On domains of $\mathcal{PT}$ symmetric operators related to $-y''(x) + (-1)^n x^{2n} y(x)$

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

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1. Introduction
In the well-known paper [1] Bender and Boettcher considered the following Hamiltonians $\tau_\epsilon$:

$$\tau_\epsilon(y)(x) := -y''(x) + x^2 (ix)^\epsilon y(x), \quad \epsilon > 0. \quad (1)$$

These complex Hamiltonians, possessing $\mathcal{PT}$ symmetry (the product of parity and time reversal), can have a 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 [2] and references therein. During the past 10 years $\mathcal{PT}$ models have been analyzed intensively, e.g. Bethe Ansatz techniques were considered in [3], various global approaches based on the extension of the above operators into the complex plane are presented in [4–7], $\mathcal{PT}$ symmetric perturbations of Hermitian operators can be found in [8–11], extension theory for singular perturbations of $\mathcal{PT}$ symmetric operators in [12, 13] and considerations on spectral
degeneracies in [14–17]. In [18] $PT$ 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 [19–24].

Starting from the pioneering work of Bender and Boettcher [1], the above Hamiltonian $\tau_\epsilon$ 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 [25] this approach was extended to different parametrizations and in [26–28] this approach was mapped back to the real axis using a real parametrization of a suitable contour within the defined along an appropriate complex contour within Stokes wedges. In [25] the problem degeneracies in [14–17]. In [18] $PT$ symmetric if $H$ commutes with $PT$. For unbounded operators this is also a condition on the domains. It is the aim of this paper to specify $PT$ symmetric operators connected with the differential expression $\tau_\epsilon$ in (1).

Here we will restrict ourselves to the most simple case. We will consider the differential expression $\tau_\epsilon$ only in the case of $\epsilon$ even. Moreover, we will consider the differential expression only for real $x$. For these cases we will show that there are two fundamentally different situations (limit point/limit circle) which both can be treated mathematically rigorously and illustrate the cases where the real line belongs to the Stokes wedges or not. We believe that the results obtained in this paper give strong indications on how to treat the more difficult cases mentioned above in an operator theoretic framework.

The above differential expression $\tau_\epsilon$ 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 the case $\epsilon = 4n + 2$.

We will describe all domains giving rise to a self-adjoint (Hermitian) operator in $L^2(\mathbb{R})$ associated with $\tau_\epsilon$ which is at the same time $PT$ 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 $\tilde{D}$ 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 $\alpha_k := (4n + 5 - k)k^{-4n-5}e^k$ and $\beta_k := (4n + 6 - k)\frac{1}{5}k^{-4n-5}e^k$ 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 $\tilde{D}$. 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 $\tilde{D}$. 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.
The densely defined operator $H$ defined via $\text{dom } H := \bar{D}$, $Hy := \tau_{4n+2}(y)$ for $f \in \text{dom } H$, 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 with $\tau_{4n}$ 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 $\tau_{4n}$ is in the limit point case at $+\infty$ and $-\infty$, it turns out that there is only one self-adjoint operator connected to $\tau_{4n}$ which is also $PT$ symmetric.

The more interesting case is $\epsilon = 4n + 2$. The differential expression $\tau_{4n+2}$ is in the 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 with $\epsilon = 4n + 2$. However, as a main result of this paper we characterize precisely which of these ‘boundary conditions at $+\infty$ and $-\infty$’ give rise to $PT$ symmetric extensions. It turns out, see section 4, that surprisingly only a rather small class of boundary conditions gives rise to $PT$ symmetric extensions. Hence, in order to obtain a $PT$ symmetric operator associated with $\tau_{4n+2}$, 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 [30–33]. 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 with $\tau_{4n}$ and $\tau_{4n+2}$ share one common property. They commute also with the parity operator $P$; hence, they are also self-adjoint in a Krein space where the inner product is given by

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

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 $\epsilon$ not even in a subsequent paper. A short introduction to self-adjoint operators in Krein spaces is given in the next section.

2. $PT$ 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 [34–36])

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

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 [37, proposition 11.2]. 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 [34, 35] and, in the context of \(\mathcal{PT}\) symmetry, we refer to [22].

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 \(\text{dom } A^*\) 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., [37, 38])

\[ A^* = JA^*J, \]

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 \(\lambda_0\) 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 [37, 39–43], 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 1 which corresponds to an eigenvalue of \(A\) of positive type (or of negative type). This classification of real isolated eigenvalues is used frequently; we mention here only [11, 21, 22, 44–46].

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

\[ (Pf)(x) = f(-x) \quad \text{and} \quad (Tf)(x) = \overline{f(x)}, \quad f \in L^2(\mathbb{R}). \]

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

Usually, see e.g. [1, 2, 4], 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., [2, 9, 11]). We denote by \(\text{dom } H\) 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 \(f \in \text{dom } H\) we have

\[ \mathcal{PT}f \in \text{dom } H \quad \text{and} \quad \mathcal{PT}Hf = H\mathcal{PT}f. \]

Obviously, it follows from definition 1:

\[ \text{dom } H = \text{dom } H\mathcal{PT}. \]

To investigate the property of \(\mathcal{PT}\) symmetric operators we will need in the following the next lemma.
Theorem 1. Let $H$ be a closed densely defined operator $H$ in $L^2(\mathbb{R})$ and assume $\tau \in \text{dom } H$. The operator $H$ is $PT$ symmetric if and only if

\[ \forall \ f \in \text{dom } H \quad \text{and} \quad \forall \ f \in \text{dom } H, \ P\tau H f = HPT f \]

Proof. Let $f \in \text{dom } H$. Let $H$ be $PT$ symmetric. By assumption we have $\tau f \in \text{dom } H$ and, from the $PT$ symmetry, we conclude $\tau \tau f = \tau f$ is in $\text{dom } H$.

Contrary, for $f \in \text{dom } H$, we have by assumption $\tau f \in \text{dom } H$ and, hence, $\tau f \in \text{dom } H$, that is, $H$ is $PT$ symmetric.

The operator $P$ 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

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

(6)

With respect to this inner product, $L^2(\mathbb{R})$ becomes a Krein space. Observe that in this case the operator $P$ 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 $P$. Then $H$ is selfadjoint in the Krein space $(L^2(\mathbb{R}), [\cdot, \cdot])$.

The proof of this lemma follows immediately from (4) and $H P = P H$. We mention that such operators are called fundamental reducible, see e.g. [47], and that they possess a well-developed spectral and perturbation theory, cf [36, 40, 43, 47–52].

3. Domains of $PT$ 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 $\tau_{4n}$ defined according to (1) via

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

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

\[ D_{\text{max}} := \{ y \in L^2(\mathbb{R}) : y, y' \in AC_{\text{loc}}(\mathbb{R}), \tau_{4n}y \in L^2(\mathbb{R}) \}, \]

via

\[ \text{dom } H := D_{\text{max}}, \quad Hy := \tau_{4n}(y) \quad \text{for } f \in \text{dom } H. \]

Here and in the following $AC_{\text{loc}}(\mathbb{R})$ 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 $\tau_{4n}$ is called in the limit circle at $\infty$ (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 $\tau_{4n}$ is called in the limit point at $\infty$ (resp. at $-\infty$), if it is not in the limit circle at $\infty$ (resp. at $-\infty$), cf [32, section 13.3] or [33, 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 $\tau_{4n}$ is in the limit point case at $\infty$ and at $-\infty$. The operator $H$ with domain $\text{dom } H = D_{\text{max}}$ 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 [33, example 7.4.2 (1)] we have the limit point case at $\infty$ and at $-\infty$ and the operator $H$ with the domain $\text{dom } H = D_{\text{max}}$ is self-adjoint in the Hilbert space $L^2(\mathbb{R})$. Denote by $\tau_{4n,+}$ and $\tau_{4n,-}$ the restriction of the differential expression $\tau_{4n}$ to $\mathbb{R}^+$ and $\mathbb{R}^-$, respectively. Obviously, $\tau_{4n,+}$ is in the limit point case at $\infty$, $\tau_{4n,-}$ is in the 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 endpoint of the differential expressions $\tau_{4n,+}$ and $\tau_{4n,-}$, respectively, cf [32, section 13.1] or [30, chapters 1 and 2]. We set

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

and define $H_{\text{min}, \pm} := \tau_{4n, \pm}(y)$ for $y \in \text{dom } H_{\text{min}, \pm} = D_{\text{max}, \pm}$. It follows from [30, lemma 3.1.2] that the essential spectrum of $H_{\text{min}, \pm}$ is empty. It is easily seen that the difference of the resolvents of $H$ and the operator $H_{\text{min}, +} \oplus H_{\text{min}, -}$, considered as an operator in $L^2(\mathbb{R}) = L^2(\mathbb{R}^+) \oplus L^2(\mathbb{R}^-)$ with domain $D_{\text{max}, +} \oplus D_{\text{max}, -}$, 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 $\tau_{4n}$ is in the limit point case at $\infty$ and at $-\infty$, all eigenvalues are simple. \hfill \Box

Theorem 2. We have

$$T \text{ dom } H = \text{ dom } H \quad \text{ and } \quad \mathcal{P} \text{ dom } H = \text{ dom } H. \quad (7)$$

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

$$(\mathcal{P} H)^* = H \mathcal{P} = \mathcal{P} H. \quad (8)$$

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

$$\mathcal{P} H = H \mathcal{P} \quad \text{ and } \quad T H = H T. \quad (8)$$

From this we conclude

$$\mathcal{P} T H f = H \mathcal{P} T f \quad \text{ for all } \quad f \in \text{ dom } H$$

and, by lemma 1, $H$ is $\mathcal{P} T$ symmetric. Relation (8), theorem 1 and lemma 2 imply the self-adjointness of $H$ in the Krein space $(L^2(\mathbb{R}), [\cdot, \cdot])$. \hfill \Box

According to theorem 1 all eigenvalues of $H$ are isolated and simple. Then, see [35, corollary VI.6.6.6], 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:

$$\sigma(H) = \sigma_p(H) = \sigma_{++}(H) \cup \sigma_{--}(H).$$
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 $\tau_{4n+2}$ defined according to (1) via

$$
\tau_{4n+2}(y) := -y''(x) - x^{4n+1}y(x), \quad x \in \mathbb{R}.
$$

From [33, example 7.4.2 (2)] we conclude the following.

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

Recall that $\tau_{4n+2}$ is called in the limit circle in $\infty$ (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.

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

In order to study all self-adjoint operators associated with $\tau_{4n+2}$ we need to introduce some notations. For two functions $f, g \in AC_{\text{loc}}(\mathbb{R})$ with a continuous derivative, we define $[f, g]$, for $x \in \mathbb{R}$ via

$$
[f, g]_x := \frac{f(x)g'(x) - f'(x)g(x)}{x}, \quad [f, g]_\infty := \lim_{x \to -\infty} [f, g]_x.
$$

**Lemma 3.** There exist real valued solutions $w_1, w_2 \in D_{\text{max}}$ of the equation

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

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

$$
[w_1, w_1]_\infty = [w_2, w_2]_\infty = 1
$$

and

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

**Proof.** With each solution $z \in D_{\text{max}}$ 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 $z_1, z_2 \in D_{\text{max}}$ of the equation $\tau_{4n+2}(y) = 0$. Denote by $z_{1, \text{odd}}$ and $z_{1, \text{ev}}$ the odd part of $z_1$ and the even part of $z_1$, respectively. That is

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

We have $z_1 = z_{1, \text{odd}} + z_{1, \text{ev}}$. Similarly, we denote by $z_{2, \text{odd}}$ and $z_{2, \text{ev}}$ the odd and even part of $z_2$. The functions $x \mapsto z_1(-x)$ and $x \mapsto z_2(-x)$ belong to $D_{\text{max}}$ and are solutions of $\tau_{4n+2}(y) = 0$. Hence, $z_{1, \text{odd}}, z_{1, \text{ev}}, z_{2, \text{odd}}$ and $z_{2, \text{ev}}$ belong to $D_{\text{max}}$ and are real valued solutions of $\tau_{4n+2}(y) = 0$. Assume that $z_{1, \text{odd}}$ and $z_{2, \text{odd}}$ are zero functions. Then $z_1, z_2$ are even functions, and their derivatives $z'_1, z'_2$ are odd solutions. We conclude for $x \in \mathbb{R}$

$$
[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}.
$$

(9)

3 In the formulation of [33, example 7.4.1] and, hence, in [33, example 7.4.2 (2)] a minus sign is missing.
As \( z_1, z_2 \) are two real-valued, linearly independent solutions of \( \tau_{4n+2}(y) = 0 \), their Wronskian \( [z_1, z_2]_x \) is constant for all \( x \in \mathbb{R} \) and nonzero, a contradiction. Hence \( z_{1, \text{odd}} \) or \( z_{2, \text{odd}} \) is not equal to zero. For simplicity, assume that \( z_{1, \text{odd}} \) is not equal to zero. We set
\[
 w_1 := z_{1, \text{odd}}.
\]
By a calculation similar to (9) we see that at least one of the functions \( z_{1, \text{ev}} \) and \( z_{2, \text{ev}} \) is nonzero. Let us assume that \( z_{2, \text{ev}} \) is not identically zero. Obviously, \( z_{2, \text{ev}} \) and \( w_1 \) are linearly independent solutions of \( \tau_{4n+2}(y) = 0 \), and their Wronskian \( W(w_1, z_{2, \text{ev}}) \) is constant and nonzero. We set
\[
 w_2 := W(w_1, z_{2, \text{ev}})^{-1} z_{2, \text{ev}}.
\]
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 \( D_{\max} \) 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.

For simplicity we set for \( f \in D_{\max} \)
\[
\begin{align*}
\alpha_1(f) &= [w_1, f]_{-\infty}, & \alpha_2(f) &= [w_2, f]_{-\infty}, \\
\beta_1(f) &= [w_1, f]_{\infty}, & \beta_2(f) &= [w_2, f]_{\infty}.
\end{align*}
\]
The next lemma describes the behavior of the above numbers under the operators \( \mathcal{P} \) and \( T \).

**Lemma 4.** For \( f \in D_{\max} \) we have
\[
\begin{align*}
\alpha_1(\mathcal{P} f) &= \beta_1(f), & \alpha_2(\mathcal{P} f) &= -\beta_2(f), \\
\beta_1(\mathcal{P} f) &= \alpha_1(f), & \beta_2(\mathcal{P} f) &= -\alpha_2(f), \\
\alpha_1(T f) &= \beta_1(f), & \alpha_2(T f) &= -\beta_2(f), \\
\beta_1(T f) &= \alpha_1(f), & \beta_2(T f) &= -\alpha_2(f).
\end{align*}
\]

**Proof.** Taking into account that \( w_1 \) is odd and \( w_1' \) is even, we see
\[
\begin{align*}
\alpha_1(\mathcal{P} f) &= \lim_{x \to -\infty} -f'(x)w_1(x) - f(x)w_1'(x) \\
&= \lim_{x \to -\infty} f'(x)w_1(x) - f(x)w_1'(x) = \beta_1(f)
\end{align*}
\]
and \( \beta_1(\mathcal{P} f) = \alpha_1(\mathcal{P} \mathcal{P} f) = \alpha_1(f) \). Similarly, as \( w_2 \) is even and \( w_2' \) is odd,
\[
\begin{align*}
\alpha_2(\mathcal{P} f) &= \lim_{x \to -\infty} -f'(x)w_2(x) - f(x)w_2'(x) \\
&= \lim_{x \to -\infty} f'(x)w_2(x) + f(x)w_2'(x) = -\beta_2(f)
\end{align*}
\]
and \( \beta_2(\mathcal{P} f) = -\alpha_2(\mathcal{P} \mathcal{P} f) = -\alpha_2(f) \). The remaining statements of lemma 4 follow immediately from the definition of the operator \( T \).

In what follows we will use the functions \( w_1 \) and \( w_2 \) from lemma 4 to describe all boundary conditions for self-adjoint operators associated with the differential expression \( \tau_{4n+2} \).

The following is from \([32, p 64], [53, III.5]\); see also \([33, chapter 10, section 4.4]\). As usual, we will consider two different kinds of boundary conditions: mixed and separated.

All self-adjoint operators \( H_{\alpha, \beta} \) associated with the differential expression \( \tau_{4n+2} \) with separated boundary conditions are of the following form. For \( \alpha, \beta \in [0, \pi) \) we set
\[
\text{dom } H_{\alpha, \beta} := \left\{ f \in D_{\max} : \begin{array}{l}
\alpha_1(f) \cos \alpha - \alpha_2(f) \sin \alpha = 0, \\
\beta_1(f) \cos \beta - \beta_2(f) \sin \beta = 0.
\end{array} \right\}.
\] (10)

Then (cf \([32, Satz 13.21] \) and also \([33, chapter 10, section 4.5]\)) the operator \( H_{\alpha, \beta} \),
\[
H_{\alpha, \beta} f = \tau_{4n+2}(f) \quad \text{for } f \in \text{dom } H_{\alpha, \beta}.
\] (11)
is self-adjoint in the Hilbert space $L^2(\mathbb{R})$ and the spectrum of $H_{\alpha,\beta}$ consists of isolated simple eigenvalues $\lambda_n$, $n \in \mathbb{N}$,
\[ \sigma(H) = \sigma_p(H) = \{\lambda_1, \lambda_2, \ldots\} \subset \mathbb{R} \quad \text{with} \quad \sum_{n \in \mathbb{N} : \lambda_n \neq 0} |\lambda_n|^2 < \infty. \]

All self-adjoint operators $H_B$ associated with the differential expression $\tau_{4n^2}$ 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
\[ B := e^{i\phi} \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad (12) \]
\[ \text{dom } H_B := \left\{ f \in \mathcal{D}_\text{max} : \begin{pmatrix} \beta_1(f) \\ \beta_2(f) \end{pmatrix} = B \begin{pmatrix} \alpha_1(f) \\ \alpha_2(f) \end{pmatrix} \right\}. \quad (13) \]

Then (cf. e.g., [32, Satz 13.21]) the operator $H_B$,
\[ H_B f = \tau_{4n^2}(f) \quad \text{for} \quad f \in \text{dom } H_B, \quad (14) \]
is self-adjoint in the Hilbert space $L^2(\mathbb{R})$ and the spectrum of $H_B$ consists of isolated eigenvalues $\lambda_n$, $n \in \mathbb{N}$, with multiplicity equal or less than 2,
\[ \sigma(H) = \sigma_p(H) = \{\lambda_1, \lambda_2, \ldots\} \subset \mathbb{R} \quad \text{with} \quad \sum_{n \in \mathbb{N} : \lambda_n \neq 0} |\lambda_n|^2 < \infty. \]

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
\[ \alpha + \beta = \pi \quad \text{or} \quad \alpha \beta = 0. \]

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:
\[ \sigma(H_{\alpha,\beta}) = \sigma_p(H_{\alpha,\beta}) = \sigma_{++}(H_{\alpha,\beta}) \cup \sigma_{--}(H_{\alpha,\beta}). \quad (15) \]

**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 $f \in \text{dom } H_{\alpha,\beta}$ we have $\alpha_2(f) = \beta_2(f) = 0$ and, by lemma 4, $\mathcal{P} f \in \text{dom } H_{\alpha,\beta}$.

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 $\alpha + \beta = 0$, we have $\mathcal{P} \text{dom } H_{\alpha,\beta} \subset \text{dom } H_{\alpha,\beta}$. Moreover, dom $H_{\alpha,\beta} = \mathcal{P} \text{dom } H_{\alpha,\beta} \subset \text{dom } H_{\alpha,\beta}$, 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
\[ T \text{ dom } H_{\alpha,\beta} = \text{ dom } H_{\alpha,\beta}, \quad \text{and} \quad T H_{\alpha,\beta} = H_{\alpha,\beta} T. \]

Hence
\[ \mathcal{P} T H_{\alpha,\beta} f = H_{\alpha,\beta} \mathcal{P} T f \quad \text{for all} \quad f \in \text{dom } H_{\alpha,\beta}. \]
By lemma 1, $H_{a,\beta}$ is $\mathcal{PT}$ symmetric. Lemma 2 implies the self-adjointness of $H_{a,\beta}$ in the Krein space $(L^2(\mathbb{R}), \cdot, \cdot)$. Relation (15) follows from the fact that the spectrum of $H_{a,\beta}$ consists only of isolated, simple eigenvalues and from [35, corollary VI.6.6].

It remains to show that $H_{a,\beta}$ is not $\mathcal{PT}$ symmetric if $\alpha + \beta \neq \pi$ and $\alpha + \beta = 0$. 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,

$$\alpha_1(y) = \sin \alpha, \quad \alpha_2(y) = \cos \alpha,$$

$$\beta_1(y) = \sin \beta, \quad \beta_2(y) = \cos \beta.$$

From this we conclude $y \in \text{dom } H_{a,\beta}$ and with lemma 4

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

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

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

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

(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 1 or 2.

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

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

(17)

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

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

and $\mathcal{P}f$ is in $\text{dom } H_B$ 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

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

(18)
Similarly as in theorem 4 we consider functions $y_1, y_2, z_1, z_2$ from $D_{\text{max}}$ 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 $(1, \infty)$ and equal 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 $y, z \in \text{dom} \ HB$, 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 $c = 0$), $\phi$ is either zero or $\pi$. This shows that $\cal P \text{ dom} \ HB \subset \text{ dom} \ HB$ if and only if (16) holds.

Hence, if (16) does not hold, there exists $f \in \text{ dom} \ HB$ with $\cal P f \notin \text{ dom} \ HB$ and then it follows from lemma 1 that $\text{ HKr }$ is not $\cal PT$ symmetric.

Conversely, if (16) holds, then we have $\cal P \text{ dom} \ HB \subset \text{ dom} \ HB$ and dom $\text{ HKr } = \cal P \text{ dom} \ HB \subset \cal P \text{ dom} \ HB$, that is $\cal P \text{ dom} \ HB = \text{ dom} \ HB$. An easy calculation gives $\text{ HKr } \cal P = \cal P \text{ HKr }$ and lemma 4 gives
\[
T \text{ dom} \ HB = \text{ dom} \ HB \quad \text{and} \quad T \text{ HKr } = \text{ HKr } T;
\]
hence $\cal P \text{ HKr } f = \text{ HKr } \cal P f$ for all $f \in \text{ dom} \ HB$. By lemma 1, $\text{ HKr }$ is $\cal PT$ symmetric. Lemma 2 implies the self-adjointness of $\text{ HKr }$ in the Krein space $(L^2(\mathbb{R}), [\cdot, \cdot])$. \qed

As mentioned above, the spectrum of $\text{ HKr }$ consists only of isolated eigenvalues with multiplicity less or equal to $2$. We have the following.

**Proposition 2.** Let the operator $\text{ HKr }$ be $\cal PT$ symmetric and let $\lambda_0 \in \sigma_p(\text{ HKr })$ with dim Ker $(\text{ HKr } - \lambda_0) = 1$; then
\[
\lambda_0 \in \sigma_+(\text{ HKr }) \cup \sigma_-(\text{ HKr }). \tag{19}
\]
If $\lambda_0 \in \sigma_p(\text{ HKr })$ with dim Ker $(\text{ HKr } - \lambda_0) = 2$, then
\[
\lambda_0 \notin \sigma_+(\text{ HKr }) \cup \sigma_-(\text{ HKr }). \tag{20}
\]

**Proof.** Relation (19) follows from the fact that isolated eigenvalues with multiplicity $1$ in the Krein space $(L^2(\mathbb{R}), [\cdot, \cdot])$ are not neutral, see [35, corollary VI.6.6]. Using the reasoning in the proof of lemma 3 applied to the equation $\tau_{\text{ HKr } + 2}(y) - \lambda_0 y = 0$, we find an odd and an even eigenfunction of $\text{ HKr }$ corresponding to the eigenvalue $\lambda_0$. 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. \qed

**Remark 3.** Let the operator $\text{ HKr }$ be $\cal PT$ symmetric. It is usual in the perturbation theory in Krein spaces to consider spectral points of type $\pi_+$ and $\pi_-$, denoted by $\sigma_+(\text{ HKr })$ and $\sigma_-(\text{ HKr })$, see [39, 43, 47]. 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 types $\pi_+$ and $\pi_-$. Hence
\[
\sigma(\text{ HKr }) = \sigma_p(\text{ HKr }) = \sigma_+(\text{ HKr }) \cup \sigma_-(\text{ HKr }).
\]
With theorems 4 and 5 all self-adjoint operators associated with the differential expression \( \tau_{n+2} \) 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 \( \mathcal{H}_{\alpha,\beta} \) is not \( \mathcal{PT} \) symmetric.

**Corollary 2.** If \( d \neq \alpha \) or \( \phi \) is not zero or \( \pi \), then the operator \( \mathcal{H}_d \) is not \( \mathcal{PT} \) symmetric.

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