Operator-based approach to $\mathcal{PT}$-symmetric problems on a wedge-shaped contour

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Abstract We consider a second-order differential equation

$$-y''(z) - (iz)^{N+2}y(z) = \lambda y(z), \quad z \in \Gamma$$

with an eigenvalue parameter $\lambda \in \mathbb{C}$. In $\mathcal{PT}$ quantum mechanics $z$ runs through a complex contour $\Gamma \subset \mathbb{C}$, which is in general not the real line nor a real half-line. Via a parametrization we map the problem back to the real line and obtain two differential equations on $[0, \infty)$ and on $(-\infty, 0]$. They are coupled in zero by boundary conditions and their potentials are not real-valued. The main result is a classification of this problem along the well-known limit-point/limit-circle scheme for complex potentials introduced by Sims 60 years ago. Moreover, we associate operators to the two half-line problems and to the full axis problem and study their spectra.

Keywords Non-Hermitian Hamiltonian · Stokes wedges · Limit point · Limit circle · $\mathcal{PT}$ symmetric operator · Spectrum · Eigenvalues

1 Introduction

In classical quantum mechanics Hamiltonians are Hermitian. Recently this has been questioned to be too restrictive. In 1998 Bender and Boettcher in the pioneering work [8] noticed that a large class of non-Hermitian Hamiltonians possesses real spectra and suggested to construct a non-Hermitian quantum mechanic, see [8, 10, 14, 36] or for an overview [5, 7, 32]. They adopted all axioms of quantum mechanics except the one that restricted the Hamiltonian to be Hermitian. Instead, one assumes the Hamiltonian to satisfy $\mathcal{PT}$-symmetry. In [8] they consider a non-Hermitian Hamiltonian corresponding to

$$p^2 - (iz)^{N+2}, \quad z \in \Gamma,$$

where $N$ is a natural number greater than zero. Contrary to standard quantum mechanics, $z$ runs along a complex contour $\Gamma$.
Hamiltonians of the form (1) are not Hermitian, but possess an antilinear $\mathcal{PT}$-symmetry, which is the combined invariance under simultaneous spatial reflection $\mathcal{P}$ and time reversal $\mathcal{T}$. The condition that the Hamiltonian is $\mathcal{PT}$-symmetric is a physical condition, because $\mathcal{P}$ and $\mathcal{T}$ both are elements of the homogenous Lorentz group of Lorentz boost and spatial rotation. Nowadays there are a lot of papers in diverse research areas about $\mathcal{PT}$-symmetric Hamiltonians, see [6,7,12,14,23,27,33,35,36]. E.g., a close relation to metamaterials was discovered as $\mathcal{PT}$-symmetric operators are capable to incorporate negative permittivity and permeability, cf. [23,27,33].

In general one can not expect that the Hamiltonian (1) is Hermitian in the Hilbert space $L^2$ and has real spectrum. However, in, e.g. [5,8,10,19], Hamiltonians with complex potential and real spectra were discussed. The eigenfunctions of different eigenvalues of a Hermitian Hamiltonian are mutually orthogonal. This orthonormal set is even complete and, therefore, a basis, if the Parseval equality is fulfilled. The existence of this eigenbasis of a Hermitian Hamiltonian is essential for quantum mechanics. However, eigenfunctions of non-Hermitian Hamiltonians are in general not orthogonal and they do not form a basis. Moreover, [24,25,29,37] show that even the eigenfunctions of the imaginary cubic oscillator $p^2 + ix^3, \ x \in \mathbb{R}$ do not form a Riesz basis despite possessing real spectra, cf. [36]. Therefore, a new approach beyond standard quantum theory is required.

In (1) the contour $\Gamma$ is located in regions of the complex plane, such that the eigenfunctions $\phi : \Gamma \rightarrow \mathbb{C}$ of (1) vanish exponentially as $|z| \rightarrow \infty$ along $\Gamma$. The regions in the complex plane where the solutions of (1) vanish exponentially are wedges, which are called Stokes wedges. Stokes wedges correspond to sectors in the complex plane. The opening angle and, hence the number of wedges, correspond only to the number $N$, for details we refer to Fig. 2. They are bounded by lines, the so-called Stokes lines, cf. [5,8,10]. Both, Stokes wedges and Stokes lines are symmetric to the action of $\mathcal{PT}$.

It is our main aim to relate this Stokes wedge/Stokes line dichotomy to the classical limit point/limit circle classification from the Sturm–Liouville theory with complex potentials.

For simplicity, we choose here the special contour (cf. [4])

$$\Gamma := \left\{ z = xe^{i\phi \text{sgn}(x)} : x \in \mathbb{R} \right\}, \ \ \phi \in (-\pi/2, \pi/2),$$

see Fig. 1 and treat this problem via a Sturm–Liouville approach. Namely (1) leads to the associated eigenvalue equation

$$-y''(z) - (iz)^{N+2}y(z) = \lambda y(z), \ z \in \Gamma.$$  \hspace{1cm} (2)

Via the parametrization $z(x) := xe^{i\phi \text{sgn}(x)}$, $x \in \mathbb{R}$, we obtain Sturm–Liouville differential equations on $[0, \infty)$ and on $(-\infty, 0]$, respectively,

$$\tau_+ w(x) := -e^{-2i\phi}w''(x) - (ix)^{N+2}e^{(N+2)i\phi}w(x) = \lambda w(x), \ x \in \mathbb{R}_+$$  \hspace{1cm} (3)

$$\tau_- w(x) := -e^{2i\phi}w''(x) - (ix)^{N+2}e^{-(N+2)i\phi}w(x) = \lambda w(x), \ x \in \mathbb{R}_-.$$  \hspace{1cm} (4)

It is our aim to treat (3) and (4) from an operator-based perspective. This is new compared with the above cited literature from theoretical physics.

Equations (3) and (4) correspond to a Sturm–Liouville problem $- (py')' + qy = \lambda y$ with non-real $p$ and non-real $q$ on a half-axis. But, before we consider this case, we recall the classical Sturm–Liouville theory on a half-axis (see [26,40]) for real-valued coefficients $p$, $q$ and regular end-point 0. Classical Sturm–Liouville theory for $p$, $q$ real follows the following (rough) scheme:
(a) Determine the number of $L^2$-solutions of $-(py')' + qy = \lambda y$ for $\lambda \in \mathbb{C} \setminus \mathbb{R}$. According to the famous Weyl alternative (cf. [40]) we obtain either one or two linearly independent $L^2$-solutions. The corresponding situation is then called the limit-point case (in case of one solution) or the limit-circle (two solutions).

(b) Define minimal and maximal operator corresponding to the differential expression $-(py')' + qy$. Roughly speaking, the elements in the domain of the minimal operator vanishes at the endpoint zero and the elements in the domain of the maximal operator satisfy no boundary conditions.

(c) Show that the minimal operator is symmetric and its adjoint is the maximal operator.

(d) Describe all self-adjoint extensions $A_\theta$ of the minimal operator via a suitable parameter $\theta$ and solve the spectral problem $A_\theta y = \lambda y$.

The above scheme was adopted to various more general situations, see, e.g., the monographs [20, 22, 28, 34, 41]. An analogous theory was subsequently developed for non-real potentials $q$ by Sims [38]. In a first step, item (a) was generalized by Sims [38] to $\text{Im} q \leq 0$. It states that there exists at least one solution of (3) in the weighted space $L^2(0, \infty, \text{Im}(\lambda - q))$, where $\text{Im}(\lambda - q)$ is the weight, and this solution is also in $L^2(0, \infty)$ for $\lambda$ in the upper complex plane. Contrary to the above Weyl alternative in item (a) from above, now there are three cases possible:

1. Limit-point I: There is (up to a constant) exactly one solution of $-(py')' + qy = \lambda y$ which is simultaneously in $L^2(0, \infty, \text{Im}(\lambda - q))$ and in $L^2(0, \infty)$.
2. Limit-point II: There is one solution in $L^2(0, \infty, \text{Im}(\lambda - q))$, but all are in $L^2(0, \infty)$.
3. Limit-circle: All solutions are simultaneously in $L^2(0, \infty, \text{Im}(\lambda - q))$ and in $L^2(0, \infty)$.

The above approach from Sims [38] is restricted to potentials $q$ with $\text{Im} q \leq 0$. Instead, here we use a generalisation which allows more general potential $q$ and a complex-valued function $p$, cf. [15]. Again one obtains three cases, which corresponds to the above limit-point I, II and limit-circle cases (and which are called cases I, II and III in [15, Theorem 2.1]). We use this result to give a complete classification into limit-point/limit-circle of the two differential equations (3) and (4). This is done with the help of asymptotic analysis, cf. [21]. Depending on the location of the contour $\Gamma$ in terms of its angle, we specify limit-point I, II or limit-circle case. In the limit-point I case we do not need boundary conditions at $\pm \infty$, i.e. the functions $\phi$ of the domain fulfill $|\phi(x)| \to 0$ if $|x| \to \infty$ and if $\phi$ is additionally a solution of (3) or (4), then $\phi(x)$ vanishes even exponentially for $|x| \to \infty$. So we reduce the (physical) notion of Stokes wedges and Stokes lines to the limit-point/limit-circle classification in the following way:
Equations (3), (4) in limit-point case I ⇔ Γ lies in two Stokes wedges.
Limit-point case II is never possible.
Equations (3), (4) in limit-circle case ⇔ Γ lies on two Stokes lines.

This correspondence between \( \mathcal{PT} \) quantum mechanics and well-known notion from the Sturm–Liouville theory with complex-valued potentials is one of the main findings of this paper.

Moreover, in this paper, we then develop for the non-Hermitian Hamiltonian (1) a spectral theory which takes as a guiding principle the items (b)–(d) from above. For simplicity, we restrict ourselves to the physically relevant limit-point case I or, what is the same, to the case when Γ lies in two Stokes wedges (see [2,3] for some investigations in the limit-circle case).

Similar as in item (b) from above, we characterize the domains of the minimal operator \( A_{0\pm}(\tau_{\pm}) \) and the maximal operator \( A_{\text{max}\pm}(\tau_{\pm}) \) as
\[
\text{dom } A_{\text{max}\pm}(\tau_{\pm}) := \{ w \in L^2(\mathbb{R}_{\pm}) : \tau_{\pm}w \in L^2(\mathbb{R}_{\pm}), w, w' \in AC_{\text{loc}}(\mathbb{R}_{\pm}) \}
\]
and
\[
\text{dom } A_{0\pm}(\tau_{\pm}) := \{ w \in \text{dom } A_{\text{max}\pm}(\tau_{\pm}) : w(0) = w'(0) = 0 \}
\]
(in the limit-point case I). The minimal operator is now \( T \)-symmetric and its adjoint is the maximal operator, i.e. we show
\[
A_{\text{max}\pm}(\tau_{\pm})^* = A_{0\pm}(\tau_{\pm}).
\]

In the literature, e.g. [22], instead of \( T \)-symmetric it is common to use \( J \)-symmetric, that is, symmetric under complex conjugation, see also Sect. 3. Observe, that \( J \) in this meaning has nothing to do with the fundamental symmetry from Krein spaces, which is also often named \( J \). The maximal/minimal operators \( A_{\text{max}+}(\tau_+) \) and \( A_{0+}(\tau_+) \) correspond to the differential expression \( \tau_+ \) on the positive real axis, cf. (3), whereas \( A_{\text{max}-}(\tau_-) \) and \( A_{0-}(\tau_-) \) correspond to \( \tau_- \) on \( \mathbb{R}_- \), cf. (4). However, the problem under consideration is (2), which corresponds (after parametrization) to the joint problems (3) and (4) on the real line with a (so far) unspecified boundary condition in zero.

Hence, we will use the maximal/minimal operators \( A_{\text{max}\pm}(\tau_{\pm}) \) and \( A_{0\pm}(\tau_{\pm}) \) as the building blocks for operators on the full axis. We define the maximal operator on the full-axis via the direct sum of the maximal operators on the half-axis:
\[
A_{\text{max}} = A_{\text{max}-}(\tau_-) \oplus A_{\text{max}+}(\tau_+)
\]
and domain
\[
D_{\text{max}} = \left\{ w \in L^2(\mathbb{R}) : Aw \in L^2(\mathbb{R}), w|_{\mathbb{R}_{\pm}}, w'|_{\mathbb{R}_{\pm}} \in AC_{\text{loc}}(\mathbb{R}_{\pm}) \right\}.
\]
Moreover, we obtain in the same way the minimal operator
\[
A_0 = A_{0-}(\tau_-) \oplus A_{0+}(\tau_+)
\]
with domain
\[
\text{dom } A_0 = \{ w \in D_{\text{max}} : w(0+) = w(0-), w'(0+) = w'(0-) = 0 \}.
\]
It turns out that the operators \( A_{\text{max}} \) and \( A_0 \) are adjoint to each other in the new inner product \( \langle \cdot, \cdot \rangle \), see, e.g., [30–32,39], where \( \langle \cdot, \cdot \rangle \) is a new inner product defined via
\[
\langle \cdot, \cdot \rangle := (P\cdot, \cdot).
\]
Here \( (\cdot, \cdot) \) stands for the classical \( L^2 \)-inner product. However, when it comes to the spectrum, both operators, the maximal \( A_{\text{max}} \) and the minimal \( A_0 \), are not suitable as it is easy to see that their spectra cover the complex plane. Therefore, it is natural to assume some coupling at \( z = 0 \) for the half-axis operators. This is done by boundary
conditions in zero. From the physical point of view we always assume continuity in zero, whereas we allow some freedom for the derivative in zero. Therefore, we introduce a parameter $\alpha$ and obtain finally the wanted operator $A$:

$$\text{dom}(A) := \{ w \in D_{\max} : w(0+) = w(0-), w'(0+) = \alpha w'(0-) \}$$

and

$$A w(x) := \begin{cases} -e^{-2i\phi} w''(x) - (ix)^{N+2} e^{(N+2)i\phi} w(x), & x \geq 0 \\ -e^{2i\phi} w''(x) - (ix)^{N+2} e^{-(N+2)i\phi} w(x), & x \leq 0 \end{cases}$$

We show that the operator $A$ is indeed $PT$-symmetric and even self-adjoint in the new inner product $[\cdot, \cdot]$, for the right choice of $\alpha$.

In a next step, it is our aim to discuss the spectrum of $A$. For non-self-adjoint operators like $A$ there is no standard theory to do this. Therefore, we use a different extension of the minimal operator $A_0$ as an aid. For this we introduce the operators $A_{\pm}$ which are extensions of the half-axis minimal operators (or, what is the same, restrictions of the half-axis maximal operators) with domain:

$$\text{dom} A_{\pm} := \{ w \in \text{dom} A_{\max_{\pm}}(\tau_{\pm}) : w(0) = 0 \}.$$ 

From [15] it is known that the operators $A_{\pm}$ are $T$-self-adjoint and their spectra consist only of isolated eigenvalues with finite algebraic multiplicity and empty essential spectrum.

Obviously $A$ and the direct sum of $A_- \oplus A_+$ differ only by two dimensions. As a second main result of this note we show that $A$ has the same spectral properties as the direct sum $A_- \oplus A_+$, i.e. the spectrum $\sigma(A)$ of $A$ consists only of isolated eigenvalues with finite algebraic multiplicity, that is, $\sigma(A) = \sigma_p(A)$, the essential spectrum is empty and the resolvent set $\rho(A)$ is non-empty.

Summing up, to some extent it is a surprise that in the physical literature, starting from the seminal paper of Bender and Boettcher [8], the above presented techniques from the Sturm–Liouville theory for complex potentials were never exploited. It is the aim of this paper to recall those techniques and, hence, provide a setting of the (nowadays) classical Bender–Boettcher-theory in terms of the spectral extension theory for Sturm–Liouville expressions with a complex potential.

2 Limit-point/limit-circle and Stokes wedges and lines

We consider the Hamiltonian

$$H = \frac{1}{2m} p^2 - (iz)^{N+2}, \quad z \in \Gamma,$$

with a natural number $N > 0$, cf. [5,8] and a wedge-shaped contour,

$$\Gamma := \{ z = xe^{i\phi \text{sgn}(x)} : x \in \mathbb{R} \}$$

for some angle $\phi \in (-\pi/2, \pi/2)$, see also [4]. We refer to [16,30,33] where a similar contour was used. The associated Schrödinger eigenvalue problem is

$$-y''(z) - (iz)^{N+2} y(z) = \lambda y(z), \quad z \in \Gamma,$$

for some complex number $\lambda$. We map the problem back to the real line via the parametrization
Thus \( y \) solves (5) if and only if \( w, w(x) := y(z(x)) \), solves

\[-e^{\mp 2i\phi} w''(x) - (ix)^{N+2} e^{\pm (N+2)i\phi} w(x) = \lambda w(x), \quad x \in \mathbb{R}_\pm.\]  

Here and in the following we set \( \mathbb{R}_+ := [0, \infty) \) and \( \mathbb{R}_- := (-\infty, 0] \). For a complex number \( z \) with argument \( \theta \in (-\pi, \pi] \), we choose as the \( n \)th root \( z^{1/n} = r^{1/n} e^{i\theta/n} \). In the following theorem we give a classification of this equation into two cases, namely limit-point case and limit-circle case:

**Theorem 1** For all \( \lambda \in \mathbb{C} \), exactly one of the following holds:

(I) If \( \phi \neq -\frac{N+2}{2N+8} \pi + \frac{2k}{4+N} \pi, \ k = 0, \ldots, N + 3 \), there exists, up to a constant, unique solution \( w \) of (7) satisfying \( w \in L^2(\mathbb{R}_\pm) \). In particular, there is one solution of (7) which is not in \( L^2(\mathbb{R}_\pm) \).

(II) If \( \phi = -\frac{N+2}{2N+8} \pi + \frac{2k}{4+N} \pi, \ k = 0, \ldots, N + 3 \), all solutions \( w \) of (7) satisfy \( w \in L^2(\mathbb{R}_\pm) \).

Case (I) is called limit-point case I and case (II) is called limit-circle case.

**Proof** We consider Eq. (7) on \( \mathbb{R}_+ \) only. The results for \( \mathbb{R}_- \) are obtained by an analogous argument by replacing \( x \) by \( -x \). This theorem is a special case of [15, Theorem 2.1]. The two corresponding linear independent solutions \( w_1 \) and \( w_2 \) of the Schrödinger eigenvalue differential equation \(-w''(x) - (ix)^{N+2} e^{(N+4)i\phi} w(x) = \lambda w(x), \ x \in \mathbb{R}_+, \tilde{\lambda} = e^{2i\phi} \lambda, \) satisfy [21, Corollary 2.2.1]

\[w_{1,2}(x) \sim q(x)^{-1/4} \exp \left( \pm \int_1^x \Re(q(t)^{1/2}) \, dt \right) \text{ for } x \to \infty\]  

with \( q(x) := -(ix)^{N+2} e^{(N+4)i\phi} - \lambda e^{2i\phi} \). The notation \( f(x) \sim g(x) \) means that \( f(x)/g(x) \to 1 \) as \( x \to \infty \).

We compute \( \Re(q(t)^{1/2}) \). For \( \lambda = 0 \) we obtain

\[
\Re(q(t)^{1/2}) = \Re((-ix)^{N+2} e^{(N+4)i\phi})^{1/2} = \Re((e^{i\pi+(N+2)i\phi/2+(N+4)i\phi})^{1/2} x^{(N+2)/2}) \]
\[
= \Re(e^{i\pi/2+(N+2)i\phi/4+(N+4)i\phi/2}) x^{(N+2)/2} = -\sin((N+2)\pi/4 + (N+4)\phi/2) x^{(N+2)/2}
\]

It is easy to see that

\[
\sin((N+2)\pi/4 + (N+4)\phi/2) = 0
\]

if and only if

\[
\phi = -\frac{N+2}{2N+8} \pi + \frac{2k}{4+N} \pi, \quad \text{for } k \in \mathbb{Z}.
\]

Hence, if \( \phi \neq -\frac{N+2}{2N+8} \pi + \frac{2k}{4+N} \pi \) and if \( \lambda = 0 \) then \( \Re(q(t)^{1/2}) \neq 0 \) and there exists exactly one solution in \( L^2(\mathbb{R}_+) \) or \( L^2(\mathbb{R}_-) \), respectively. This implies, see [15, Theorem 2.1], that we have case (I), limit-point case I for \( \lambda = 0 \) and with [15, Remark 2.2] even for all \( \lambda \in \mathbb{C} \). This shows (I).
It remains to consider the following case: \( \phi = - \frac{N+2}{2N+8} \pi + \frac{2k}{4+N} \pi \) and \( k \in \mathbb{Z} \). We obtain
\[
q(x) = -(ix)^{N+2}e^{-(N+2)i\pi/2+2ki\pi} - \tilde{\lambda} = -x^{N+2} - \tilde{\lambda}.
\]
and the Schrödinger eigenvalue equation
\[
-w''(x) - x^{N+2}w(x) = \tilde{\lambda}w(x)
\]
and we know from (8) that both (linearly independent) solutions of (7) are in \( L^2(\mathbb{R}_+) \), because for \( \tilde{\lambda} = 0 \) we obtain \( \text{Re}(q(x)^{1/2}) = 0 \). Therefore, from [15, Theorem 2.1] we have to examine whether
\[
\int_0^\infty \text{Re} e^{i\eta \left( |w'(x)|^2 + (-x^{N+2} - K)|w(x)|^2 \right)} \, dx + \int_0^\infty |w(x)|^2 \, dx < \infty
\]
is for one or both solutions of (7) fulfilled, where \( \eta \) and \( K \) are suitable variables, which we explain in the following, in order to decide whether we are in the limit-point case I, II or limit-circle case. In our setting the set
\[
Q_+ := \text{clconv} \left\{ r - x^{N+2} : x \in [0, \infty), 0 < r < \infty \right\},
\]
where clconv denotes the closed convex hull, is the real line and \( K \) is the number in \( Q_+ \) with the shortest distance to \( \lambda \); hence \( K = \text{Re} \lambda \). And \( \eta \) corresponds to the angle which rotates \( Q_+ \) into the right (closed) half-plane, such that \( \lambda \) is located in the left half-plane; hence \( \eta = \pm \frac{\pi}{2} \). So
\[
\pm \int_0^\infty \text{Re} \left( |w'(x)|^2 + (-x^{N+2} - \text{Re} \lambda)|w(x)|^2 \right) \, dx = 0.
\]
Condition (9) is fulfilled for both solutions. Thus we are in the limit-circle case (i.e. case III in [15]) (Fig. 2). \( \square \)

**Remark 1** In particular, limit-point case II (cf. Sect. 1) is not possible, which corresponds to case (II) in [15, Theorem 2.1].

**Remark 2** The limit-point case I, II and limit-circle case correspond to the cases I, II and III from [38] and [15].

In the limit-point case there is exactly one solution of (7) which is in \( L^2(\mathbb{R}_+) \) resp. \( L^2(\mathbb{R}_-) \) and because of the asymptotics (8) we even know that this solution goes exponentially to 0 for \( |x| \to \infty \). The regions in the complex plane where \( \Gamma \) fulfills this condition are wedges, see, e.g. [8,30,32].

We decompose the complex plane according to the angle \( \theta = -\frac{N+2}{2N+8} \pi + \frac{2k}{4+N} \pi \) in \( N + 4 \) sectors
\[
S_k := \left\{ z \in \mathbb{C} : -\frac{N + 2}{2N + 8} \pi + \frac{2k - 2}{4 + N} \pi < \text{arg}(z) < -\frac{N + 2}{2N + 8} \pi + \frac{2k}{4 + N} \pi \right\}, \ k = 0, \ldots, N + 3.
\]
The boundary of each \( S_k \) consists of two rays \( L_k \):
\[
L_k := \left\{ z \in \mathbb{C} : \text{arg}(z) = -\frac{N + 2}{2N + 8} \pi + \frac{2k}{4 + N} \pi \right\}, \ k = 0, \ldots, N + 3.
\]

In the sectors \( S_k \), \( k = 0, \ldots, N + 3 \) one solution of (7) decays exponentially, whereas on the lines \( L_k \) both solutions decay polynomially. The regions \( S_k \) are called **Stokes wedges** \( S_k \) (see, i.e. [5,8,9]) and the rays \( L_k \) are called **Stokes lines**. Hence we have \( N + 4 \) Stokes lines and Stokes wedges.

By definition, \( \Gamma \) is either contained in two Stokes wedges or corresponds to two Stokes lines. This means we can classify our problem depending on the angle \( \phi \) of the contour \( \Gamma \).

**Theorem 2** (i) If \( \Gamma \) is located in two Stokes wedges, which are symmetric with respect to the imaginary axis, then (7) is in the limit-point case for all \( \lambda \in \mathbb{C} \), cf. case (I) in Theorem 1. In particular, this implies that only one solution of (7) is in \( L^2(\mathbb{R}_+) \) resp. \( L^2(\mathbb{R}_-) \).

(ii) If \( \Gamma \) is located on Stokes lines, then (7) is in the limit-circle case for all \( \lambda \in \mathbb{C} \), cf. case (III) in Theorem 1. In particular, this implies that all solutions of (7) are in \( L^2(\mathbb{R}_+) \) resp. \( L^2(\mathbb{R}_-) \).
3 Maximal and minimal operators on the semi-axis

From now on we restrict ourselves to the limit-point case, i.e. \( \Gamma \) lies in two Stokes wedges and (7) has exactly one solution which is in \( L^2(\mathbb{R}_\pm) \), cf. Theorem 2. Here we will define three different kinds of operators on \( \mathbb{R}_+ \) and \( \mathbb{R}_- \): The maximal, the minimal and the preminimal operator. This is motivated by the classical procedure for Sturm–Liouville expressions in the limit-point case. In the classical Sturm–Liouville situation, where the coefficients are real, the minimal operator is the closure of the preminimal, it is a symmetric operator in a Hilbert space and its adjoint is the maximal operator.

Here, the situation is slightly different. However, the definitions of the corresponding operators are formally the same as in the classical Sturm–Liouville case, but due to the complex-valued coefficients the adjoints behave differently.

**Definition 1** The operator \( T \) defined on the Hilbert space \( L^2(I) \), where \( I \subset \mathbb{R} \) is an interval, is called *time reverse* operator, if for all \( u \in L^2 \) we have
\[
Tu(x) = \overline{u}(x).
\]
We mention that in [22] \( T \) equals \( J \).

We consider the following differential expressions:
\[
\tau_\pm w(x) := -e^{\mp 2i\phi} w''(x) - (i x)^{N+2} e^{\pm(N+2)i\phi} w(x)
\]
and the formal adjoint
\[
\tau_\pm^* w(x) := -e^{\pm 2i\phi} w''(x) - (-i x)^{N+2} e^{\mp(N+2)i\phi} w(x)
\]
on \( \mathbb{R}_\pm \). Obviously
\[
\tau_\pm^* = \tau_\pm, \quad \text{where} \quad \tau_\pm = T \tau_\pm T.
\]

We assume that \( \tau_\pm \) is in the limit-point case, that is, \( \phi \neq -\frac{N+2}{2N+8}\pi + \frac{2k}{N+4}\pi \), cf. Theorem 2. Observe that then also the following lemma holds:
Lemma 1 If $\tau_{\pm}$ is in the limit-point case, then $\tau_{\pm}^* = T \tau_{\pm} T$ is in the limit-point case.

Proof Recall for $z = re^{i\arg z} \in \mathbb{C}$ with $-\pi < \arg z \leq \pi$ the square root of $z$ is $z^{1/2} = \sqrt{re^{i\arg z}/2}$. As in the proof of Theorem 1 we use the asymptotics (8) from [21, Corollary 2.2.1] and calculate for the potential in (10) its real part for $x \in \mathbb{R}_+$:

$$\text{Re}(q(t))^{1/2} = \text{Re}((-(-ix))^{N+2} + (N+4)i\phi)^{1/2} = \text{Re}((e^{i\pi-(N+2)i\pi/2-(N+4)i\phi/2})x^{(N+2)/2}$$

Hence

$$\sin((N+2)\pi/4 + (N+4)\phi/2)x^{(N+2)/2} = 0,$$

if and only if

$$\phi = -\frac{N+2}{2N+8} \pi + \frac{2k}{N+4} \pi, \quad k \in \mathbb{Z},$$

which is exactly the condition for $\tau_+$ to be in the limit-point case, see Theorems 1 and 2. In the same way we obtain the result for $x \in \mathbb{R}_-$. \hfill \Box

Define the following operators with

$$\text{dom} \; (A_{0\pm}(\tau_{\pm})) := \{ w \in L^2(\mathbb{R}_\pm) : \tau_{\pm} w \in L^2(\mathbb{R}_\pm), \; w, w' \in AC_{loc}(\mathbb{R}_\pm), \; w(0) = w'(0) = 0, \; w \text{ has compact support in } \mathbb{R}_\pm \}$$

$$A_{0\pm}'(\tau_{\pm}) w(x) := \tau_{\pm} w(x).$$

By $A_{0\pm}(\tau_{\pm})$ we denote the closure of $A_{0\pm}'(\tau_{\pm})$ ($A_{0\pm}'(\tau_{\pm})$ is closable by Edmunds and Evans [22, III Theorem 10.7]). The operators $A_{0\pm}'(\tau_{\pm})$ correspond to the preminimal operators in classical Sturm–Liouville theory, whereas $A_{0\pm}(\tau_{\pm})$ correspond to the minimal operators.

Additionally we define the maximal operators

$$\text{dom} \; (A_{max\pm}(\tau_{\pm})) := \{ w \in L^2(\mathbb{R}_\pm) : \tau_{\pm} w \in L^2(\mathbb{R}_\pm), \; w, w' \in AC_{loc}(\mathbb{R}_\pm) \}$$

$$A_{max\pm}(\tau_{\pm}) w(x) := \tau_{\pm} w(x).$$

Recall that for a closed operator $T : \text{dom} (T) \subset L^2 \to L^2$ the deficiency of $T$ is defined as $\deficiency T := \dim L^2/\text{ran} (T)$. Moreover, we recall that the notion of the set $\Pi (T)$ of regular points of $T$ (cf., e.g., [22, pg. 101]) is

$$\Pi (T) := \{ \lambda : \exists \; k(\lambda) > 0 \text{ with } \| (T - \lambda) u \| \geq k(\lambda) \| u \| \text{ for all } u \in \text{dom} (T) \}.$$

Theorem 3 We have

$$A_{max\pm}(\tau_{\pm})^* = A_{0\pm}(\tau_{\pm}^*) \text{ and } A_{0\pm}(\tau_{\pm})^* = A_{max\pm}(\tau_{\pm}^*). \quad (12)$$

Moreover, $TA_{0\pm}(\tau_{\pm}) T \subset A_{0\pm}(\tau_{\pm})^*$ and $\deficiency (A_{0\pm}(\tau_{\pm}) - \lambda) = \deficiency (A_{0\pm}(\tau_{\pm}^*) - \lambda)$ is either 1 or 2 for all $\lambda \in \Pi (A_{0\pm}(\tau_{\pm}))$. In the limit-point case we obtain $\deficiency (A_{0\pm}(\tau_{\pm}) - \lambda) = 1$ and

$$\dim \text{dom} A_{max\pm}(\tau_{\pm})/\text{dom} A_{0\pm}(\tau_{\pm}) = 2. \quad (13)$$

Furthermore, in the limit-point case, $\Pi (A_{0\pm}(\tau_{\pm})) \neq \emptyset$ and with

$$Q_\pm := \text{clconv} \left\{ e^{\pm 2i\phi} r - (i x)^{N+2} e^{\pm (N+2)i\phi} : 0 < r < \infty, x \in \mathbb{R}_\pm \right\}$$
we have

\[ \mathbb{C} \setminus Q_\pm \subset \Pi(A_{0\pm}(\tau_\pm)). \]  

(14)

In particular, \( Q_+ \) and \( Q_- \) are sectors in the complex plane with opening angles strictly less than \( \pi \),

\[ \Pi(A_{0-}(\tau_-)) \cap \Pi(A_{0+}(\tau_+)) \neq \emptyset. \]  

(15)

**Proof** We will use [22, III Theorem 10.7]. It cannot be used directly as the coefficient in front of the second derivative in [22, III Theorem 10.7] is assumed to be real-valued. However, a multiplication in (7) by \( e^{\pm 2i\phi} \) turns the eigenvalue problem (7) into a problem considered in [22, III Section 10] (with a shifted eigenvalue parameter). Then [22, III Theorem 10.7] holds for the shifted problem and, again by a multiplication with \( e^{\pm 2i\phi} \), we see that [22, III Theorem 10.7] is also valid for (7). Therefore, it remains only to show (14) and that in the limit-point case def \((A_{0\pm}(\tau_\pm) - \lambda) = 1 \) and (13) hold.

Observe that

\[ Q^*_- := \{ \bar{x} : x \in Q_- \} = Q_+ \]

and \( Q_\pm \) are convex sectors in the complex plane. Assume that their opening is \( \pi \); then we have for \( x \in \mathbb{R}_+ \) and for some \( k \in \mathbb{Z} \)

\[ -2\phi + 2k\pi = \frac{\pi}{2}(N + 2) + (N + 2)\phi. \]

This gives

\[ \phi = \frac{2k\pi}{N + 4} - \frac{(N + 2)\pi}{2N + 8}. \]

For \( x \in \mathbb{R}_- \) we obtain the same condition as \( Q^*_- = Q_+ \). But this condition is the condition for the limit-circle case and hence not possible, see Theorems 1 and 2. Therefore, the opening angle of \( Q_\pm \) is strictly less than \( \pi \) and we have

\[ Q_+ \cup Q_- \neq \mathbb{C}. \]  

(16)

We choose \( \lambda \in \mathbb{C} \setminus Q_\pm \). Because \( Q_\pm \) are sectors with two rays as boundary (which may coincide) the distance \( \delta(\lambda) \) between \( \lambda \) and \( Q_\pm \) is \( \delta(\lambda) = |K - \lambda| \), where \( K \) is a point of the boundary of \( Q_\pm \), i.e., \( K \in \{ e^{\pm 2i\phi} r : 0 < r < \infty \} \) or \( K \in \mathbb{R}_\pm := \{ -ix)^{N+2} e^{\pm(N+2)i\phi} : x \in \mathbb{R}_\pm \} \), cf. Fig. 3. There is a suitable angle \( \eta \in (-\pi, \pi) \) with

\[ \delta(\lambda) = |K - \lambda| = e^{i\eta}(K - \lambda). \]

The convexity of \( Q_\pm \) induces that the straight line

\[ \{ e^{\mp 2i\phi} r : r \in \mathbb{R} \} \text{ or resp. } \{ -(i)^{N+2} e^{\pm(N+2)i\phi} s : s \in \mathbb{R} \} \]

separates \( \lambda \) and \( Q_\pm \), cf. Fig. 3. Moreover we get after a rotation via the angle \( \eta \) that \( Q_\pm \) is located in the right half plane, cf. Fig. 4.

\[ \{ z = e^{i\eta} q : q \in Q_\pm \} \subset \mathbb{C}_{\Re \geq 0}. \]

We obtain

\[ \Re e^{i\eta} (e^{\mp 2i\phi} r - (i)^{N+2} e^{\pm(N+2)i\phi} K) \geq 0, \quad \text{for } 0 < r < \infty, x \in \mathbb{R}_\pm \]  

(17)

For \( \lambda \in \mathbb{C} \setminus Q_\pm \) we get for \( u \in \text{dom}(A_{0\pm}'\lambda) \) and \( \|u\| = 1 \)

\[ \lbrack \mathcal{B} \rbrack \text{ Springer} \]
Fig. 3 The line \( \{ e^{-2i\phi}r : r \in \mathbb{R} \} \) separates \( \lambda \) and \( Q_+ \).

Fig. 4 Rotation via the angle \( \eta \) and \( e^{i\eta}Q_+ \) lies in the right half plane

\[
\| (A'_{0\pm}(\tau_{\pm}) - \lambda) u \| \geq |(A'_{0\pm}(\tau_{\pm}) u, u) - \lambda| = \left| \int_0^\infty e^{\mp 2i\phi} u'' \overline{u} - (ix)^{N+2} e^{\mp (N+2)i\phi} |u|^2 \, dx - \lambda \right| = \left| \int_0^\infty e^{\mp 2i\phi} |u'|^2 - \lambda \right| \geq \text{Re} e^{i\eta} \left( \int_0^\infty e^{\mp 2i\phi} |u'|^2 - (ix)^{N+2} e^{\mp (N+2)i\phi} |u|^2 \, dx + K - \lambda \right)
\]

Now (17) implies

\[
\int_0^\infty \text{Re} e^{i\eta} \left( e^{\mp 2i\phi} |u'|^2 - (ix)^{N+2} e^{\mp (N+2)i\phi} |u|^2 - K |u|^2 \right) \, dx + \text{Re} e^{i\eta} (K - \lambda) \geq \delta(\lambda) > 0.
\]

Hence \( \mathbb{C} \setminus Q_\pm \subset \Pi(A'_{0\pm}(\tau_{\pm})) \) and in particular we have \( \Pi(A'_{0\pm}(\tau_{\pm})) \neq \emptyset \). Now we choose for \( y \in \text{dom} \, A_{0\pm}(\tau_{\pm}) \) a sequence \((x_n)_{n} \subset \text{dom} \, A'_{0\pm}(\tau_{\pm})\) such that \( x_n \to y \) and \( A'_{0\pm}(\tau_{\pm}) x_n \to A_{0\pm}(\tau_{\pm}) y \). Moreover, for \( \varepsilon > 0 \) choose \( n \) large enough, such that \( \| A'_{0\pm}(\tau_{\pm}) x_n - A_{0\pm}(\tau_{\pm}) y \| \leq \varepsilon \) and \( k(\lambda) \| x_n - y \| \leq \varepsilon \). Then we obtain
\[ \| (A_{0\pm}(\tau_{\pm}) - \lambda) y \| = \| (A_{0\pm}(\tau_{\pm}) - \lambda)(y - x_n) + (A'_{0\pm}(\tau_{\pm}) - \lambda)x_n \| \geq \| (A'_{0\pm}(\tau_{\pm}) - \lambda)x_n \| - \varepsilon \geq k(\lambda)\|x_n\| - \varepsilon \geq k(\lambda)\|y\| - 2\varepsilon, \]

and (14) follows. Moreover, from this and (16) we obtain (15).

Now we can apply [22, III Theorem 5.6] and obtain

\[ \dim \text{dom } (TA_{0\pm}(\tau_{\pm})T)/\text{dom } A_{0\pm}(\tau_{\pm}) = 2 \text{def } (A_{0\pm}(\tau_{\pm}) - \lambda) \]

and from the same result in [22] we have

\[ \text{dom } (TA_{0\pm}(\tau_{\pm})^*T) = \text{dom } A_{0\pm}(\tau_{\pm}) + \text{ker } ((A_{0\pm}(\tau_{\pm})^* - \overline{\lambda})(TA_{0\pm}(\tau_{\pm})^*T - \lambda)). \]

With \( A'_{0\pm}(\tau_{\pm}) = A_{max\pm}(\tau_{\pm})^+ = A_{max\pm}(\tau_{\pm}) \) and

\[ TA'_{0\pm}(\tau_{\pm})T = TA_{max\pm}(\tau_{\pm})T = A_{max\pm}(\tau_{\pm}) \]

we obtain

\[ \dim \text{dom } A_{max\pm}(\tau_{\pm})/\text{dom } A_{0\pm}(\tau_{\pm}) = 2 \text{def } (A_{0\pm}(\tau_{\pm}) - \lambda) \]

and

\[ \dim (A_{max\pm}(\tau_{\pm})) = \dim \text{dom } A_{0\pm}(\tau_{\pm}) + \dim \text{ker } ((TA_{max\pm}(\tau_{\pm})T - \overline{\lambda})(A_{max\pm}(\tau_{\pm}) - \lambda)). \quad (18) \]

Because \( \tau_{\pm} \) and \( \overline{\tau} \) are in the limit-point case, cf. Lemma 1, the equations \( (\tau_{\pm} - \lambda)u = 0 \) and \( (\overline{\tau}_{\pm} T - \overline{\lambda})u = 0 \), have only one solution in \( L^2(\mathbb{R}_\pm) \). Therefore, there is only one function \( u \) with \( (A_{max\pm}(\tau_{\pm}) - \lambda)u = 0 \). Moreover, we have from [22, III Theorem 5.6],

\[ \dim \text{dom } A_{max\pm}(\tau_{\pm})/\text{dom } A_{0\pm}(\tau_{\pm}) = 2 \text{def } (A_{0\pm}(\tau_{\pm}) - \lambda) \]

plus Eqs. (12) and (18), that \( \dim \text{ker } ((TA_{max\pm}(\tau_{\pm})T - \overline{\lambda})(A_{max\pm}(\tau_{\pm}) - \lambda)) \) is even and because of the limit-point case at most 2. Hence

\[ \dim \text{ker } ((TA_{max\pm}(\tau_{\pm})T - \overline{\lambda})(A_{max\pm}(\tau_{\pm}) - \lambda)) = 2, \]

and we obtain

\[ 2 = \dim \text{dom } A_{max\pm}(\tau_{\pm})/\text{dom } A_{0\pm}(\tau_{\pm}) = 2 \text{def } (A_{0\pm}(\tau_{\pm}) - \lambda). \]

\[ \square \]

With [22, III Theorem 10.13] the following proposition follows immediately:

**Proposition 1** We obtain in the limit-point case

\[ \text{dom } A_{0\pm}(\tau_{\pm}) = \{ w \in \text{dom } A_{0\pm}(\tau_{\pm}) : w(0) = w'(0) = 0 \} \]

and for \( u \in \text{dom } A_{max\pm}(\tau_{\pm}) \) and \( v \in \text{dom } A_{max\pm}(\tau_{\pm}^+) \)

\[ \lim_{x \to \pm \infty} (u\overline{v}' - u'\overline{v}) (x) = 0. \]
4 Maximal and minimal operators on the full axis

Here we define and study the maximal and the minimal operator on the real line. We do this by composition of the corresponding operators on the semi-axis from Sect. 3.

The maximal operator on $\mathbb{R}$ is given by

$$D_{\text{max}} := \{ w \in L^2(\mathbb{R}) : \tau_\pm w|_{\mathbb{R}_\pm} \in L^2(\mathbb{R}), w|_{\mathbb{R}_\pm}, w'|_{\mathbb{R}_\pm} \in AC_{\text{loc}}(\mathbb{R}_\pm) \}$$

and

$$A_{\text{max}} w(x) := \begin{cases} \tau_+ w(x), & x \geq 0, \\ \tau_- w(x), & x \leq 0. \end{cases}$$

or, what is the same,

$$A_{\text{max}} = A_{\text{max}}^-(\tau_-) \oplus A_{\text{max}}^+(\tau_+).$$

We define the parity $\mathcal{P}$. One has to be careful how to define it. In the literature it is quite often just defined by the (somehow sloppy) notion $x \mapsto -x$. More precisely, we have for a function $f \in L^2(\mathbb{R})$ with $f_+ := f|_{\mathbb{R}_+}$ and $f_- := f|_{\mathbb{R}_-}$

$$(\mathcal{P} f)(x) := \begin{cases} f_-(x) & \text{if } x \geq 0, \\ f_+(x) & \text{if } x < 0. \end{cases}$$

The parity $\mathcal{P}$ gives rise to a new inner product, which was considered in many papers; we mention here only [30–32,39]. It is the right inner product in which the operators exhibit symmetry properties, as we will show below:

$$[\cdot, \cdot] = (\mathcal{P} \cdot, \cdot).$$

**Lemma 2** For $v, w \in D_{\text{max}}$ we have

$$[A_{\text{max}} w, v] - [w, A_{\text{max}} v] = e^{2i\phi}((w'(0+)+\overline{v}(0)) + w(0+)) - e^{-2i\phi}((w'(0-)+\overline{v}(0)) + w(0-)).$$

**Proof** As $\tau_\pm = T \tau_\pm T$ (see (11)) we have $\overline{v}|_{\mathbb{R}_\pm} \in \text{dom } A_{\text{max}}(\tau_\pm)$. From

$$\tau_\pm w(-x) = \tau_\mp w(x),$$

we see that the function $x \mapsto \overline{w(-x)}$ for $x \in \mathbb{R}_\pm$ is in $\text{dom } A_{\text{max}}(\tau_\pm)$. Then Proposition 1 gives

$$\lim_{x \to \pm \infty} \overline{w(-x)} v'(x) - w'(-x) v(x) = 0. \quad (19)$$

We have

$$[A_{\text{max}} w, v] - [w, A_{\text{max}} v] = (\mathcal{P} A_{\text{max}} w, v) - (\mathcal{P} w, A_{\text{max}} v)$$

$$= \int_{-\infty}^0 \tau_+ w_-(x) \overline{\mathcal{P} v}(x) \, dx + \int_0^\infty \tau_- w_-(x) \overline{\mathcal{P} v}(x) \, dx - \int_{-\infty}^0 w_-(x) \tau_+ \overline{v}(x) \, dx - \int_0^\infty w_-(x) \tau_+ \overline{v}(x) \, dx$$

$$= \int_{-\infty}^0 \left( e^{2i\phi} w_-'(-x) - (-ix)^{N+2} e^{-2i\phi} w(-x) \right) \overline{\mathcal{P} v}(x) \, dx + \int_0^\infty \left( e^{-2i\phi} w_-'(-x) - (-ix)^{N+2} e^{2i\phi} w(-x) \right) \overline{\mathcal{P} v}(x) \, dx$$
We refer to the monographs [1,13]. We mention here only that the operator

\[ A \]


And Theorem 3 gives for \( \text{def} \) (\( \text{dom} \))

Then (19) (after taking the complex conjugate) shows the statement of the lemma.

Similar as the maximal operator on the real line, we define the minimal operator \( A_0 \) on the real line as the direct sum of the corresponding minimal operators on the half-axis:

\[ A_0 = A_{0-}(\tau_-) \oplus A_{0+}(\tau_+). \]

Observe that with Proposition 1 the domain of \( A_0 \) is given via

\[ \text{dom} \ A_0 = \{ w \in D_{\text{max}} : w(0+) = w(0-) = w'(0+) = w'(0-) = 0 \}. \]

And Theorem 3 gives for \( \lambda \in \Pi(A_0) = \Pi(A_{0-}(\tau_-)) \cap \Pi(A_{0+}(\tau_+)) \), which is by (15) non-empty,

\[ \text{def} \ (A_0 - \lambda) = \text{def} \ (A_{0-}(\tau_-) - \lambda) + \text{def} \ (A_{0+}(\tau_+) - \lambda) = 2. \]
5 Operator-based approach to $\mathcal{PT}$-symmetric Hamiltonians

In this section we define the operator $A$ corresponding to (5) and (7) on the full real axis with a coupling condition in 0. It is an extension of the minimal operator $A_0$ and a restriction of the maximal operator $A_{\text{max}}$, both studied in Sect. 4.

Here we restrict ourselves to a coupling of the form $w(0^+) = w(0^-)$ and $w'(0^+) = \alpha w'(0^-)$ in zero as we want $w$, and hence $y$ (see (5)), to be continuous. As we will see below, it is reasonable to allow a jump of $w'$ in 0. So we define for a fixed complex number $\alpha$ an extension $A$ of $A_0$ by

$$\text{dom} \,(A) := \{ w \in D_{\text{max}} : w(0^+) = w(0^-), \, w'(0^+) = \alpha w'(0^-) \}$$

$$Au := A_{\text{max}}u.$$

**Definition 2** We call a closed densely defined operator $A$ defined on $L^2(\mathbb{R})$ $\mathcal{PT}$-symmetric if and only if for all $f \in \text{dom} \, A$ we have $\mathcal{PT} f \in \text{dom} \, A$ and $\mathcal{PT} Af = A\mathcal{PT} f$, see also [28, III. 5.6].

**Theorem 4** Let $w \in \text{dom} \, A$ and let $y$ satisfy $w(x) = y(z(x))$, where $z$ is given by (6). Then we have

(i) $y'$ is continuous if and only if $\alpha = e^{2i\phi}$.

(ii) $A$ is $\mathcal{PT}$-symmetric if and only if $|\alpha| = 1$.

(iii) $A$ is self-adjoint with respect to $[\cdot, \cdot]$, if and only if $\alpha = e^{-4i\phi}$.

**Proof** We obtain

$$w'(x) = z'(x)y'(z(x)) = e^{i\phi \text{sgn}(x)}y'(z(x)),$$

for $x \neq 0$. Then $y'(0^+) = y'(0^-)$ is equivalent to

$$e^{-i\phi} w'(0^+) = y'(0^+) = y'(0^-) = e^{i\phi} w'(0^-).$$

This shows (i).

We choose $y \in \text{dom} \, A$ and obtain $\alpha(\mathcal{PT} y)'(0^-) = -\alpha y'(0^-)$, because of the definition of the action of $\mathcal{PT}$. From the matching condition in zero follows $y'(0^+) = \alpha y'(0^-)$ and again with the definition of $\mathcal{PT}$ we get $\alpha y'(0^-) = -\alpha(\mathcal{PT} y)'(0^+)$. In conclusion with $y \in \text{dom} \, A$,

$$\mathcal{PT} y(0^+) = y(0^-) = y(0^+) = \mathcal{PT} y(0^-)$$

and

$$\alpha(\mathcal{PT} y)'(0^-) = -\alpha y'(0^+) = -\alpha \alpha y'(0^-) = |\alpha|^2 (\mathcal{PT} y)'(0^+)$$

we get $\mathcal{PT} y \in \text{dom} \, A$ if and only if $|\alpha| = 1$. Moreover, for $x > 0$ we have

$$\mathcal{PT} Ay(x) = -e^{2i\phi} \sqrt{x} y'(-x) - e^{-(N+2)i\phi} (ix)^{N+2} y(-x) = A\mathcal{PT} y(x)$$

A similar calculation holds for $x < 0$ and (ii) follows.

It remains to show (iii). From Lemma 2 follows that $A$ is $[\cdot, \cdot]$-symmetric. Because def $(A_0 - \lambda) = 2$ (see (20)) and $A$ is a two-dimensional extension of $A_0$, $A$ is $[\cdot, \cdot]$-self-adjoint.

Obviously, the coupling condition $\alpha$ in zero satisfies simultaneously items (i), (ii), (iii) from Theorem 4 if and only if $\phi = \pm \frac{\pi}{4}$. We refer to [11] for similar considerations of coupling constants in the case of coupled quantum systems.

**Proposition 3** Let $\lambda \in \sigma_p(A)$ and let $|\alpha| = 1$, which implies $\mathcal{PT}$-symmetry for $A$, see Theorem 4. If $y$ is the corresponding eigenfunction, then $\mathcal{PT} y$ is also an eigenfunction for $\tilde{\lambda}$.

**Proof** From $y \in \text{dom} \, A$ it follows that $\mathcal{PT} y \in \text{dom} \, A$ and $A\mathcal{PT} y = \mathcal{PT} Ay = \mathcal{PT} \lambda y = \tilde{\lambda} \mathcal{PT} y$. □
The following theorem is our main result:

**Theorem 5** Let $\alpha = e^{-4i\phi}$. We assume $\phi \neq 0$ and we assume that one of the following two conditions is satisfied:

- If $\phi > 0$, then there exists a natural number $k$, $k \geq 0$, with
  \[
  \frac{2k\pi}{N+2} - \frac{\pi}{2} < \phi < \frac{2k\pi}{N+2} - \frac{\pi}{2}.
  \]
- If $\phi < 0$, then there exists $k \in \mathbb{Z}$, $k \leq 0$, with
  \[
  \frac{(2k-1)\pi}{N+2} - \frac{\pi}{2} < \phi < \frac{2k\pi}{N+2} - \frac{\pi}{2}.
  \]

Then $A$ is $[\cdot, \cdot]$-self-adjoint and $\mathcal{PT}$-symmetric with $\rho(A) \neq \emptyset$, and $\sigma(A) = \sigma_p(A)$.

The spectrum of $A$ is symmetric to the real line; it consists only of discrete eigenvalues of finite algebraic multiplicity with no finite accumulation point and $\dim \ker (A - \lambda) = 1$ for $\lambda \in \sigma_p(A)$.

**Proof** The self-adjointness and the $\mathcal{PT}$-symmetry follow from Theorem 4. In order to show that the resolvent set of $A$ is non-empty, we introduce two auxiliary operators $A_{\pm}$ via

\[
\text{dom } A_{\pm} := \{w \in \text{dom } A_{\text{max}}(\tau_{\pm}) : w(0) = 0\}, \quad A_{\pm}w(x) := \tau_{\pm}w(x)
\]

From [15, Theorems 4.4 and 4.5] we know that the spectrum consists at most of isolated eigenvalues with finite algebraic multiplicity and it is located in the set $Q_{\pm}$,

\[
\sigma(A_{\pm}) = \sigma_p(A_{\pm}) \subset Q_{\pm}.
\]  \hfill \text{(21)}

In particular, the essential spectrum is empty.

The assumption on $\phi$ implies that for $\phi > 0$ we obtain $\sin((N + 2)\phi + (N + 2)\frac{\pi}{2}) > 0$ and, hence, $\text{Im} \left(-(ix)^{N+2}e^{(N+2)i\phi}\right) < 0$. As $\phi > 0$, it is, by definition, in the interval $(0, \pi/2)$, we have $\text{Im} e^{-2i\phi} < 0$ and, therefore, $Q_+$ is contained in the lower half plane.

If $\phi < 0$ we have $\text{Im} \left(-(ix)^{N+2}e^{(N+2)i\phi}\right) > 0$ and $\text{Im} e^{-2i\phi} > 0$ and $Q_+$ is contained in the upper half plane. As $Q_- = Q_+^*$, we obtain $Q_+ \cap Q_- = \{0\}$.

**Claim** For $\lambda \notin \sigma_p(A_+) \cup \sigma_p(A_-)$ we have $v_{\lambda, +}(0) \neq 0$ and $v_{\lambda, -}(0) \neq 0$, where $v_{\lambda, +}$ and $v_{\lambda, -}$ are the non-zero $L^2$-solutions of $(\tau_{\pm} - \lambda)v = 0$. In this case

\[
\lambda \in \sigma_p(A) \iff \frac{v'_{\lambda, +}(0)}{v_{\lambda, +}(0)} = e^{-4i\phi} \frac{v'_{\lambda, -}(0)}{v_{\lambda, -}(0)}.
\]  \hfill \text{(22)}

**Proof of the claim** Suppose that the right-hand side of (22) holds. Set

\[
v(x) := \begin{cases} 
  v_{\lambda, +}(x), & x \geq 0 \\
  v_{\lambda, -}(0), & x < 0;
\end{cases}
\]

then $v(0+) = v(0-)$ and

\[
v'(0-) = \frac{v_{\lambda, +}(0)}{v_{\lambda, -}(0)} v'_{\lambda, -}(0) = e^{4i\phi} v'_{\lambda, +}(0) = e^{4i\phi} v'(0+).
\]
So we have \( v \in \text{dom } A \) and \( \lambda \in \sigma_p(A) \).

To prove the converse choose an eigenfunction \( v \in \text{dom } A \) corresponding to the eigenvalue \( \lambda \). Due to the limit point case there exist constants with \( v|_{\partial \gamma} = \alpha_{\pm}v_{\lambda,\pm} \). Hence \( v(0) = \alpha_+v_{\lambda,+}(0) = \alpha_-v_{\lambda,-}(0) \) and \( \alpha_+v'_{\lambda,+}(0) = v'(0+) = e^{-4i\phi}v'(0-) = e^{-4i\phi}\alpha_-v'_{\lambda,-}(0) \) and we obtain
\[
\frac{v'_{\lambda,+}(0)}{v_{\lambda,+}(0)} = \frac{\alpha_+v'_{\lambda,+}(0)}{\alpha_+v_{\lambda,+}(0)} = e^{-4i\phi}\frac{\alpha_-v'_{\lambda,-}(0)}{\alpha_-v_{\lambda,-}(0)} = e^{-4i\phi}v'_{\lambda,-}(0)
\]
and the claim is proved.

We continue with the proof of Theorem 5. We have \( Q_+ \cap Q_- = \{0\} \) and, hence, by (21) we find \( \lambda \in \sigma(A_+) \setminus \sigma(A_-) \). Then we have for \( v_{\lambda,+}, v_{\lambda,-} \) as in the claim from above that \( v_{\lambda,+}(0) = 0 \) and \( v_{\lambda,-}(0) \neq 0 \). According to the uniqueness theorem \( v'_{\lambda,+}(0) \neq 0 \) holds. Moreover, \( \lambda \) is an isolated singularity of the function \( \lambda \mapsto \frac{v'_{\lambda,+}(0)}{v_{\lambda,+}(0)} \). Recall that \( v_{\lambda,+} \) depends holomorphic on \( \lambda \), cf. [26, Theorem 3.4.2.]. But the right-hand side of (22) has no singularity at \( \lambda \). Hence there exists an open set \( O \) with \( O \cap \sigma(A) = \emptyset \) due to the claim above. It is easy to see that \( \lambda \) is an eigenvalue of \( A_- \) but, due to the fact that the opening of \( Q_+ \) is less than \( \pi \), cf. Theorem 3, \( \lambda \) is no eigenvalue of \( A_+ \). We obtain with the same arguments from above \( O^* := \{ \lambda \in O : \sigma(A) \} \) with \( (O \cup O^*) \cap \sigma(A) = \emptyset \), so \( (O \cup O^*) \cap \sigma(A) = \emptyset \).

Now assume that \( \rho(A) = \emptyset \), that is, \( \sigma(A) = \mathbb{C} \). If \( \lambda \) is a point from the residual spectrum of \( A \) (i.e., the operator \( A - \lambda \) has zero kernel but a non-dense range), then [13, VI Theorem 6.1] implies \( \lambda \in \sigma_p(A) \). Therefore, \( O \cup O^* \subset \sigma_c(A) \),
\[
(23)
\]
where \( \sigma_c(A) \) denote the set of all \( \lambda \in \mathbb{C} \) such that the operator \( A - \lambda \) has zero kernel and a dense but non-closed range. We choose now \( \lambda \in (O \cup O^*) \cap \rho(A_+ \cap A_-) \). Then we have \( \lambda \in \rho(A_- \oplus A_+) \). As \( A_- \oplus A_+ \subset A_{\max} \), we see \( \text{ran } (A_{\max} - \lambda) = L^2(\mathbb{R}) \). As the minimal operator \( A_0 \) is the direct sum of two closed operators (cf. Theorem 3) it is a closed operator. With \( \rho(A_\pm) \subset \Pi(A_\pm) \subset \Pi(A_{0\pm}) \) we get \( \lambda \in \Pi(A_0) \) and from (20) we obtain
\[
\text{def } (A_0 - \lambda) = 2;
\]

hence the operator \( A_0 - \lambda \) has a closed range. As \( A_0 \subset A \) and \( \text{dim } A/A_0 = 2 \) also the range of \( A - \lambda \) is closed, a contradiction to (23) and we have \( \rho(A) \neq \emptyset \). Moreover, we have for \( \lambda \in \rho(A) \cap \rho(A_- \oplus A_+) \)
\[
\text{rank } ((A - \lambda)^{-1} - (A_- \oplus A_+ - \lambda)^{-1}) \leq 2
\]
and thus the essential spectra coincide, cf. [22, IX Theorem 2.4].

According to limit-point/limit-circle classification we have for \( \lambda \in \sigma_p(A) \)
\[
\text{dim ker } (A - \lambda) = 1.
\]
The symmetry of the spectrum follows from Proposition 3.

\[\square\]

6 Conclusion

Summing up, our main results include

1. A limit-point/limit-circle classification of (3) and (4), plus a mathematical meaning of Stokes wedges and Stokes lines, which is the limit-point/limit-circle classification.
2. The operator \( A \), which corresponds to the full axis problem (2) with a coupling condition in zero, is self-adjoint in the inner product \([\cdot, \cdot]\) and it is \(PT\)-symmetric.
3. The spectrum of \( A \) consists at most of isolated eigenvalues with finite algebraic multiplicity, the essential spectrum is empty and \( A \) has a non-empty resolvent set.

Compliance with ethical standards

Conflict of interest On behalf of all authors, the corresponding author states that there is no conflict of interest.
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