4n,-}$ is in limit point case at $-\infty$ and at the other, finite, end point zero the potential $x \mapsto x^{4n+2}$ is integrable over every interval $(-a,0)$ and $(0,a)$ for $a > 0$. Hence, zero is a regular end point of the differential expressions $\tau_{4n,+}$ and $\tau_{4n,-}$, respectively, cf. [45, Section 13.1] or [37, Chapters 1 and 2]. We set

$$\mathcal{D}_{\max,\pm} := \{y \in L^2(\mathbb{R}^{\pm}) : y, y' \in AC_{loc}(\mathbb{R}^{\pm}), y(0) = 0, \tau_{4n} y \in L^2(\mathbb{R}^{\pm})\}$$

and define $H_{4n,\pm} y := \tau_{4n,\pm}(y)$ for $y \in \operatorname{dom} H_{4n,\pm} = \mathcal{D}_{\max,\pm}$. It follows from [37, Lemma 3.1.2] that the essential spectrum of $H_{4n,\pm}$ is empty. It is easily seen that the difference of the resolvents of H and the operator $H_{4n,+} \oplus H_{4n,-}$, considered as an operator in $L^2(\mathbb{R}) = L^2(\mathbb{R}^+) \oplus L^2(\mathbb{R}^-)$ with domain $\mathcal{D}_{\max,+} \oplus \mathcal{D}_{\max,-}$, is a finite rank operator. Hence, the essential spectrum of H is empty, that is, the spectrum of H consists of isolated eigenvalues only. Obviously, we have $H \geq 0$. Therefore all eigenvalues are non-negative and, as τ_{4n} is in the limit point case at ∞ and at $-\infty$, all eigenvalues are simple. $\qquad\square$

Theorem 2 *We have*

$$\mathcal{T} \operatorname{dom} H = \operatorname{dom} H \quad and \quad \mathcal{P} \operatorname{dom} H = \operatorname{dom} H. \tag{7}$$

Moreover H commutes with $\mathcal{P}$, with $\mathcal{T}$ and with $\mathcal{PT}$. Hence H is $\mathcal{PT}$ symmetric and self-adjoint in the Krein space $(L^2(\mathbb{R}), [\cdot, \cdot])$. In particular we have

$$(\mathcal{P}H)^* = H\mathcal{P} = \mathcal{P}H.$$

Proof.

Relation (7) follows immediately from the definition of the operators $\mathcal{P}$ and $\mathcal{T}$ and, hence, H commutes with $\mathcal{P}$ and with $\mathcal{T}$,

$$\mathcal{P}H = H\mathcal{P} \quad and \quad \mathcal{T}H = H\mathcal{T}. \tag{8}$$

From this we conclude

$$\mathcal{PT}Hf = H\mathcal{PT}f \quad \text{for all } f \in \operatorname{dom} H$$

and, by Lemma 1, H is $\mathcal{PT}$ symmetric. Relation (8), Theorem 1 and Lemma 2 imply the selfadjointness of H in the Krein space $(L^2(\mathbb{R}), [\cdot, \cdot])$. $\qquad\square$

According to Theorem 1 all eigenvalues of H are isolated and simple. Then, see [16, Corollary VI.6.6], the corresponding eigenvectors are not neutral vectors in the Krein space $(L^2(\mathbb{R}), [\cdot, \cdot])$ and we obtain the following.

Theorem 3 *All eigenvalues of H are either of positive or of negative type,*

$$\sigma(H) = \sigma_p(H) = \sigma_{++}(H) \cup \sigma_{--}(H).$$

Remark 2 *We mention that the sets $\sigma_{++}(H)$ and $\sigma_{--}(H)$ are stable under perturbations small in gap, we refer to [5, 7, 32, 35].*

4. Domains of $\mathcal{PT}$ symmetric operators in the case $\epsilon = 4n + 2$

Now we discuss the case $\epsilon = 4n + 2$ for some $n \in \mathbb{N}$, that is, we consider τ_{4n+2} defined according to (1) via

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

From [46, Example 7.4.2 (2)]§ we conclude the following.

Proposition 1 *The differential expression τ_{4n+2} is in the limit circle case at ∞ and at $-\infty$.*

Recall that τ_{4n+2} is called in limit circle at ∞ (at $-\infty$) if all solutions of the equation $\tau_{4n+2}(y) - \lambda y = 0$, $\lambda \in \mathbb{C}$, are in $L^2((a, \infty))$ (resp. $L^2((-\infty, a))$) for some $a \in \mathbb{R}$.

Again, we consider the maximal domain, i.e.,

$$\mathcal{D}_{\max} := \{y \in L^2(\mathbb{R}) : y, y' \in AC_{loc}(\mathbb{R}), \tau_{4n+2}(y) \in L^2(\mathbb{R})\}.$$

In order to study all self-adjoint operators associated with τ_{4n+2} we need to introduce some notations. For two functions $f, g \in AC_{loc}(\mathbb{R})$ with continuous derivative, we define $[f, g]_x$ 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 that the limit of $[f, g]_x$ as $x \to \infty$ and $x \to -\infty$ exists for $f, g \in \mathcal{D}_{\max}$, see [45, Satz 13.4] or [46, p. 184]. We set

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

Lemma 3 *There exist real valued solutions $w_1, w_2 \in \mathcal{D}_{\max}$ of the equation*

$$\tau_{4n+2}(y) = 0$$

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

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

§ In the formulation of [46, Example 7.4.1] and, hence, in [46, Example 7.4.2 (2)] a minus sign is missing.

Proof.

With each solution $z \in \mathcal{D}_{\max}$ of the equation $\tau_{4n+2}(y) = 0$ also the function $x \mapsto \overline{z(x)}$ is a solution of $\tau_{4n+2}(y) = 0$. Hence, by Proposition 1, there exist two linearly independent real valued solutions $z_1, z_2 \in \mathcal{D}_{\max}$ of the equation $\tau_{4n+2}(y) = 0$. Denote by $z_{1,odd}$ and $z_{1,ev}$ the odd part of z_1 and the even part of z_1, respectively. That is

$$z_{1,odd}(x) := \frac{z_1(x) - z_1(-x)}{2} \quad \text{and} \quad z_{1,ev} := \frac{z_1(x) + z_1(-x)}{2} \quad x \in \mathbb{R}.$$

We have $z_1 = z_{1,odd} + z_{1,ev}$. Similarly, we denote by $z_{2,odd}$ and $z_{2,ev}$ the odd and even part of z_2. The functions $x \mapsto z_1(-x)$ and $x \mapsto z_2(-x)$ belong to $\mathcal{D}_{\max}$ and are solutions of $\tau_{4n+2}(y) = 0$. Hence, $z_{1,odd}, z_{1,ev}, z_{2,odd}$ and $z_{2,ev}$ belong to $\mathcal{D}_{\max}$ and are real valued solutions of $\tau_{4n+2}(y) = 0$. Assume that $z_{1,odd}$ and $z_{2,odd}$ are zero functions. Then z_1, z_2 are even functions and their derivatives z_1', z_2' are odd functions. We conclude for $x \in \mathbb{R}$

$$\begin{aligned}
[z_1, z_2]_x &= z_1(x) z_2'(x) - z_1'(x) z_2(x) \\
&= -z_1(-x) z_2'(-x) + z_1'(-x) z_2(-x) \\
&= -[z_1, z_2]_{-x}.
\end{aligned} \tag{9}$$

As z_1, z_2 are two real valued, linearly independent solution of $\tau_{4n+2}(y) = 0$, their Wronskian $[z_1, z_2]_x$ is constant for all $x \in \mathbb{R}$ and non zero, a contradiction. Hence $z_{1,odd}$ or $z_{2,odd}$ is not equal to zero. For simplicity, assume that $z_{1,odd}$ is not equal to zero. We set

$$w_1 := z_{1,odd}.$$

By a calculation similar to (9) we see that at least one of the functions $z_{1,ev}$ and $z_{2,ev}$ is non zero. Let us assume that $z_{2,ev}$ is not identically zero. Obviously, $z_{2,ev}$ and w_1 are linearly independent solutions of $\tau_{4n+2}(y) = 0$, and their Wronskian $W(w_1, z_{2,ev})$ is constant and non zero. We set

$$w_2 := W(w_1, z_{2,ev})^{-1} z_{2,ev}.$$

Therefore, $[w_1, w_2]_{-\infty} = [w_1, w_2]_\infty = 1$, w_1 is an odd, w_2 an even function and w_1, w_2 are solutions from $\mathcal{D}_{\max}$ of the equation $\tau_{4n+2}(y) = 0$. The remaining assertion of Lemma 4 follows from the fact that w_1 and w_2 are real valued functions. $\qquad \square$

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

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

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

Lemma 4 *For $f \in \mathcal{D}_{\max}$ we have*

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

Proof.

Taking into account that w_1 is odd and w_1' is even, we see

$$\begin{aligned} \alpha_1(\mathcal{P}f) &= \lim_{x \to -\infty} -f'(-x)w_1(x) - f(-x)w_1'(x) \\ &= \lim_{x \to \infty} f'(x)w_1(x) - f(x)w_1'(x) = \beta_1(f) \end{aligned}$$

and $\beta_1(\mathcal{P}f) = \alpha_1(\mathcal{PP}f) = \alpha_1(f)$. Similarly, as w_2 is even and w_2' is odd,

$$\begin{aligned} \alpha_2(\mathcal{P}f) &= \lim_{x \to -\infty} -f'(-x)w_2(x) - f(-x)w_2'(x) \\ &= \lim_{x \to \infty} -f'(x)w_2(x) + f(x)w_2'(x) = -\beta_2(f) \end{aligned}$$

and $\beta_2(\mathcal{P}f) = -\alpha_2(\mathcal{PP}f) = -\alpha_2(f)$. The remaining statements of Lemma 4 follow immediately from the definition of the operator $\mathcal{T}$. $\qquad\square$

In the sequel we will use the functions w_1 and w_2 from Lemma 4 to describe all boundary conditions for self-adjoint operators associated to the differential expression τ_{4n+2}.

The following is from [45, p. 64], [27, III.5] see also [46, Chapter 10, Section 4.4]. As usual, we will consider two different kinds of boundary conditions: mixed and separated.

All self-adjoint operators $H_{\alpha,\beta}$ associated to the differential expression τ_{4n+2} with separated boundary conditions are of the following form. For $\alpha, \beta \in [0, \pi)$ we set

$$\operatorname{dom} H_{\alpha,\beta} := \left\{ f \in \mathcal{D}_{\max} : \begin{array}{l} \alpha_1(f)\cos\alpha - \alpha_2(f)\sin\alpha = 0, \\ \beta_1(f)\cos\beta - \beta_2(f)\sin\beta = 0. \end{array} \right\}. \tag{10}$$

Then (cf. [45, Satz 13.21] and also [46, Chapter 10, Section 4.5]) the operator $H_{\alpha,\beta}$,

$$H_{\alpha,\beta}f = \tau_{4n+2}(f) \quad \text{for } f \in \operatorname{dom} H_{\alpha,\beta}, \tag{11}$$

is self-adjoint in the Hilbert space $L^2(\mathbb{R})$ and the spectrum of $H_{\alpha,\beta}$ consists of isolated simple eigenvalues λ_n, $n \in \mathbb{N}$,

$$\sigma(H) = \sigma_p(H) = \{\lambda_1, \lambda_2, \ldots\} \subset \mathbb{R} \quad \text{with} \quad \sum_{n \in \mathbb{N}} |\lambda_n|^{-2} < \infty.$$

All self-adjoint operators H_B associated to the differential expression τ_{4n+2} with mixed boundary conditions are of the following form. For $\phi \in [0, 2\pi)$, $a, b, c, d \in \mathbb{R}$ with $ad - bc = 1$ we set

$$B := e^{i\phi} \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \tag{12}$$

$$\operatorname{dom} H_B := \left\{ f \in \mathcal{D}_{\max} : \begin{pmatrix} \beta_1(f) \\ \beta_2(f) \end{pmatrix} = B \begin{pmatrix} \alpha_1(f) \\ \alpha_2(f) \end{pmatrix} \right\}. \tag{13}$$

Then (cf., e.g., [45, Satz 13.21]) the operator H_B,

$$H_B f = \tau_{4n+2}(f) \quad \text{for } f \in \operatorname{dom} H_B, \tag{14}$$

is self-adjoint in the Hilbert space $L^2(\mathbb{R})$ and the spectrum of H_B consists of isolated eigenvalues λ_n, $n \in \mathbb{N}$, with multiplicity equal or less than two,

$$\sigma(H) = \sigma_p(H) = \{\lambda_1, \lambda_2, \ldots\} \subset \mathbb{R} \quad \text{with} \quad \sum_{n \in \mathbb{N}} |\lambda_n|^{-2} < \infty.$$

We now formulate the main results of this section. We start with the case of separated boundary conditions.

Theorem 4 *The operator $H_{\alpha,\beta}$ defined via (10) and (11) with $\alpha, \beta \in [0, \pi)$ is $\mathcal{PT}$ symmetric if and only if*

$$\alpha + \beta = \pi \quad or \quad \alpha + \beta = 0.$$

In this case, $H_{\alpha,\beta}$ commutes with $\mathcal{P}$ and with $\mathcal{T}$. Hence $H_{\alpha,\beta}$ is self-adjoint in the Krein space $(L^2(\mathbb{R}), [\cdot, \cdot])$. In particular, all eigenvalues of $H_{\alpha,\beta}$ are either of positive or of negative type,

$$\sigma(H_{\alpha,\beta}) = \sigma_p(H_{\alpha,\beta}) = \sigma_{++}(H_{\alpha,\beta}) \cup \sigma_{--}(H_{\alpha,\beta}). \tag{15}$$

Proof.
Assume $\alpha + \beta = \pi$. If, in addition, $\alpha \neq \frac{\pi}{2}$, then we have $\sin \beta = \sin \alpha$ and $\cos \beta = -\cos \alpha$ and with Lemma 4 we conclude for $f \in \text{dom} \, H_{\alpha,\beta}$

$$\alpha_1(\mathcal{P}f) \cos \alpha - \alpha_2(\mathcal{P}f) \sin \alpha = -\beta_1(f) \cos \beta + \beta_2(f) \sin \beta = 0$$
$$\beta_1(\mathcal{P}f) \cos \beta - \beta_2(\mathcal{P}f) \sin \beta = -\alpha_1(f) \cos \alpha + \alpha_2(f) \sin \alpha = 0.$$

Hence, $\mathcal{P}f \in \text{dom} \, H_{\alpha,\beta}$. If $\alpha = \beta = \frac{\pi}{2}$ then for $f \in \text{dom} \, H_{\frac{\pi}{2}, \frac{\pi}{2}}$ we have $\alpha_2(f) = \beta_2(f) = 0$ and, by Lemma 4, $\mathcal{P}f \in \text{dom} \, H_{\frac{\pi}{2}, \frac{\pi}{2}}$.

Assume $\alpha + \beta = 0$. Then for $f \in \text{dom} \, H_{0,0}$ we have $\alpha_1(f) = \beta_1(f) = 0$ and, by Lemma 4, $\mathcal{P}f \in \text{dom} \, H_{0,0}$.

Hence, if $\alpha + \beta = \pi$ or $\alpha + \beta = 0$ and we have $\mathcal{P}\text{dom} \, H_{\alpha,\beta} \subset \text{dom} \, H_{\alpha,\beta}$. Moreover, $\text{dom} \, H_{\alpha,\beta} = \mathcal{PP}\text{dom} \, H_{\alpha,\beta} \subset \mathcal{P}\text{dom} \, H_{\alpha,\beta}$, that is

$$\mathcal{P}\text{dom} \, H_{\alpha,\beta} = \text{dom} \, H_{\alpha,\beta}.$$

An easy calculation gives $H_{\alpha,\beta}\mathcal{P} = \mathcal{P}H_{\alpha,\beta}$ and Lemma 4 gives

$$\mathcal{T}\text{dom} \, H_{\alpha,\beta} = \text{dom} \, H_{\alpha,\beta}, \quad \text{and} \quad \mathcal{T}H_{\alpha,\beta} = H_{\alpha,\beta}\mathcal{T}.$$

Hence

$$\mathcal{PT}H_{\alpha,\beta}f = H_{\alpha,\beta}\mathcal{PT}f \quad \text{for all } f \in \text{dom} \, H_{\alpha,\beta}.$$

By Lemma 1, $H_{\alpha,\beta}$ is $\mathcal{PT}$ symmetric. Lemma 2 implies the selfadjointness of $H_{\alpha,\beta}$ in the Krein space $(L^2(\mathbb{R}), [\cdot, \cdot])$. Relation (15) follows from the fact that the spectrum of $H_{\alpha,\beta}$ consists only of isolated, simple eigenvalues and from [16, Corollary VI.6.6].

It remains to show that $H_{\alpha,\beta}$ is not $\mathcal{PT}$ symmetric if $\alpha + \beta \neq \pi$ and $\alpha + \beta \neq 0$. For this we consider functions y_1, y_2, z_1, z_2 from $\mathcal{D}_{\max}$ such that y_j, $j = 1, 2$ equal w_j on

the interval $(1, \infty)$, equal zero on the interval $(-\infty, -1)$ and the functions z_j, $j = 1, 2$ equal w_j on the interval $(-\infty, -1)$ and equal zero on the interval $(1, \infty)$. Set

$$y := -\cos \beta y_1 + \sin \beta y_2 - \cos \alpha z_1 + \sin \alpha z_2.$$

We have $y \in \mathcal{D}_{\max}$ and, by Lemma 3,

$$\alpha_1(y) = \sin \alpha, \qquad \alpha_2(y) = \cos \alpha,$$
$$\beta_1(y) = \sin \beta, \qquad \beta_2(y) = \cos \beta.$$

From this we conclude $y \in \operatorname{dom} H_{\alpha, \beta}$ and with Lemma 4

$$\alpha_1(\mathcal{P}y) \cos \alpha - \alpha_2(\mathcal{P}y) \sin \alpha = \beta_1(y) \cos \alpha + \beta_2(y) \sin \alpha$$
$$= \sin \beta \cos \alpha + \cos \beta \sin \alpha$$
$$= \sin(\alpha + \beta) \neq 0,$$

as $\alpha + \beta \in (0, 2\pi)$ with $\alpha + \beta \neq \pi$. Hence $\mathcal{P}y \notin \operatorname{dom} H_{\alpha, \beta}$ and we see with Lemma 1 that $H_{\alpha, \beta}$ is not $\mathcal{PT}$ symmetric. $\qquad \square$

Now we formulate a similar result for the case of mixed boundary conditions.

Theorem 5 *The operator H_B defined via (12), (13) and (14) is $\mathcal{PT}$ symmetric if and only if*

$$B = \pm \begin{pmatrix} a & b \\ c & a \end{pmatrix} \quad \text{with } a^2 - bc = 1. \tag{16}$$

In this case, H_B commutes with $\mathcal{P}$ and with $\mathcal{T}$. Hence H_B is self-adjoint in the Krein space $(L^2(\mathbb{R}), [\cdot, \cdot])$. The spectrum of H_B consists only of isolated eigenvalues with multiplicity one or two.

Proof.
Let $f \in \operatorname{dom} H_B$, i.e.

$$\begin{pmatrix} \beta_1(f) \\ \beta_2(f) \end{pmatrix} = e^{i\phi} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \alpha_1(f) \\ \alpha_2(f) \end{pmatrix}, \tag{17}$$

for some $\phi \in [0, 2\pi)$, $a, b, c, d \in \mathbb{R}$ with $ad - bc = 1$. Lemma 4 implies

$$\begin{pmatrix} \beta_1(\mathcal{P}f) \\ \beta_2(\mathcal{P}f) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \alpha_1(f) \\ \alpha_2(f) \end{pmatrix}, \begin{pmatrix} \alpha_1(\mathcal{P}f) \\ \alpha_2(\mathcal{P}f) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \beta_1(f) \\ \beta_2(f) \end{pmatrix}$$

and $\mathcal{P}f$ is in $\operatorname{dom} H_B$ if and only if

$$\begin{pmatrix} \alpha_1(f) \\ \alpha_2(f) \end{pmatrix} = e^{i\phi} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \beta_1(f) \\ \beta_2(f) \end{pmatrix}.$$

With (17) we see that this is the case if and only if

$$\begin{pmatrix} \alpha_1(f) \\ \alpha_2(f) \end{pmatrix} = e^{2i\phi} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \alpha_1(f) \\ \alpha_2(f) \end{pmatrix}$$

which is equivalent to

$$\begin{pmatrix} \alpha_1(f) \\ \alpha_2(f) \end{pmatrix} = e^{2i\phi} \begin{pmatrix} a^2 - bc & b(a-d) \\ c(d-a) & d^2 - bc \end{pmatrix} \begin{pmatrix} \alpha_1(f) \\ \alpha_2(f) \end{pmatrix}. \tag{18}$$

Similar as in Theorem 4 we consider functions y_1, y_2, z_1, z_2 from $\mathcal{D}_{\max}$ such that y_j, $j = 1, 2$, equals w_j on the interval $(1, \infty)$, equals zero on the interval $(-\infty, -1)$ and the functions z_j, $j = 1, 2$, equals w_j on the interval $(-\infty, -1)$ and equals zero on the interval $(1, \infty)$. Set

$$y := -ce^{i\phi}y_1 + ae^{i\phi}y_2 + z_2, \quad \text{and} \quad z := -de^{i\phi}y_1 + be^{i\phi}y_2 + z_1$$

We have $y, z \in \mathcal{D}_{\max}$ and

$$\begin{array}{llll} \alpha_1(y) = 1, & \beta_1(y) = ae^{i\phi}, & \alpha_1(z) = 0, & \beta_1(z) = be^{i\phi}, \\ \alpha_2(y) = 0, & \beta_2(y) = ce^{i\phi}, & \alpha_2(z) = 1, & \beta_2(z) = de^{i\phi}. \end{array}$$

Hence, $y, z \in \operatorname{dom} H_B$, see (17). Inserting y and z in (18) we see

$$e^{2i\phi}(a^2 - bc) = 1, \quad b(a-d) = 0 = c(d-a), \quad e^{2i\phi}(d^2 - bc) = 1.$$

For $c \neq 0$ it follows $a = d$ and, from $ad - bc = 1$, we obtain $a^2 - bc = 1$. For $c = 0$ it follows $a^2 = d^2 = 1$ and $ad = 1$ This gives $a = d = \pm 1$. Moreover, in both cases (i.e. $c \neq 0$ and $c = 0$) ϕ is either zero or π. This shows that $\mathcal{P}\operatorname{dom} H_B \subset \operatorname{dom} H_B$ if and only if (16) holds.

Hence, if (16) does not hold, there exists $f \in \operatorname{dom} H_B$ with $\mathcal{P}f$ is not in $\operatorname{dom} H_B$ and we see with Lemma 1 that H_B is not $\mathcal{PT}$ symmetric.

Conversely, if (16) hold, then we have $\mathcal{P}\operatorname{dom} H_B \subset \operatorname{dom} H_B$ and $\operatorname{dom} H_B = \mathcal{PP}\operatorname{dom} H_B \subset \mathcal{P}\operatorname{dom} H_B$, that is $\mathcal{P}\operatorname{dom} H_B = \operatorname{dom} H_B$. An easy calculation gives $H_B\mathcal{P} = \mathcal{P}H_B$ and Lemma 4 gives

$$\mathcal{T}\operatorname{dom} H_B = \operatorname{dom} H_B, \quad \text{and} \quad \mathcal{T}H_B = H_B\mathcal{T},$$

hence $\mathcal{PT}H_Bf = H_B\mathcal{PT}f$ for all $f \in \operatorname{dom} H_B$. By Lemma 1, H_B is $\mathcal{PT}$ symmetric. Lemma 2 implies the selfadjointness of H_B in the Krein space $(L^2(\mathbb{R}), [\cdot, \cdot])$. $\qquad \square$

As mentioned above, the spectrum of H_B consists only of isolated eigenvalues with multiplicity less or equal to two. We have the following.

Proposition 2 *Let the operator H_B be $\mathcal{PT}$ symmetric and let $\lambda_0 \in \sigma_p(H_B)$ with* $\dim \operatorname{Ker}(H_B - \lambda_0) = 1$, *then*

$$\lambda_0 \in \sigma_{++}(H_B) \cup \sigma_{--}(H_B). \tag{19}$$

If $\lambda_0 \in \sigma_p(H_B)$ with $\dim \operatorname{Ker}(H_B - \lambda_0) = 2$, *then*

$$\lambda_0 \notin \sigma_{++}(H_B) \cup \sigma_{--}(H_B). \tag{20}$$

Proof.

Relation (19) follows from the fact that isolated eigenvalues with multiplicity one in the Krein space $(L^2(\mathbb{R}), [\cdot, \cdot])$ are not neutral, see [16, Corollary VI.6.6]. Using the reasoning in the proof of Lemma 3 applied to the equation $\tau_{4n+2}(y) - \lambda_0 y = 0$, we find an odd and an even eigenfunction of H_B corresponding to the eigenvalue λ_0. Then the odd eigenfunction is a negative vector in the Krein space $(L^2(\mathbb{R}), [\cdot, \cdot])$ and the even eigenfunction is a positive vector in the Krein space $(L^2(\mathbb{R}), [\cdot, \cdot])$ and (20) holds. $\square$

Remark 3 *Let the operator H_B be $\mathcal{PT}$ symmetric. It is usual in the perturbation theory in Krein spaces to consider spectral points of type π_+ and π_-, denoted by $\sigma_{\pi_+}(H_B)$ and $\sigma_{\pi_-}(H_B)$, see [7, 28, 35]. The main property of these points is that they are invariant under compact perturbations and perturbations small in norm or small in the gap metric. We mention here only that isolated eigenvalues of finite algebraic multiplicity are spectral points of type π_+ and π_+. Hence*

$$\sigma(H_B) = \sigma_p(H_B) = \sigma_{\pi_+}(H_B) \cup \sigma_{\pi_-}(H_B).$$

With Theorems 4 and 5 all self-adjoint operators associated to the differential expression τ_{4n+2} which give rise to a $\mathcal{PT}$ symmetric operator can precisely be characterized. We wish to emphasize the following.

Corollary 1 *If $\alpha\beta \neq 0$ and $\alpha + \beta \neq \pi$, then the operator $H_{\alpha,\beta}$ is not $\mathcal{PT}$ symmetric.*

Corollary 2 *If $d \neq a$ or ϕ is not zero or π, then the operator H_B is not $\mathcal{PT}$ symmetric.*

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