On the S-matrix of Schrödinger operators with non-symmetric zero-range potentials

P A Cojuhari, A Grod and S Kuzhel

1 AGH University of Science and Technology, 30-059 Krakow, Poland
2 Institute of Mathematics of the National Academy of Sciences of Ukraine, Kiev, Ukraine

E-mail: cojuhari@agh.edu.pl, andriy.grod@yandex.ua and kuzhel@mat.agh.edu.pl

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Abstract
Non-self-adjoint Schrödinger operators $A_\varepsilon$ which correspond to non-symmetric zero-range potentials are investigated. We show that various properties of $A_\varepsilon$ (eigenvalues, exceptional points, spectral singularities and the property of similarity to a self-adjoint operator) are completely determined by poles of the corresponding S-matrix.

Keywords: poles of S-matrix, similarity to a self-adjoint operator, exceptional points
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1. Introduction

This work was inspired by an intensive development of pseudo-Hermitian quantum mechanics (PHQM) during the past few decades [1]. The key point of this theory is the employment of non-self-adjoint operators for the description of experimentally observable data. Briefly speaking, a given non-self-adjoint operator $A$ in a Hilbert space $H$ can be interpreted as a physically meaningful Hamiltonian if its spectrum is real and there exists a new inner product that ensures the (hidden) self-adjointness of $A$.

As usual, in PHQM studies, a non-self-adjoint operator $A$ admits a representation $A = A_0 + V$, where $A_0$ is an (unperturbed) self-adjoint operator in $H$ and $V$ is a non-symmetric potential characterized by a set $\mathcal{Y} = \{\varepsilon\}$ of complex parameters $\varepsilon$. One of the most important problems is the description of quantitative and qualitative changes of spectrum $\sigma(A)$ when $\varepsilon$ runs $\mathcal{Y}$. A typical evolution of properties is the following:
An operator from domain I cannot be realized as a self-adjoint operator for any choice of inner product, while an operator from domain III turns out to be self-adjoint with respect to a new inner product of $\mathcal{H}$ which is equivalent to the initial one. Domain II can be interpreted as a boundary between I and III and the corresponding operators will keep only part of the properties of I and III. For instance, if an operator $A$ corresponds to II, then its spectrum is real (similar to III) but $A$ cannot be made self-adjoint by an appropriate choice of equivalent inner product of $\mathcal{H}$ (in spirit of I). This phenomenon deals with the appearance of ‘wrong’ spectral points of $A$ which are impossible for the spectra of self-adjoint operators. Traditionally, these spectral points are called exceptional points if they are located at the discrete spectrum of $A$ and spectral singularities, in the case of the continuous spectrum.

In the present paper, we show that the evolution of spectral properties (1.1) can be successfully and easily described in terms of poles of $S$-matrices of operators $A$. We illustrate this point by considering the set of operators $A$ generated by the Schrödinger type differential expression

$$A = -\frac{d^2}{dx^2} + V$$

with zero-range potential

$$V = a < \delta, \cdot > + b < \delta', \cdot > + c < \delta', \delta > + d < \delta', \delta' >,$$

where $\delta$ and $\delta'$ are, respectively, the Dirac $\delta$-function and its derivative and $a, b, c, d$ are complex numbers.

The Schrödinger operator with zero-range potential fits well the Lax–Phillips scattering scheme [5] since the potential is concentrated at one point (so-called 0-perturbations [6]). In that case the $S$-matrix (the Lax–Phillips scattering matrix) of $A$ coincides with the meromorphic matrix-valued function

$$S(k) = \left[ \sigma_0 - 2(1 - ik)\Sigma \right]^{-1} \left[ \sigma_0 - 2(1 + ik)\Sigma \right], \quad k \in \mathbb{C}, \quad \sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

(1.2)

where $(2 \times 2)$-matrix $\Sigma$ is expressed in terms of parameters $a, b, c, d$ and it determines the domain of definition of $A$ (see (2.6)). If the matrix $\Sigma$ is Hermitian, then the corresponding operator $A = A_\Sigma$ is self-adjoint and the $S$-matrix (1.2) is the direct consequence of mathematically rigorous arguments of scattering theory: establishing the existence of wave operators with subsequent representation of the scattering operator in the spectral representation of unperturbed dynamics [7]. In the case of a non-self-adjoint operator $A_\Sigma$ we define the $S$-matrix by analogy, considering an arbitrary matrix $\Sigma$ in (1.2) and do not take care about auxiliary mathematical constructions (see [8, 9] for details). We found this definition useful because a) the formula (1.2) for the $S$-matrix enables us to determine explicitly the matrix $\Sigma$ characterizing the operator $A_\Sigma$; b) the formula (1.2) can be easily rewritten in terms of right/left reflection and transmission coefficients of the corresponding traveling wave functions (cf. subsection 2.4).

The Lax–Phillips scattering scheme allows us to define $S$-matrices for Schrödinger operators with local (i.e., the support of potential is a bounded interval) non-symmetric potentials. The obtained formulas are similar to (1.2) and they can also be rewritten via
reflection/transmission coefficients [9]. We believe that such an interpretation of the $S$-matrix that comes from the Lax–Phillips scattering theory makes it possible to establish more a informative connection between poles of the $S$-matrix and spectral properties of Schrödinger operators with local non-symmetric potentials.

In this paper, using the decomposition of the $S$-matrix (1.2) with respect to the Pauli matrices (subsection 2.3), we show that the location of poles of the $S$-matrix $S(\cdot)$ completely determines the spectral properties of non-self-adjoint operators $A_T$ outlined in (1.1).

Our proof of the similarity of $A_T$ to a self-adjoint operator in section 3 does not contain an algorithm of the construction of an appropriate metric operator $e^{Q}$ which guarantees the self-adjointness of $A_T$. However, in the particular case where the $S$-matrix of a non-self-adjoint operator $A_T$ has simple imaginary poles, we ‘guessat’ an explicit expression of the metric operator (section 4). Sections 5 and 6 are devoted to spectral singularities and exceptional points, respectively.

Throughout the paper $D(A)$ denotes the domain and $\text{ker}A$ denotes the null-space of a linear operator $A$. The resolvent set and the spectrum of $A$ are denoted by $\rho(A)$ and $\sigma(A)$, respectively.

2. Schrödinger operator with non-symmetric zero-range potentials

2.1. Preliminaries

A one-dimensional Schrödinger operator with general zero-range potential at the point $x = 0$ can be defined by the formal expression

$$-rac{d^2}{dx^2} + a < \delta, \cdot > \delta(x) + b < \delta', \cdot > \delta(x) + c < \delta, \cdot > \delta'(x) + d < \delta', \cdot > \delta'(x), \tag{2.1}$$

where $\delta$ and $\delta'$ are, respectively, the Dirac $\delta$-function and its derivative (with support at 0) and $a, b, c, d$ are complex numbers. Using the regularization method suggested in [10], a direct relationship between parameters $a, b, c, d$ of the singular potential

$$V = a < \delta, \cdot > \delta(x) + b < \delta', \cdot > \delta(x) + c < \delta, \cdot > \delta'(x) + d < \delta', \cdot > \delta'(x) \tag{2.2}$$

and operator-realizations of (2.1) in the Hilbert space $L_2(\mathbb{R})$ can be established [11]. Precisely, the formal expression (2.1) gives rise to the operator

$$A_T = -\frac{d^2}{dx^2}, \quad T = \begin{pmatrix} a & b \\ c & d \end{pmatrix}. \tag{2.3}$$

defined on smooth functions $f \in W^2_2(\mathbb{R} \setminus \{0\})$ which satisfy the boundary condition

$$T \begin{pmatrix} f(0 + ) + f(0 - ) \\ -f'(0 + ) - f'(0 - ) \end{pmatrix} = \begin{pmatrix} f'(0 + ) - f'(0 - ) \\ f(0 + ) - f(0 - ) \end{pmatrix}. \tag{2.4}$$

Remark 2.1. The matrix $T$ in (2.4) relates the mean values of functions $f, f'$ at point 0 with their jumps. Another description of point interaction at point 0 can be given by the matching conditions
which connect the left-side and the right-side boundary values of the functions \( f, f' \) at point 0 [12]. The sets of operators defined via the boundary conditions (2.4) and (2.5) do not coincide. For instance, in view of (2.4), the operator \( A_T \) with \( T = \begin{pmatrix} 0 & -2 \\ 2 & 0 \end{pmatrix} \) is defined on functions \( f \in W^2_2(\mathbb{R}\setminus\{0\}) \) with boundary condition \( f(0-) = f'(0-) = 0 \) that cannot be realized with the use of (2.5).

2.2. Definition and elementary properties of S-matrix

The S-matrix \( S(\cdot) \) of \( A_T \) can be directly expressed in terms of \( T \) since the potential \( V \) is supported at point 0. However, the obtained formula looks quite cumbersome. Having simplification of the expression for \( S(\cdot) \) in mind, we rewrite the boundary condition (2.4) in the form

\[
\mathcal{T}
\begin{pmatrix}
 f(0^+) + f'(0^+)
 f(0^-) - f'(0^-)
\end{pmatrix}
= \frac{1}{2}
\begin{pmatrix}
 f(0^+)
 f(0^-)
\end{pmatrix},
\mathcal{T} = \begin{pmatrix} 1_{11} & 1_{12} \\ 1_{21} & 1_{22} \end{pmatrix}
\]

(2.6)

It should be noted that the set of operators \( A_T = -\frac{d^2}{dx^2} \) determined by the boundary condition (2.6) does not coincide with the set of operators \( A_T \) defined by (2.3), (2.4). Namely, the domain of definition of \( A_T \) is characterized by (2.6) if and only if \(-1\) does not belong to the point spectrum of \( A_T \) or, that is equivalent [13], if

\[
\mathcal{E} = 4 - \det T + 2(a - d) \neq 0, \quad \det T = ad - bc.
\]

(2.7)

In that case, it is easy to verify by comparing (2.4) and (2.6) that the matrix \( \mathcal{T} \) is expressed directly in terms of \( T \)

\[
\mathcal{T} = \frac{1}{4\mathcal{E}} \begin{pmatrix}
 \mathcal{E} + 2(b + c - a - d) & 4 + \det T - 2(b - c) \\
 4 + \det T + 2(b - c) & 4 - 2(b + c + a + d) 
\end{pmatrix}
\]

(2.8)

On the other hand, not every operator \( A_T \) can be rewritten as \( A_T \) (for example \( A_T \) with \( \mathcal{E} = 0 \) does not belong to the set of operators \( A_T \)).

The operators \( A_T \) fit well the Lax–Phillips scattering scheme and the corresponding S-matrix of \( A_T \) coincides with the matrix-valued function

\[
S(k) = \begin{bmatrix}
\sigma_0 - 2(1 - ik)\mathcal{E} & \sigma_0 - 2(1 + ik)\mathcal{E}^{-1} \\
0 & 1
\end{bmatrix}, \quad \sigma_0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}
\]

(2.9)

determined for all \( k \in \mathbb{C}_+ = \{ k \in \mathbb{C} : \text{Im} \ k > 0 \} \) where (2.9) is well posed [8, 9].

The expression (2.9) enables to determine the S-matrix \( S(\cdot) \) of \( A_T \) for any \((2 \times 2)\)-matrix \( \mathcal{E} \). In the particular case where \( \mathcal{E} \) admits the representation (2.8) (i.e., the matrix \( \mathcal{E} \) can be expressed via \( T \) and hence, \( A_T \equiv A_T \) we will say that \( S(\cdot) \) is the S-matrix of \( A_T \).

Remark 2.2.

(i) In the Lax–Phillips scattering scheme the free evolution is determined by the Friedrichs extension of the symmetric operator

\[
A_s = -\frac{d^2}{dx^2}, \quad \mathcal{D}(A_s) = \left\{ f \in W^2_2(\mathbb{R}\setminus\{0\}) : f(0^+) = f(0^-) = 0, f'(0^+) = f'(0^-) = 0 \right\}
\]

(2.10)

associated with the given differential expression (2.1). Namely, the Friedrichs extension
coincides with the operator

\[ A_f = -\frac{d^2}{dx^2}, \quad \mathcal{D}(A_f) = \left\{ f \in W^2_2\left(\mathbb{R}\backslash\{0\}\right) : f(0^+) = f(0^-) = 0 \right\}. \quad (2.11) \]

The self-adjoint operator \( A_f \) is determined by \( \mathcal{I} = 0 \) in (2.6). Thus, the matrix \( \mathcal{I} \) characterizes 'a deviation' of \( A_f \) from the unperturbed Hamiltonian \( A_f \). In a sense, this explains why the matrix \( \mathcal{I} \) (rather than \( T \)) appears in (2.9).

(ii) The self-adjoint operator

\[ A_k = -\frac{d^2}{dx^2}, \quad \mathcal{D}(A_k) = \left\{ f \in W^2_2\left(\mathbb{R}\backslash\{0\}\right) : f'(0^+) = f'(0^-) = 0 \right\} \quad (2.12) \]

is determined by \( \mathcal{I} = \frac{1}{2}\sigma_0 \) in (2.6) and it is the Krein extension of the symmetric operator \( A_s \). Similarly to the Friedrichs extension \( A_f \), the Krein extension \( A_k \) determines a free evolution in the Lax–Phillips scattering scheme [14]. The corresponding \( S \)-matrices are: \( S(k) = \sigma_0 \) for \( A_f \) and \( S(k) = -\sigma_0 \) for \( A_k \).

(iii) The expression (2.9) determines the \( S \)-matrix for \( A_s \) only in the case where \(-1 \in \rho(A_f)\).

It turns out that the formula (2.9) and the results below can be easily modified for any operator \( A \) with a nonempty resolvent set.

It follows from (2.9) that the \( S \)-matrix \( S(\cdot) \) is a meromorphic matrix-function on \( \mathbb{C}_+ \). It can be established that poles of \( S(\cdot) \) correspond to eigenvalues of \( A_f \). Precisely, \( k \in \mathbb{C}_+ \) is a pole of \( S(\cdot) \) if and only if \( k^2 \) is an eigenvalue of \( A_f \) [13]. The formula (2.9) allows us to extend the definition of \( S \)-matrix of \( A_f \) to all complex numbers \( k \in \mathbb{C} \). Obviously, the extended \( S \)-matrix remains a meromorphic matrix-function.

We will say that \( S(\cdot) \) has a pole at infinity if at least one of entries of \( S(k) \) tend to infinity when \( k \to \infty \). We will say that \( S(k) \) is defined on the physical sheet if \( k \in \mathbb{C}_+ \) and \( S(k) \) is defined on the nonphysical sheet if \( k \in \mathbb{C}_- = \{ k \in \mathbb{C} : \text{Im } k < 0 \} \).

According to the above discussion the discrete spectrum of \( A_f \) is completely determined by the corresponding \( S \)-matrix on the physical sheet \( \mathbb{C}_+ \).

2.3. The presentations of \( S \)-matrix with the use of Pauli matrices

The \( S \)-matrix for a non-self-adjoint operator \( A_f \) may have new unusual properties. For this reason, an additional representation of \( S(\cdot) \) can be useful. First of all, we are interested in the decomposition of \( S(\cdot) \) with respect to the Pauli matrices

\[ \sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_i = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \]

Let \( X \) be an arbitrary \((2 \times 2)\)-matrix. Then \( X \) admits the presentation \( X = \sum_{j=1}^{3} x_j \sigma_j \), where \( x_j \in \mathbb{C} \). In that case

\[ \det X = x_0^2 - \sum_{j=1}^{3} x_j^2 \quad \text{and} \quad X^{-1} = \frac{1}{\det X} \left( x_0 \sigma_0 - \sum_{j=1}^{3} x_j \sigma_j \right). \quad (2.13) \]

In particular, if \( X = \sigma_0 - 2(1 + ik)\mathcal{I} \), then

\[ \det \left( \sigma_0 - 2(1 + ik)\mathcal{I} \right) = 4(1 + ik)^2 \det \mathcal{I} - 4(1 + ik) \gamma_0 + 1 \quad (2.14) \]
\[
\sigma_0 - 2(1 + ik) \Sigma^{-1} = \frac{(1 - 2(1 + ik)\gamma_j)\sigma_0 + 2(1 + ik) \sum_{j=1}^{3} \gamma_j \sigma_j}{4(1 + ik)^2 \det \Sigma - 4(1 + ik)\gamma_0 + 1}, \tag{2.15}
\]

where \( \gamma_j \in \mathbb{C} \) are determined uniquely by the decomposition

\[
\Sigma = \sum_{j=0}^{3} \gamma_j \sigma_j, \quad \text{and} \quad \det \Sigma = \gamma_0^2 - \sum_{j=1}^{3} \gamma_j^2.
\]

Substituting (2.15) into (2.9) and making elementary calculations we obtain another representation of \( S \)-matrix of \( A_\Sigma \)

\[
S(k) = \sigma_0 + \text{4ik} \frac{\Sigma - 2(1 + ik)\det \Sigma \sigma_0}{4(1 + ik)^2 \det \Sigma - 4(1 + ik)\gamma_0 + 1}.
\tag{2.16}
\]

The general formula (2.16) can be simplified if we will consider separately the cases \( \det \Sigma \neq 0 \) and \( \det \Sigma = 0 \). Denote \( \theta_+ = 2(1 + ik) \) and assume that \( \det \Sigma \neq 0 \). Then

\[
4(1 + ik)^2 \det \Sigma - 4(1 + ik)\gamma_0 + 1 = \frac{(\theta_+ - \theta_-)(\theta_+ - \theta_-)}{\theta_+ \theta_-},
\tag{2.17}
\]

where

\[
\theta_+ = \frac{1}{\gamma_0 + \sqrt{\sum_{j=1}^{3} \gamma_j^2}}, \quad \theta_- = \frac{1}{\gamma_0 - \sqrt{\sum_{j=1}^{3} \gamma_j^2}}, \quad \det \Sigma = \frac{1}{\theta_+ \theta_-}.
\tag{2.18}
\]

Therefore, (2.16) can be rewritten as

\[
S(k) = \sigma_0 + \text{4ik} \frac{\theta_+ \theta_- \Sigma - \theta_- \sigma_0}{(\theta_+ - \theta_-)(\theta_+ - \theta_-)}. \tag{2.19}
\]

The decomposition of \( S(k) \) with respect to the Pauli matrices has the form

\[
S(k) = \sum_{j=0}^{3} s_j(k) \sigma_j, \tag{2.20}
\]

where

\[
s_0(k) = 1 + \text{4ik} \frac{\theta_+ \theta_- \gamma_0 - \theta_-}{(\theta_+ - \theta_-)(\theta_+ - \theta_-)}, \quad s_j(k) = \text{4ik} \frac{\theta_+ \gamma_j}{(\theta_+ - \theta_-)(\theta_+ - \theta_-)}, \quad j \geq 1. \tag{2.21}
\]

Let \( \det \Sigma = 0 \). Then at least one of \( \theta_- \) is equal to \( \infty \) and (2.19) is reduced to

\[
S(k) = \sigma_0 + \frac{\text{4ik}}{1 - \frac{2\theta_+ \gamma_0}{\theta_-}}. \tag{2.22}
\]

Sometimes it is useful to calculate the \( S \)-matrix directly in terms of coefficients \( a, b, c, d \) of the initial singular potential (2.2). This means that we consider the particular case where \( A_\Sigma \equiv A_\Sigma \) and \( \Sigma \) is defined by (2.8). In that case the coefficients \( \gamma_j \) of the decomposition \( \Sigma = \sum_{j=0}^{3} \gamma_j \sigma_j \) have the form
\[
\gamma_0 = \frac{1}{4\Xi} (\Xi - 2(a + d)), \\
\gamma_2 = -\frac{i}{2\Xi} (b - c), \\
\gamma_3 = \frac{1}{2\Xi} (b + c),
\]

(2.23)

where \( \Xi = 4 - \det T + 2(a - d) \). Furthermore, the identities

\[
\det \Xi = -\frac{d}{2\Xi}, \quad \sum_{j=1}^3 f_j^2 = \frac{(4 + \det T)^2 + 16bc}{16\Xi^2}
\]

(2.24)

are deduced directly from (2.8) and (2.23). Substituting the obtained relations into (2.16) we obtain the expression of \( S(\cdot) \) in terms of the coefficients \( a, b, c, d \). In particular, if \( d = 0 \), then \( \det \Xi = 0 \) and the expression (2.16) is reduced to

\[
S(k) = \sigma_0 + \frac{4ik\Xi}{2a(1 + ik) - ik\Xi}.
\]

(2.25)

**Example I.** \( \delta \)-potential with a complex coupling. Let \( a \in \mathbb{C} \) and \( b = c = d = 0 \). Then (2.1) takes the form

\[
-\frac{d^2}{dx^2} + a < \delta, \cdot > \delta(x), \quad a \in \mathbb{C}
\]

and (2.4) determines the operators \( A_T \equiv A_a = -\frac{\delta^2}{\delta x^2} \) with domains of definition

\[
\mathcal{D}(A_a) = \left\{ f \in W^2_2(\mathbb{R} \setminus \{0\}) \mid \begin{cases} f(0+) = f(0-) \ (\equiv f(0)) \\
 f'(0+) - f'(0-) = af(0) \end{cases} \right\}
\]

The matrix \( \Xi \) in (2.8) and \( \Xi \) are

\[
\Xi = \frac{1}{4 + 2a} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad \Xi = 4 + 2a.
\]

By virtue of (2.25),

\[
S(k) = \frac{1}{2k + ia} \begin{pmatrix} ia & -2k \\ -2k & ia \end{pmatrix}.
\]

**Example II.** Mixed complex \( \delta \)-potential. Let \( b \in \mathbb{C} \) and \( a = c = d = 0 \). Then (2.1) is reduced to

\[
-\frac{d^2}{dx^2} + b < \delta, \cdot > \delta(x), \quad b \in \mathbb{C}
\]

and the domains of definition of the corresponding operators \( A_T \equiv A_b = -\frac{\delta^2}{\delta x^2} \) take the form

\[
\mathcal{D}(A_b) = \left\{ f \in W^2_2(\mathbb{R} \setminus \{0\}) \mid \begin{cases} f(0+) = f(0-) \ (\equiv f(0)) \\
(2 + b)f'(0+) = (2 - b)f'(0-) \end{cases} \right\}
\]

The matrix \( \Xi \) and \( \Xi \) are

\[
\Xi = \frac{1}{8} \begin{pmatrix} 2 + b & 2 - b \\ 2 + b & 2 - b \end{pmatrix}, \quad \Xi = 4.
\]

Using (2.25) again we obtain

\[
S(k) = \frac{-1}{2} \begin{pmatrix} b & 2 - b \\ 2 + b & -b \end{pmatrix}
\]

**Example III.** The case where the S-matrix is a constant on \( \mathbb{C} \). The S-matrices of operators \( A_b \) in example II do not depend on \( k \) and they are constants on \( \mathbb{C} \).
Let \( A \) be an operator defined by \( 2.6 \) and let \( S_T(\cdot) \) be the corresponding \( S \)-matrix. An elementary analysis of \( 2.19, 2.21, \) and \( 2.22 \) shows that \( S_T(k) \) does not depend on \( k \in \mathbb{C} \) if and only if \( \mathcal{T} = 0, \mathcal{T} = \tau \sigma_0 \), or

\[
\mathcal{T} = \frac{1}{4} \sigma_0 + \sum_{j=1}^{3} \gamma_j \sigma_j \quad \text{where} \quad \sum_{j=1}^{3} \gamma_j^2 = \frac{1}{16}.
\]

In these cases, respectively,

\[
S_0(k) = \sigma_0, \quad S_{-\tau}(k) = -\sigma_0, \quad S_\tau(k) = -4 \sum_{j=1}^{3} \gamma_j \sigma_j.
\]

Assume now that the matrix \( \mathcal{T} \) can be expressed via \( T \) and hence, \( T \equiv A \). Using \( 2.23, 2.24, \) and \( 2.25 \), we conclude that the \( S \)-matrix \( S_T(k) \) of \( A_T \) is a constant on \( C \) if and only if \( a = d = 0 \).

2.4. The presentation of \( S \)-matrix in terms of transmission and reflection coefficients

The expression \( 2.9 \) of the \( S \)-matrix was obtained within the framework of the Lax–Phillips scattering theory and, certainly, it looks quite unusual. Our aim now is to rewrite \( 2.9 \) in terms of transmission and reflection coefficients of the wave functions

\[
f_1 = \begin{cases} e^{-ikx} + R_k^r e^{ikx}, & x > 0 \\ T_k^t e^{-ikx}, & x < 0 \end{cases}, \quad f_2 = \begin{cases} T_k^l e^{ikx}, & x > 0 \\ e^{ikx} + R_k^l e^{-ikx}, & x < 0 \end{cases}
\]

where \( k \in \mathbb{C} \backslash \mathbb{R} = \{ k \in \mathbb{C} : \Re k \neq 0 \} \).

It follows from \( 2.26 \) that:

\[
f_1(0 +) = 1 + R_k^r, \quad f_1(0 -) = T_k^t, \quad f_1'(0 +) = i(-k^2 + kR_k^r), \quad f_1'(0 -) = -ikT_k^t,
\]

\[
f_2(0 +) = T_k^l, \quad f_2(0 -) = 1 + R_k^l, \quad f_2'(0 +) = ikT_k^l, \quad f_2'(0 -) = i(-k^2 - kR_k^l).
\]

Substituting these values in \( 2.6 \) and solving the corresponding systems of linear equations, we get

\[
t_{11} = \frac{1}{\theta_k \Delta_k} \begin{bmatrix} \Delta_k - (e^{iu} - 1)(R_k^l + e^{i\alpha}) \end{bmatrix}, \quad t_{12} = \frac{T_k^l}{\theta_k \Delta_k} (e^{iu} - 1),
\]

\[
t_{22} = \frac{1}{\theta_k \Delta_k} \begin{bmatrix} \Delta_k - (e^{iu} - 1)(R_k^r + e^{i\alpha}) \end{bmatrix}, \quad t_{21} = \frac{T_k^r}{\theta_k \Delta_k} (e^{iu} - 1),
\]

where \( \theta_k = 2(1 + ik), \quad e^{iu} = \frac{\pi}{\theta_k}, \quad k \in \mathbb{C} \backslash \mathbb{R}, \) and

\[
\Delta_k = \begin{bmatrix} R_k^r + e^{iu}, & T_k^l \\ T_k^t, & R_k^l + e^{iu} \end{bmatrix}.
\]

Then

\[
\sigma_0 - 2(1 + ik)\mathcal{T} = \frac{e^{iu} - 1}{\Delta_k} \begin{bmatrix} R_k^l + e^{iu} & -T_k^l \\ -T_k^t & R_k^r + e^{iu} \end{bmatrix}
\]

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and
\[
\det[\sigma_0 - 2(1 + ik)\Sigma] = \frac{(e^{\alpha} - 1)^2}{\Delta_i}.
\]

Hence,
\[
[\sigma_0 - 2(1 + ik)\Sigma]^{-1} = \frac{1}{e^{\alpha} - 1} \begin{pmatrix} R_k + e^{\alpha} & T_k^l \\ T_k^l & R_k^l + e^{\alpha} \end{pmatrix}.
\] (2.27)

Rewriting (2.9) as
\[
S(k) = \frac{1 - ik}{1 + ik} \sigma_0 + \frac{2ik}{1 + ik} \left[ \delta_0 - 2(1 + ik)\Sigma \right]^{-1}, \quad k \in \mathbb{C}^\prime,
\]
using (2.27), and taking into account that
\[
\frac{2ik}{1 + ik} \cdot \frac{1}{e^{\alpha} - 1} = -\frac{k}{\text{Re} k} \cdot \frac{1 - ik}{1 + ik} - \frac{k e^{\alpha}}{\text{Re} k} = -\frac{\text{Im} k}{\text{Re} k}.
\]

we obtain
\[
S(k) = -\frac{k}{\text{Re} k} \begin{pmatrix} R_k + \frac{\text{Im} k}{k} & T_k \\ T_k^l & R_k^l + \frac{\text{Im} k}{k} \end{pmatrix}.
\] (2.28)

The expression (2.28) coincides with the $S$-matrix of $T_{\alpha}$ for all $k \in \mathbb{C}^\prime$ such that
\[
\Delta_k = \begin{vmatrix} R_k + e^{\alpha} & T_k^l \\ T_k & R_k^l + e^{\alpha} \end{vmatrix} \neq 0, \quad e^{\alpha} = \frac{1 - ik}{1 + ik}.
\]

3. Similarity to self-adjoint operators

An operator $A$ acting in a Hilbert space $\mathcal{H}$ is called similar to a self-adjoint operator $H$ if there exists a bounded and boundedly invertible operator $Z$ such that
\[
A = Z^{-1}HZ.
\] (3.1)

It is known (see, for example, [15]) that the similarity of $A$ to a self-adjoint operator means that $A$ is self-adjoint for a certain choice of inner product of the Hilbert space $\mathcal{H}$, which is equivalent to the initial inner product $(\cdot, \cdot)$.

The following integral-resolvent criterion of similarity can be useful:

**Lemma 3.1.** ([16]). A closed densely defined operator $A$ acting in $\mathcal{H}$ is similar to a self-adjoint one if and only if the spectrum of $A$ is real and there exists a constant $M$ such that
\[
\sup_{\gamma, \delta} \int_{-\infty}^{+\infty} \| (A - zI)^{\gamma} g \| \| dx \leq M \| g \|^2,
\]
\[
\sup_{\gamma, \delta} \int_{-\infty}^{+\infty} \| (A^* - zI)^{\gamma} g \| \| dx \leq M \| g \|^2, \quad \forall g \in \mathcal{H},
\] (3.2)

where the integrals are taken along the line $z = \xi + i\varepsilon$ ($\varepsilon > 0$ is fixed) of $C_{\varepsilon}$.

In order to use lemma 3.1 we need an explicit form of the resolvent $(A_{\alpha} - zI)^{-1}$.  


Lemma 3.2. Let $A_T$ and $A_F$ be linear operators in $L_2(\mathbb{R})$ defined, respectively, by (2.6) and (2.11). Then, for all $g \in L_2(\mathbb{R})$ and for all $z = k^2$ ($k \in \mathbb{C}_+$) from the resolvent set of $A_T$

$$\left\| \left[ (A_T - zI)^{-1} - (A_F - zI)^{-1} \right] g \right\|^2 = \frac{1}{\text{Im} \ k} \left\| \left( \sigma_0 + i\sigma_3 [\Sigma - \theta_i \det \Sigma \sigma_0] \right) F_g \right\|^2_{\mathbb{C}^2},$$

where $\theta_i = 2(1 + ik)$, $\| \cdot \|_{\mathbb{C}^2}$ is the norm in $\mathbb{C}^2$, $F_g = \begin{cases} \int_{0}^{\infty} e^{ikx} g(s) ds, \\ \int_{-\infty}^{0} e^{-ikx} g(s) ds \end{cases}$ and

$$p_z(k) = 4(1 + ik)^2 \det (\Sigma - (1 + ik) \chi) + 1.$$  \hspace{1cm} (3.3)

Proof. Let us fix $k \in \mathbb{C}_+$ and consider the functions

$$h_{1k}(x) = \begin{cases} e^{ikx}, & x > 0 \\ -e^{-ikx}, & x < 0 \end{cases}, \quad h_{2k}(x) = \begin{cases} e^{-ikx}, & x > 0 \\ e^{ikx}, & x < 0 \end{cases}$$

which belong $L_2(\mathbb{R})$ and form a basis of $\ker (A_T^* - zI)$, where $z = k^2 \in \mathbb{C} \setminus \mathbb{R}_+$ and $A_T^*$ is the adjoint of the symmetric operator $A_T$ defined by (2.10). Similar to the proof of Lemma 4 in [11], we conclude that

$$\left[ (A_T - zI)^{-1} - (A_F - zI)^{-1} \right] g = c_{1k} h_{1k} + c_{2k} h_{2k}, \quad \forall g \in L_2(\mathbb{R}),$$

where $c_{jk}$ are two parameters to be calculated. The latter relation allows one to express any function $f \in \mathcal{D}(A_T)$ as follows:

$$f(x) = f_{+}(x) + c_{1k} h_{1k}(x) + c_{2k} h_{2k}(x),$$

where $f_{+/−}(x) = f_{+/(−)}(0) = 0$ (in view of (2.11)).

The functions $f$ in (3.6) satisfy (2.6). Calculating the values of $f(0 +)$, $f'(0 +)$ with the help of (3.4) and (3.6), substituting them to (2.6) and making elementary transformations we get

$$(c_{1k} c_{2k}) = \left( \sigma_0 + i\sigma_3 [\Sigma - \theta_i \det \Sigma \sigma_0] \right)^{-1} \begin{cases} f'_{+}(0 +) \\ -f'_{−}(0 −) \end{cases}.$$ \hspace{1cm} (3.7)

Simple calculation with the use of (2.15) and properties of Pauli matrices gives

$$(\sigma_0 + i\sigma_3 [\Sigma - \theta_i \det \Sigma \sigma_0])^{-1} = \frac{(\sigma_0 + i\sigma_3 [\Sigma - \theta_i \det \Sigma \sigma_0])^{-1}}{p_z(k)}.$$  \hspace{1cm} (3.7)

On the other hand, taking into account the explicit expression of $(A_F - zI)^{-1}$:

$$(A_F - zI)^{-1} g = \begin{cases} \frac{e^{ikx}}{k} \int_{x}^{\infty} g(s) \sin ks ds + \frac{\sin kx}{k} \int_{x}^{\infty} e^{ikx} g(s) ds, & x > 0; \\ -\frac{e^{-ikx}}{k} \int_{x}^{\infty} g(s) \sin ks ds - \frac{\sin kx}{k} \int_{-\infty}^{x} e^{-ikx} g(s) ds, & x < 0 \end{cases}.$$
we obtain
\[
\left( f'(0+) - f'(0-) \right) = \left( \int_{0}^{\infty} e^{iks}g(s)ds \right).
\]
Thus, (3.7) can be rewritten as
\[
\left( \frac{c_{1k}}{c_{2k}} \right) = \left( \frac{\sigma_0 + i\sigma_2}{p_2(k)} \right) Fg, \quad \text{where} \quad Fg = \left( \int_{0}^{\infty} e^{iks}g(s)ds \right).
\]

The functions \( h_{\beta} \) in (3.4) are orthogonal in \( L_2(\mathbb{R}) \) and \( \| h_{\beta} \|^2 = \frac{1}{\text{im} k} \). Hence, (3.5) gives
\[
\left\| (A_T - zI)^{-1} - (A_F - zI)^{-1}g \right\| \leq \frac{\| c_{1k} \|^2 + \| c_{2k} \|^2}{\text{Im} k} Fg = \frac{1}{\text{Im} k} \left\| \left( \frac{\sigma_0 + i\sigma_2}{p_2(k)} \right) Fg \right\| \leq \sup_{x \in \mathbb{R}} \| g \| \leq M \| g \|^2,
\]
which completes the proof of lemma 3.2.

**Theorem 3.3.** If all poles of the S-matrix \( S(\cdot) \) of \( A_T \) lie on the nonphysical sheet \( C_\sigma \), then \( A_T \) is similar to a self-adjoint operator.

**Proof.** The operator \( A_F \) defined by (2.11) is self-adjoint. Hence, it satisfies (3.2) and the inequalities
\[
\sup_{x \geq 0} \int_{-\infty}^{\infty} \left\| (A_T - zI)^{-1} - (A_F - zI)^{-1}g \right\|^2 dz \leq M \| g \|^2,
\]
give us the necessary and sufficient condition for the similarity of \( A_T \) to a self-adjoint operator.

First we consider the auxiliary self-adjoint operator \( A_K \) defined by (2.12). Obviously, the inequalities (3.8) are true with \( A_T = A_K \). Using lemma 3.2, and taking into account that
\[
A_K = A_{\frac{1}{2}m}, \quad \det -\frac{\sigma_0}{2} = \frac{1}{4}, \quad p_{\frac{1}{2}m}(k) = -k^2
\]
we get
\[
\left\| (A_K - zI)^{-1} - (A_F - zI)^{-1}g \right\| \leq \frac{1}{\text{Im} k} \left\| \frac{\sigma_0 + i\sigma_2}{2k} Fg \right\| \leq \sup_{x \in \mathbb{R}} \| g \| \leq M \| g \|^2.
\]
Therefore, in view of (3.8),

$$
\int_{-\infty}^{\infty} \frac{\varepsilon}{\Im k} \left\| \left( \frac{\sigma_0 + i\sigma_2}{k} \right) F^2_k \right\|_{c_2}^2 \, d\xi \leq M \| g \|^2.
$$
(3.9)

We note that the integral in (3.9) is taken along the line $z = k^2 = \xi + i\varepsilon$ ($\varepsilon > 0$ is fixed) of upper half-plane $\mathbb{C}_+$. This means that

$$
\varepsilon = 2(\Re k)(\Im k) > 0, \quad \xi = (\Re k)^2 - (\Im k)^2.
$$

Therefore, the variable $k$ belongs to $\mathbb{C}_+$. Hence, the entries of the matrix

$$
\Psi(k) = \frac{k}{p_{\xi}(k)} [\Xi - \Theta_i \det \Xi_{\sigma_0}]
$$

are uniformly bounded when $k$ runs $\mathbb{C}_+$. Keeping in mind this fact, lemma 3.2 and (3.9) we obtain

$$
\varepsilon \int_{-\infty}^{\infty} \left\| \left( A_{\xi} - zI \right)^{-1} - \left( A_{\xi} - zI \right)^{-1} \right\|_2^2 \, d\xi = \int_{-\infty}^{\infty} \frac{\varepsilon}{\Im k} \left\| \left( \frac{\sigma_0 + i\sigma_2}{k} \right) \Psi(k) F^2_k \right\|_{c_2}^2 \, d\xi \leq M_1 \int_{-\infty}^{\infty} \frac{\varepsilon}{\Im k} \left\| \left( \frac{\sigma_0 + i\sigma_2}{k} \right) F^2_k \right\|_{c_2}^2 \, d\xi < MM_1 \| g \|^2
$$

that establish the first inequality in (3.8).

The second inequality can be justified in a similar manner. Indeed, it is easy to check that the domain of definition $\mathcal{D}(A_{\xi})$ has the form (2.6) with $\Xi^*$ (instead of $\Xi$). Thus,

$$
A_{\xi} = A_{\xi^*}.
$$
(3.10)

Let $S_{\xi}(\cdot)$ and $S_{\xi^*}(\cdot)$ be the $S$-matrix of operators $A_{\xi}$ and $A_{\xi^*}$, respectively. It follows from (2.9) that

$$
S_{\xi^*}(-F) = S_{\xi}^*(k), \quad k \in \mathbb{C}.
$$
(3.11)

Therefore, the $S$-matrix of $A_{\xi^*}$ also has poles within $\mathbb{C}_-$. This allows one to establish the second relation in (3.8) by repeating the previous arguments with the use of modified matrix

$$
\Psi(k) = \frac{k}{p_{\xi^*}(k)} \left[ \Xi^* - \Theta_i \det \Xi_{\sigma_0}^* \right].
$$

In view of lemma 3.1 and inequalities (3.8) the operator $A_{\xi}$ is similar to a self-adjoint one. theorem 3.3 is proved.

**Corollary 3.4.** Let the $S$-matrix of $A_{\xi}$ be a constant on $\mathbb{C}$ (see example III). Then $A_{\xi}$ is similar to a self-adjoint operator.
4. Metric operators

Unfortunately, the proof of theorem 3.3 does not contain a ‘recipe’ for construction of an appropiate metric operator which guarantees the self-adjointness of \( A_\tau \). We simply state that such an operator exists. Various approaches to the explicit determination of metric operators with the use of formal perturbative methods as well as mathematically rigid constructions can be found in \[17\].

In this section we aim to find an explicit expression for metric operators in the case where the \( S \)-matrix \( S(\cdot \cdot) \) of \( A_\tau \) has simple nonzero imaginary poles.

Assume that \( Q \) is a self-adjoint operator in \( L_2(\mathbb{R}) \). Then \( e^{i\chi Q} (\chi \in \mathbb{R}) \) is a positive self-adjoint operator in \( L_2(\mathbb{R}) \). If there exists a metric operator \( e^{i\chi Q} \) such that

\[
e^{i\chi A_\tau} = A_\tau^+ e^{i\chi}, \tag{4.1}
\]

then \( A_\tau \) turns out to be self-adjoint with respect to the new inner product

\[
\langle \cdot, \cdot \rangle_{\text{new}} = \langle e^{i\chi Q} \cdot, \cdot \rangle = \langle e^{i\chi/2} \cdot, \cdot \rangle_{L_2(\mathbb{R})}.
\]

Using (3.10) we rewrite (4.1) in the equivalent form

\[
e^{i\chi A_\tau} = A_\tau^+ e^{i\chi}, \tag{4.2}
\]

and we will seek the operator \( Q \) in (4.2) as:

\[
Q_\beta = \alpha_1 \mathcal{P} + \alpha_2 i \mathcal{P} \mathcal{R} + \alpha_3 \mathcal{R}, \quad \alpha = (\alpha_1, \alpha_2, \alpha_3) \in \mathbb{S}^2,
\]

where \( \mathbb{S}^2 = \{ \alpha \in \mathbb{R}^3 : \sum_{j=1}^3 |\alpha_j|^2 = 1 \} \) and

\[
\mathcal{P}(x) = f(x) - \chi f(x), \quad \mathcal{R}(x) = \sigma(x) f(x), \quad \forall f \in L_2(\mathbb{R}) \tag{4.3}
\]

are self-adjoint operators in \( L_2(\mathbb{R}) \).

The operators \( Q_\beta \) are self-adjoint in \( L_2(\mathbb{R}) \) and \( Q_3^2 = I \) \[8\]. Therefore,

\[
e^{i\chi Q_\beta} = (\cosh \chi I + \sinh \chi Q_3), \quad \chi \in \mathbb{R}. \tag{4.4}
\]

It follows from (4.3)-(4.5) that \( e^{i\chi Q} \) commutes with the operator

\[
A_\tau^* = -\frac{d^2}{dx^2}, \quad \mathcal{D}(A_\tau^*) = W^2_2(\mathbb{R} \setminus \{0\}).
\]

Since \( A_\tau \) and \( A_{\tau^*} \) are restrictions of \( A_\tau^* \), respectively, onto \( \mathcal{D}(A_\tau) \) and \( \mathcal{D}(A_{\tau^*}) \) the relation (4.2) holds if and only if the operator \( e^{i\chi Q} \) maps \( \mathcal{D}(A_\tau) \) into \( \mathcal{D}(A_{\tau^*}) \), Taking (2.6) into account we conclude that the relation \( e^{i\chi Q} : \mathcal{D}(A_\tau) \to \mathcal{D}(A_{\tau^*}) \) is equivalent to the following implication

\[
\mathcal{T}_f \in \mathcal{D}(A_\tau), \quad \exists \mathcal{T}_f \mathcal{I}_e e^{i\chi Q} f = \mathcal{I}_e e^{i\chi Q} f, \quad \forall f \in \mathcal{D}(A_\tau), \tag{4.6}
\]

where \( \mathcal{T}_f = \left( \begin{array}{c} f(0 +) + f'(0 +) \\ f(0 -) - f'(0 -) \end{array} \right) \) and \( \mathcal{I}_f = \left( \begin{array}{c} f(0 +) \\ f(0 -) \end{array} \right) \).

It is easy to check, using the (4.4) of operators \( \mathcal{P} \) and \( \mathcal{R} \), that

\[
\mathcal{I}_f \mathcal{P} f = \sigma_0 \mathcal{I}_f f, \quad \mathcal{I}_f \mathcal{R} f = \sigma_1 \mathcal{I}_f f, \quad \mathcal{I}_f \mathcal{P} \mathcal{R} f = i \sigma_0 \sigma_1 \mathcal{I}_f f = \sigma_2 \mathcal{I}_f f, \quad \forall f \in W^2_2(\mathbb{R} \setminus \{0\}).
\]

Therefore,

\[
\mathcal{I}_e e^{i\chi Q} f = (\cosh \chi \sigma_0 + \sinh \chi \sigma_1) \mathcal{I}_e f, \quad k = 0, 1, \quad \text{where } \sigma_0 = \sum_{j=1}^3 |\alpha_j|^2 \text{ and implication (4.6) is equivalent to equation

\[\text{3} \quad \text{The existence of zero pole means that } A_\tau \text{ has spectral singularity at } 0 \text{ and it cannot be similar to a self-adjoint operator due to proposition 5.5.}\]
\( T \chi (\cosh \chi \sigma_0 + \sinh \chi \sigma_d) = (\cosh \chi \sigma_0 + \sinh \chi \sigma_d) T \chi \)  

(4.7)

with respect to unknown \( \chi \in \mathbb{R} \) and \( \vec{a} \in \mathbb{S}^2 \).

Assume that all poles of \( S \)-matrix \( S(\cdot) \) of a non-self-adjoint operator \( A_\chi \) are simple and they belong to \( \mathbb{R} \backslash \{0\} \). In view of (2.18)–(2.22), the case of two different simple nonzero imaginary poles of \( S(\cdot) \) is characterized by the conditions

\[
\det \Xi \neq 0, \quad \chi_0 \in \mathbb{R}, \quad \sqrt{\sum_{j=1}^{3} \chi_j^2} \in \mathbb{R} \backslash \{0\},
\]

(4.8)

where (as usual) \( \Xi = \sum_{j=1}^{3} n_j \sigma_j \). Similarly the case where the \( S \)-matrix of a non-self-adjoint operator \( A_\chi \) has one simple nonzero imaginary pole corresponds to the relations

\[
\det \Xi = 0, \quad \chi_0 \in \mathbb{R}, \quad \sqrt{\sum_{j=1}^{3} \chi_j^2} \in \mathbb{R} \backslash \{0\}.
\]

(4.9)

The condition \( \chi_0 \in \mathbb{R} \) in both cases (4.8) and (4.9) allows us to rewrite the equation (4.7) as follows:

\[
\sum_{j=1}^{3} (\text{Im} \; \gamma_j) \sigma_j = \tanh \chi \left( \begin{array}{ccc}
\sigma_1 & \sigma_2 & \sigma_3 \\
\text{Re} \; \gamma_1 & \text{Re} \; \gamma_2 & \text{Re} \; \gamma_3 \\
\text{Re} \; \gamma_1 & \text{Re} \; \gamma_2 & \text{Re} \; \gamma_3 \\
\end{array} \right) - \sum_{j=1}^{3} (\text{Im} \; \gamma_j) \alpha_j \sigma_0,
\]

(4.10)

where the formal determinant

\[
\begin{vmatrix}
\sigma_1 & \sigma_2 & \sigma_3 \\
\text{Re} \; \gamma_1 & \text{Re} \; \gamma_2 & \text{Re} \; \gamma_3 \\
\text{Re} \; \gamma_1 & \text{Re} \; \gamma_2 & \text{Re} \; \gamma_3 \\
\end{vmatrix} := \begin{vmatrix}
\sigma_1 & \sigma_2 & \sigma_3 \\
\text{Re} \; \gamma_1 & \text{Re} \; \gamma_2 & \text{Re} \; \gamma_3 \\
\text{Re} \; \gamma_1 & \text{Re} \; \gamma_2 & \text{Re} \; \gamma_3 \\
\end{vmatrix} - \begin{vmatrix}
\sigma_1 & \sigma_2 & \sigma_3 \\
\text{Re} \; \gamma_1 & \text{Re} \; \gamma_2 & \text{Re} \; \gamma_3 \\
\text{Re} \; \gamma_1 & \text{Re} \; \gamma_2 & \text{Re} \; \gamma_3 \\
\end{vmatrix} + \begin{vmatrix}
\sigma_1 & \sigma_2 & \sigma_3 \\
\text{Re} \; \gamma_1 & \text{Re} \; \gamma_2 & \text{Re} \; \gamma_3 \\
\text{Re} \; \gamma_1 & \text{Re} \; \gamma_2 & \text{Re} \; \gamma_3 \\
\end{vmatrix},
\]

is the ‘cross product’ of vectors \( \text{Re} \; \vec{\gamma} = (\text{Re} \; \gamma_1, \text{Re} \; \gamma_2, \text{Re} \; \gamma_3) \) and \( \vec{a} \) which is associated with the Pauli matrices \( \sigma_1, \sigma_2, \sigma_3 \) (instead of the standard basis vectors \( i, j, k \) of the Euclidean space \( \mathbb{R}^3 \)).

We remark that the vectors

\[
\text{Re} \; \vec{\gamma} = (\text{Re} \; \gamma_1, \text{Re} \; \gamma_2, \text{Re} \; \gamma_3), \quad \text{Im} \; \vec{\gamma} = (\text{Im} \; \gamma_1, \text{Im} \; \gamma_2, \text{Im} \; \gamma_3)
\]

in (4.10) cannot be zero. Indeed, if \( \text{Re} \; \vec{\gamma} = 0 \), then \( \sqrt{\sum_{j=1}^{3} |\gamma_j|^2} = \sqrt{-\sum_{j=1}^{3} |\gamma_j|^2} \in i\mathbb{R} \backslash \{0\} \) which contradicts the third relation in (4.8), (4.9). Similarly, if \( \text{Im} \; \vec{\gamma} = 0 \), then the second relation in (4.8), (4.9) implies that \( A_\chi \) is a self-adjoint operator which is impossible.

It follows from the third relation in (4.8), (4.9) that

\[
\sum_{j=1}^{3} |\gamma_j|^2 = \sum_{j=1}^{3} (\text{Re} \; \gamma_j)^2 - \sum_{j=1}^{3} (\text{Im} \; \gamma_j)^2 + 2i \sum_{j=1}^{3} (\text{Re} \; \gamma_j)(\text{Im} \; \gamma_j) > 0.
\]

Hence,

\[
\sum_{j=1}^{3} (\text{Re} \; \gamma_j)^2 > \sum_{j=1}^{3} (\text{Im} \; \gamma_j)^2, \quad \sum_{j=1}^{3} (\text{Re} \; \gamma_j)(\text{Im} \; \gamma_j) = 0.
\]

(4.11)

This means that the vectors \( \text{Re} \; \vec{\gamma} \) and \( \text{Im} \; \vec{\gamma} \) are orthogonal in \( \mathbb{R}^3 \).

Let us fix the vector \( \vec{a} \in \mathbb{S}^2 \) in such a way that \( \vec{a} \) is orthogonal to \( \text{Re} \; \vec{\gamma} \) and \( \text{Im} \; \vec{\gamma} \). Then the standard cross product \( \text{Re} \; \vec{\gamma} \times \vec{a} = \begin{vmatrix} i & j & k \\ \text{Re} \; \gamma_1 & \text{Re} \; \gamma_2 & \text{Re} \; \gamma_3 \\ \alpha_1 & \alpha_2 & \alpha_3 \end{vmatrix} \) is collinear to \( \text{Im} \; \vec{\gamma} \). Precisely, there exists \( \kappa \in \mathbb{R} \) such that

...
Calculating the norms of vectors $\text{Im} \overrightarrow{\gamma}$ and $\text{Re} \overrightarrow{\gamma} \times \overrightarrow{a}$ in (4.12) and taking into account (4.11), we obtain

$$|k|^2 = \frac{\| \text{Im} \overrightarrow{\gamma} \|^2}{\| \text{Re} \overrightarrow{\gamma} \|^2 \| \overrightarrow{a} \|^2} = \frac{\| \text{Im} \overrightarrow{\gamma} \|^2}{\sum_{j=1}^{3} (\text{Im} \gamma_j)^2} = \frac{\sum_{j=1}^{3} (\text{Im} \gamma_j)^2}{\sum_{j=1}^{3} (\text{Re} \gamma_j)^2} < 1.$$ 

On the other hand, since $\overrightarrow{a} \perp \text{Im} \overrightarrow{\gamma}$, the equation (4.10) takes the form

$$\sum_{j=1}^{3} (\text{Im} \gamma_j) \sigma_j = \tanh \chi \begin{vmatrix} \sigma_1 & \sigma_2 & \sigma_3 \\ \text{Re} \gamma_1 & \text{Re} \gamma_2 & \text{Re} \gamma_3 \\ \alpha_1 & \alpha_2 & \alpha_3 \end{vmatrix}.$$ (4.13)

Obviously, (4.13) has a solution $\chi \in \mathbb{R}$ such that $\tanh \chi = k$. Summing the results above, we prove

**Theorem 4.1.** If the $S$-matrix $S(\cdot)$ of a non-self-adjoint operator $A_\zeta$ has simple nonzero imaginary poles, then $A_\zeta$ turns out to be self-adjoint with respect to new inner product $\| \cdot \|_{\text{new}} = (e^{i\zeta} \cdot, \cdot)$, where $\overrightarrow{a} \in \mathbb{S}^2$ is orthogonal to the vectors $\text{Re} \overrightarrow{\gamma}$, $\text{Im} \overrightarrow{\gamma}$ and $\chi$ is defined by the relation $\tanh \chi = \kappa$, where $\kappa$ is the coefficient of collinearity in (4.12).

It looks natural that the parameter $\chi$ in theorem 4.1 correlates to the distance between imaginary poles of $S(\cdot)$.

**Corollary 4.2.** Let $k_\pm$ be two imaginary poles of the $S$-matrix of $A_\zeta$. Then the parameter $\chi$ of the corresponding metric operator $e^{i\chi} \cdot$ can be determined by the relation

$$\cosh \chi = \frac{\| \text{Re} \overrightarrow{\gamma} \|}{(k_- - k_+) \det \mathcal{T}}.$$ (4.14)

**Proof.** If $k_\pm$ are poles of $S(\cdot)$, then the quantities $\theta_\pm$ in (2.18) are expressed as $\theta_\pm = 2(1 + ik_\pm)$. Denote $\xi = \sqrt{\sum_{j=1}^{3} \gamma_j^2}$. Then

$$\xi = \frac{1}{2\theta_+} - \frac{1}{2\theta_-} = i(k_- - k_+) \det \mathcal{T}.$$ 

Taking into account that $\xi^2 = \sum_{j=1}^{3} (\text{Re} \gamma_j)^2 - (\text{Im} \gamma_j)^2$, we obtain

$$\left\| \frac{\text{Re} \overrightarrow{\gamma}}{\xi} \right\|^2 - \left\| \frac{\text{Im} \overrightarrow{\gamma}}{\xi} \right\|^2 = 1.$$ 

Therefore, there exists $\omega \geq 0$ such that $\cosh \omega = \left\| \frac{\text{Re} \overrightarrow{\gamma}}{\xi} \right\|$ and $\sinh \omega = \left\| \frac{\text{Im} \overrightarrow{\gamma}}{\xi} \right\|$. It follows from (4.12) and theorem 4.1 that

$$|\tanh \chi| = |k| = \frac{\| \text{Im} \overrightarrow{\gamma} \|}{\| \text{Re} \overrightarrow{\gamma} \|} = \frac{\sinh \omega}{\cosh \omega} = \tanh \omega.$$
Without loss of generality\(^4\) we can suppose that \(k \geq 0\) in (4.12). Then \(\chi = \omega\) and \(\cosh \chi\) is determined by (4.14). \(\square\)

5. Spectral singularities

If \(A_\tau\) is a self-adjoint operator in \(L_\tau(\mathbb{R})\) or \(A_\tau\) is similar to a self-adjoint one, then the entries of the \(S\)-matrix \(S(k)\) are uniformly bounded when \(k\) runs \(\mathbb{R}\). Since the existence of spectral singularity \(z = k_0^2\) of \(A_\tau\) should mean that \(A_\tau\) cannot be similar to a self-adjoint operator, it is natural to suppose that \(S(k)\) cannot be uniformly bounded in a neighborhood of \(k_0 \in \mathbb{R}\). This leads to the following

**Definition 5.1.** A nonnegative number \(z = k_0^2\) is called the spectral singularity of \(A_\tau\) if \(k_0 \in \mathbb{R}\) is a pole of the \(S\)-matrix \(S(\cdot)\) of \(A_\tau\). The operator \(A_\tau\) has spectral singularity at \(\infty\) if \(z = \infty\) is a pole of \(S(\cdot)\).

It is known (see, e.g., [11]) that the continuous spectrum of operators \(A_\tau\) defined by (2.6) coincides with \([0, \infty)\) and there are no eigenvalues of \(A_\tau\) embedded in the continuous spectrum. Therefore, spectral singularities of \(A_\tau\) may appear on the continuous spectrum only, and (possible) existence of a spectral singularity \(z\) does not mean that \(z\) is an eigen-value \(A_\tau\).

**Proposition 5.2.** The operators \(A_\tau\) and \(A_\tau^*\) have the same set of spectral singularities.

**Proof.** Follows immediately from the relation \(A_\tau^* = A_\tau^*\) and (3.11).

The existence of spectral singularity of \(A_\tau\) can be easily described via the roots of the polynomial \(p_z(k)\) defined by (3.3).

**Proposition 5.3.** Assume that \(\Sigma \neq \frac{1}{2} \sigma_0\). A point \(z = k_0^2\) is a spectral singularity of \(A_\tau\) if and only if the polynomial (3.3) has:

(i) a root \(k_0 \in \mathbb{R}\) for the case of nonzero spectral singularity \(z \neq 0\);

(ii) a root \(k_0 = 0\) of multiplicity 2 for the case of zero spectral singularity \(z = 0\);

(iii) no roots for the case of spectral singularity at \(z = \infty\).

Let \(z = k_0^2 \neq 0\) be a spectral singularity of \(A_\tau\). Then \(k_0 \in \mathbb{R} \setminus \{0\}\) is a pole of \(S(k)\). Assume firstly that \(\det \Sigma \neq 0\). Then \(S(\cdot)\) is determined by (2.19), where \(\theta_\tau \theta_\tau \neq 0\) and \(\theta_\tau \theta_\tau \neq \infty\) due to the third relation in (2.18). The existence of pole \(k_0\) of \(S(\cdot)\) means that \(\theta_\tau \theta_\tau = 2(1 + \imath k_0)\) coincides with \(\theta_\tau\) or with \(\theta_\tau\). Then the point \(k_0\) is a root of \(p_z(k)\) due to (2.17). Conversely, if \(k_0\) is a root of \(p_z(k)\), then \(k_0\) is a pole of \(S(k)\) (this implication follows from (2.17)–(2.21)).

Assume now that \(\det \Sigma = 0\). Then \(S(\cdot)\) is determined by (2.22). The pole \(k_0\) of \(S(\cdot)\) is possible where \(-2\theta_\tau \chi_0 + 1 = -4(1 + \imath k_0)\chi_0 + 1 = 0\). Thus, \(k_0\) is a root of \(p_z(k)\). Conversely, the statement is evident. Implication (i) is proved.

Let \(z = k_0^2 = 0\) be a spectral singularity of \(A_\tau\). Then \(k_0 = 0\) is a pole of \(S(k)\). Let \(\det \Sigma \neq 0\). Then the \(S\)-matrix is determined by (2.19) and simple analysis of (2.19) shows that \(S(k)\) has a pole at \(k_0 = 0\) in the case \(\theta_\tau = \theta_\tau = \theta_\tau = 2\) only. By (2.17), \(k_0 = 0\) is a root of \(\alpha\) in (4.12).
$p_z(k)$ of multiplicity 2. Conversely, let $k_0 = 0$ be a root of $p_z(k)$ of multiplicity 2. Then $\theta_0 = \theta_1 = \theta_2 = 0$. Using (2.19) again we deduce that $S(k)$ has a pole at $k_0 = 0$. (The case $\gamma_0 = 1$ and $\gamma = \gamma_1 = \gamma_1 = 0$ is not considered here because $T \neq 0$ by the assumption of proposition 5.3.)

Assume now that $\det T = 0$. Then $S(k)$ has a pole at $k_0 = 0$. (The case $k_0 = 0$ and $\gamma = 0$ is not considered here because $T \neq 1$ by the assumption of proposition 5.3.)

Assume now that $T = \det 0$. Then $S(k)$ is determined by (2.22) and this expression does not have a pole at $k_0 = 0$. On the other hand, $k_0 = 0$ cannot be a root of $p_z(k)$ of multiplicity 2 when $T = \det 0$. Implication (ii) is proved.

To prove (iii) it suffices to note that $S(k)$ will tend to infinity when $k \to \infty$ only in the case where $p_z(k)$ does not depend on $k$. This means that $p_z(k)$ has no roots in $C$. Proposition 5.3 is proved.

The ‘exceptional’ operator $A_{\lambda_0}$ in proposition 5.3 coincides with the Krein extension of the symmetric operator $A_\sigma$ (see remark 2.2).

In the particular case where $A_\tau = A_T$, spectral singularities are described via the roots of the polynomial

$$p_z(k) = 2dk^2 + i(\det \mathbf{T} - 4)k + 2a.$$  (5.1)

**Corollary 5.4.** ([13]). A point $z = k_0^2$ is a spectral singularity of $A_T$ if and only if the polynomial (5.1) has:

(i) a real root $\lambda_0 \in \mathbb{R}$ for the case of nonzero spectral singularity $z \neq 0$;

(ii) the zero root $\lambda_0 = 0$ of multiplicity 2 for the case of spectral singularity at $z = 0$;

(iii) no roots for the case of spectral singularity at $z = \infty$.

**Proof.** First of all we note that the domain of definition of $A_k$ (= $A_{\lambda_0}$) cannot be presented in the form (2.4). Thus $A_{\lambda_0}$ cannot be realized as $A_T$. Taking the expressions of $\gamma_0$ and $\det T$ given by (2.23) and (2.24) into account, we get $p_z(k) = \frac{1}{2}p_z(k)$. This relation and proposition 5.3 complete the proof. □

**Proposition 5.5.** If $A_\tau$ has a spectral singularity, then $A_\tau$ cannot be similar to a self-adjoint operator.

**Proof.** The resolvent of an arbitrary self-adjoint operator $H$ satisfies the inequality $\| (H - zI)^{-1} \| \leq \frac{1}{\text{Im} z}$ for all $z \in C \setminus \mathbb{R}$. If $A$ is similar to a self-adjoint operator (i.e., (3.1) holds), then the inequality above takes the form

$$\| (A - zI)^{-1} \| \leq \frac{C}{\text{Im} z}, \quad C = \| Z^{-1} \| \| Z \|, \quad z \in C \setminus \mathbb{R}.$$  (5.2)

Let $A_\tau$ be similar to a self-adjoint operator. Since $A_\tau$ is self-adjoint, the relation (5.2) holds for $A_\tau$ and for $A_F$. Therefore,

$$\left\| \left[ (A_\tau - zI)^{-1} - (A_F - zI)^{-1} \right] g \right\| \leq \frac{M}{(\text{Im} z)^2} \| g \|^2,$$  (5.3)

where $M$ is a constant independent of $g \in L_2(\mathbb{R})$ and $z \in C \setminus \mathbb{R}$.

Let us consider a particular case of (5.3) with $z = k^2$ ($k \in C_+$) and $g = g_+$, where

$$g_+(x) = \begin{cases} e^{-x}, & x > 0; \\ 0, & x < 0 \end{cases}, \quad g_-(x) = \begin{cases} 0, & x > 0; \\ e^{ix}, & x < 0 \end{cases}$$

$$g(z) = \begin{cases} e^{-x}, & x > 0; \\ 0, & x < 0 \end{cases}$$

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Taking into account that
\[ \| g_z \|^2 = \frac{1}{2 \text{Im } k}, \quad (Fg_z)(k) = \frac{1}{2 \text{Im } k}, \quad \text{Im } z = 2 \text{Im } k \Re k, \quad (5.4) \]
and using lemma 3.2 we conclude that the norm of matrix\(^5\)
\[ \Phi(k) = \frac{\Re k}{p_z(k)} \left[ \Xi - \theta_i \det \Xi \sigma_i \right] \]
is uniformly bounded on \( C_+ \). This means that the entries of \( \Phi(k) \) must be uniformly bounded when \( k \) runs \( C_+ \).

Let \( A_\xi \) have a spectral singularity at \( z = \infty \). Then, according to proposition 5.3, the polynomial \( p_z(k) \) has no roots. This is possible when \( \det \Xi = 0 \) and \( \sigma_i = 0 \). In that case \( \Phi(k) = \Re \left[ \sum_j \sigma_j \Theta \sigma_j \right] \) cannot be uniformly bounded on \( C_+ \). Hence, \( A_\xi \) is not similar to a self-adjoint operator.

Let \( z = 0 \) be a spectral singularity. Then, \( A_\xi \neq A^{\omega_0}_\xi \) and in view of proposition 5.3, \( p_z(k) = \Xi \) (a is some constant). In that case, at least one of entries of \( \Phi(k) = \Re \left[ \sum_j \sigma_j \Theta \sigma_j \right] \) tends to infinity when \( k \to 0 \). So, \( A_\xi \) is not similar to a self-adjoint operator.

Let \( z = k_0^2 \) be a nonzero spectral singularity. Then \( k_0 \in \mathbb{R} \) is a root of \( p_z(k) \) and \( \Phi(k) \) tends to infinity when \( k \to k_0 \). Thus \( A_\xi \) is not similar to a self-adjoint operator. Proposition 5.5 is proved.

**Example IV.** \( \delta' \)-potential with a complex coupling. Let \( d \in \mathbb{C} \) and \( a = b = c = 0 \). Then the expression
\[ -\frac{d^2}{dx^2} + d < \delta', \cdot > \delta' (x), \quad d \in \mathbb{C} \]
determines the operators \( A_d = -\frac{d^2}{dx^2} \) in \( L_2(\mathbb{R}) \), which are defined on
\[ \mathcal{D}(A_d) = \left\{ f \in W^2_2(\mathbb{R} \setminus \{0\}) \mid f'(0+) = f'(0-) (\equiv f'(0)) \right\} \]
In that case
\[ \Xi = \frac{1}{4 - 2d} \begin{pmatrix} 1 - d & 1 \\ 1 & 1 - d \end{pmatrix}, \quad \det \Xi = -\frac{d}{2(4 - 2d)}, \quad \gamma_0 = \frac{1 - d}{4 - 2d} \]
Substituting these quantities in (2.16) we obtain
\[ S(k) = \frac{1}{d k - 2i} \begin{pmatrix} -d k & 2i \\ 2i & -d k \end{pmatrix}. \]
The \( S \)-matrix has a real pole \( k_0 = \frac{z}{d} \) when \( d \in i \mathbb{R} \setminus \{0\} \). In that case \( z = k_0^2 = \frac{4}{\text{Im } z} \) is a spectral singularity of \( A_d \).

### 6. Exceptional points

Let \( A \) be a linear operator acting in a Hilbert space \( \mathcal{H} \). A nonzero vector \( f \in \mathcal{D}(A) \) is called a root vector of \( A \) corresponding to the eigenvalue \( z \) if \((A - z J)f = 0 \) for some \( n \in \mathbb{N} \). The set of all root vectors of \( A \) corresponding to a given eigenvalue \( z \), together with a zero vector,
forms a linear subspace $L_z$, which is called the root subspace. The dimension of the root subspace $L_z$ is called the algebraic multiplicity of the eigenvalue $z$. The geometric multiplicity of $z$ is defined as the dimension of the kernel subspace $\ker(A - zI)$ (i.e., as the dimension of the linear subspace of eigenfunctions of $A$ corresponding to $z$).

The algebraic and the geometric multiplicities of $z$ coincide in the case where $A$ is similar to a self-adjoint operator.

The existence of exceptional points deals with the possible occurrence of nontrivial Jordan blocks in discrete spectra. For operators $A_z$ depending on parameters $t \in \{t_0\}$ this means that two eigenvalues $z_1(\Sigma)$, $z_2(\Sigma)$ may coalesce (degenerate) at certain parameter hypersurfaces of the linear set $\{t_0\}$ under simultaneous coalescence of the corresponding eigenvectors $f_1(\Sigma)$, $f_2(\Sigma)$ see e.g. [2] or [3], where the general theory of exceptional and diabolical points in multiparameter families of complex matrices was developed. We formalize these ideas as follows:

**Definition 6.1.** Let $A$ be a linear operator acting in a Hilbert space $\mathcal{H}$. An eigenvalue $z$ of $A$ is called the exceptional point if the geometric multiplicity of $z$ does not coincide with its algebraic multiplicity.

The presence of an exceptional point means that the operator $A$ is not self-adjoint in $\mathcal{H}$ and, moreover, it cannot be self-adjoint for any choice of (equivalent) inner product of $\mathcal{H}$.

**Theorem 6.2.** Let $S(\cdot)$ be the $S$-matrix of $A_z$. Then $k_0 \in \mathbb{C}_+$ is a pole of order 2 of $S(\cdot)$ if and only if $z_0 = k_0^2$ is an exceptional point of $A_z$.

**Proof.** The resolvent $(A_z - zI)^{-1}$ of a self-adjoint operator $A_f$ (see (2.11)) is a holomorphic operator-valued function on $\mathbb{C} \setminus \mathbb{R}_+$. On the other hand, if $A_z$ is defined by (2.6), then the resolvent $(A_z - zI)^{-1}$ may be a meromorphic function on $\mathbb{C} \setminus \mathbb{R}_+$ and an eigenvalue $z_0 = k_0^2$ of $A_z$ will be exceptional if and only if $(A_z - zI)^{-1}$ has a pole $z_0$ of order greater than one [18]. Hence, the existence of an exceptional point $z_0 = k_0^2$ of $A_z$ is equivalent to the existence of pole $z_0$ of order 2 for the operator-valued function

$$(A_z - zI)^{-1} - (A_f - zI)^{-1}.$$ 

Taking the proof of lemma 3.2 into account (especially (3.5) and (3.7)) we conclude that this condition is equivalent to the existence of pole $k_0 \in \mathbb{C}_+$ of order 2 for the matrix-valued function $\Sigma (\sigma_0 - \theta_0 \Sigma)^{-1}$.

It should be noted that $z_0 = -1$ cannot be an exceptional point of $A_z$ (because $-1 \in \rho(A_f)$ for any operator $A_f$ defined by (2.6)). Hence, the possible pole $k_0 \neq i$ and we can suppose that $\theta_i \neq 0$ in some neighbourhood of $\theta_i = 2(1 + ik_0)$. Then

$$\Sigma (\sigma_0 - \theta_0 \Sigma)^{-1} = -\frac{1}{\theta_i} \sigma_0 + \frac{1}{\theta_k} (\sigma_0 - \theta_i \Sigma)^{-1}.$$ 

Comparing the obtained decomposition with (2.9) we conclude that $k_0$ is a pole of order 2 of $\Sigma (\sigma_0 - \theta_0 \Sigma)^{-1}$ if and only if $k_0$ is a pole of order 2 of the $S$-matrix $S(\cdot)$, theorem 6.2 is proved.

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6 In our case, the order must be 2 because the defect indices of the symmetric operator $A_s$ are $<2, 2>$. 
Corollary 6.3. The point \( z_0 = k_0^2 \) is an exceptional point of \( A \) if and only if the matrix \( \sigma_0 - \theta_{k_0} \vec{\xi} \) is nonzero and nilpotent.

Proof. Let \( z_0 = k_0^2 \) be an exceptional point of \( A \). Then \( k_0 \in \mathbb{C}_+ \) is a pole of order 2 for \( S(\cdot) \). Taking (2.16) into account, we conclude that \( \det \vec{\xi} \neq 0 \) and \( k_0 \neq i \). So, \( S(\cdot) \) is defined by (2.19) and \( \theta_{k_0} = 2(1 + ik_0) \neq 0 \).

The \( S \)-matrix \( S(\cdot) \) has a pole \( k_0 \) of order 2 if and only if at least one of functions \( s_j(\cdot) \) in the decomposition (2.20) has pole \( k_0 \) of order 2. In that case, the simple analysis of (2.21) shows that \( \theta_+ = \theta = \theta_{k_0} \). Then, in view of (2.18),

\[
\sum_{j=1}^{3} \gamma_j^2 = 0, \quad \theta_+ = \theta = \theta_{k_0} = \frac{1}{\gamma_0}. \tag{6.1}
\]

We note that not all coefficients \( \gamma_j \) are equal to zero in the first relation of (6.1). Indeed, suppose that \( \gamma_1 = \gamma_2 = \gamma_3 = 0 \). Then \( \vec{\xi} = \gamma_0 \sigma_0 \) and \( \theta_\sigma \theta_\sigma = 1/\gamma_0^2 \). Substituting these quantities into (2.19), we obtain

\[
S(k) = \left[ 1 - \frac{4ik}{\theta_\sigma - 1/\gamma_0} \right] \sigma_0 = - \frac{k + k_0}{k - k_0} \sigma_0.
\]

Therefore, \( k_0 \) cannot be a pole of order 2. The obtained contradiction means that at least one of coefficients \( k, \gamma_1, \gamma_2, \gamma_3 \) differs from zero. In that case, the matrix

\[
\sigma_0 - \theta_{k_0} \vec{\xi} = (1 - \theta_{k_0} \gamma_0) \sigma_0 - \theta_{k_0} \sum_{j=1}^{3} \gamma_j \sigma_j = - \theta_{k_0} \sum_{j=1}^{3} \gamma_j \sigma_j
\]

is nonzero.

On the other hand, taking (6.1) and properties of Pauli matrices into account,

\[
(\sigma_0 - \theta_{k_0} \vec{\xi})^2 = \theta_{k_0}^2 \left( \sum_{j=1}^{3} \gamma_j \sigma_j \right)^2 = \theta_{k_0}^2 \left( \sum_{j=1}^{3} \gamma_j^2 \right) \sigma_0 = 0.
\]

Conversely, let \( \sigma_0 - \theta_{k_0} \vec{\xi} \) be a nonzero and nilpotent matrix. In that case

\[
\sigma_0 - \theta_{k_0} \vec{\xi} = (1 - \theta_{k_0} \gamma_0) \sigma_0 - \theta_{k_0} \sum_{j=1}^{3} \gamma_j \sigma_j \neq 0
\]

and

\[
0 = (\sigma_0 - \theta_{k_0} \vec{\xi})^2 = \left[ (1 - \theta_{k_0} \gamma_0) \sigma_0 - \theta_{k_0} \sum_{j=1}^{3} \gamma_j \sigma_j \right]^2 = \\
\left[ (1 - \theta_{k_0} \gamma_0)^2 + \theta_{k_0}^2 \sum_{j=1}^{3} \gamma_j^2 \right] \sigma_0 + 2 \left( 1 - \theta_{k_0} \gamma_0 \right) \theta_{k_0} \sum_{j=1}^{3} \gamma_j \sigma_j.
\]

These relations are possible only in the case: \( 1 - \theta_{k_0} \gamma_0 \neq 0 \) and \( \sum_{j=1}^{3} \gamma_j^2 = 0 \), where at least one \( \gamma_j \) differs from zero. Then \( \theta_{k_0} = \theta_\sigma = \theta = 1/\gamma_0 \), and \( k_0 = i - \frac{1}{2\gamma_0} \) is a pole of order 2 of \( S(\cdot) \). Corollary 6.3 is proved. \( \square \)

In the particular case where \( A_\sigma = A_\tau \), the (possible) appearance of exceptional points is determined by parameters \( a, d \).
Corollary 6.4. Let \( z_0 = k_0^2 \) be an exceptional point of \( A_T \). Then
\[
k_0 = -\frac{i (4 - \det T + 4a)}{4 - \det T - 4d} = \frac{i (4 - \det T)}{4d}
\]
and \( z = k_0^2 = \frac{a}{d} \).

**Proof.** If \( z_0 = k_0^2 \) is an exceptional point of \( A_T \), then \( k_0 \in \mathbb{C}_+ \) is a pole of order 2 of \( S(\cdot) \). Then \( k_0 = i \frac{a}{d} \) and the first relation in (6.2) follows from (2.23).

Using (2.24), (6.1) and taking into account that
\[
(4 - \det T)^2 + 16ad = (4 - ad + bc)^2 + 16ad = (4 + ad - bc)^2 + 16bc = (4 + \det T)^2 + 16bc
\]
we conclude that \( (4 - \det T)^2 + 16ad = 0 \). Therefore,
\[
k_0 = -\frac{i (4 - \det T + 4d)}{4 - \det T - 4d} = -\frac{i (4 - \det T + 4d)}{4 - \det T - 4d} = \frac{i (4 - \det T)}{4d}.
\]
To complete the proof it suffices to calculate
\[
z = k_0^2 = -\frac{(4 - \det T)^2}{16d^2} = \frac{16ad}{16d^2} = \frac{a}{d}.
\]

The \( S \)-matrices in examples I–IV do not have poles of order 2. Hence, the corresponding operators \( A_T \) do not have exceptional points.

**Example V.** Let \( a = -e^\phi \), \( b = -1 \), \( c=1 \), and \( d = e^{-i\phi} \). Then (2.1) takes the form
\[
-\frac{d^2}{dx^2} - e^\phi < \delta(x) - < \delta', \cdot > \delta(x) + < \delta, \cdot > \delta'(x) + e^{i\phi} < \delta', \cdot > \delta(x)
\]
and (2.4) determines the operators \( A_\phi = -\frac{x^2}{dx^2} \) with domains of definition
\[
\mathcal{D}(A_\phi) = \left\{ f \in W^2_2(\mathbb{R}\setminus\{0\}) \mid f(0+) + e^{-i\phi}f'(0+1) = 2f(0-1) \right\}.
\]
If \( \phi \in (0, 2\pi) \), then \( \mathcal{D}(A_\phi) \) can be presented in the form (2.6), where
\[
\Xi = \frac{1}{8 \sin^2\phi/2} \begin{pmatrix} 1 - e^{-i\phi} & 2 \\ 0 & 1 - e^{-i\phi} \end{pmatrix}.
\]
In that case
\[
\theta_\sigma = 2(1 - e^\phi), \quad \det \Xi = \frac{1}{4(1 - e^\phi)} \neq 0.
\]

Substituting these quantities in (2.19) we obtain
\[
S(k) = -\frac{k + ie^\phi \sigma_0}{k - ie^\phi \sigma_0} + \frac{2ik}{(k - ie^\phi)^2} \begin{pmatrix} 0 & 2e^\phi \\ 0 & 0 \end{pmatrix}.
\]

The \( S \)-matrix has pole \( k_0 = ie^\phi \) of order 2 in the physical sheet \( \mathbb{C}_+ \), when \( \phi \in \left(0, \frac{\pi}{2}\right) \cup \left(\frac{3\pi}{2}, 2\pi\right) \). In that case \( z_0 = -e^{2i\phi} \) is an exceptional point of \( A_\phi \). If \( \phi \) coincides other than with \( \frac{\pi}{2} \) or with \( \frac{3\pi}{2} \), then the \( S \)-matrix has the real pole \( k_0 = -1 = k_0 \), respectively. The operator \( A_\phi \) has spectral singularity \( z_0 = 1 \). If \( \phi \in \left(\frac{\pi}{2}, \frac{3\pi}{2}\right) \), then the pole \( k_0 \) of the \( S \)-matrix belongs to the nonphysical sheet \( \mathbb{C}_- \). In this case \( A_\phi \) is similar to a self-adjoint operator.
7. Conclusions

This paper shows that poles of $S$-matrix $S(\cdot)$ completely characterize the properties of Schrödinger operators $T_A$ with non-symmetric zero-range potentials (2.2). Precisely, poles of $S(\cdot)$ on the physical sheet $\mathbb{C}_+$ describe the discrete spectrum $\sigma_p$ of $T_A$. The (possible) appearance of exceptional points on $\sigma_p$ is distinguished by poles of order 2 on the physical sheet. The existence of spectral singularities on the continuous spectrum $\sigma_c$ of $T_A$ is determined by poles of $S(\cdot)$ on the extended real line $\mathbb{R} = \mathbb{R} \cup \{\infty\}$. The property of similarity of $T_A$ to a self-adjoint operator means that the $S$-matrix $S(\cdot)$ has poles in the nonphysical sheet $\mathbb{C}_-$ or $S(\cdot)$ has simple nonzero imaginary poles.

Not every operator $T_A$ defined by (2.6) can be interpreted as pseudo-Hermitian or $\mathcal{PT}$-symmetric. The operators $T_A$ are examples of quasi-self-adjoint operators [19]. It should be noted that the notion of quasi-self-adjoint operators in mathematical literature completely differs from the Dieudonné’s notion of quasi-Hermitian operators [20]. Precisely, let $A_s$ be a symmetric operator with deficiency indices $(m, m)$ ($m < \infty$) acting in a Hilbert space $\mathcal{H}$. An operator $A$ is a quasi-self-adjoint extension of $A_s$ if $A_s \subseteq A \subseteq A_s^*$ (i.e., $A$ is a proper extension of $A_s$) and $\dim \mathcal{D}(A) = m$ (mod $\mathcal{D}(A_s)$).

Our studies show that techniques based on the decomposition of an $S$-matrix with respect to the Pauli matrices turned out to be very useful for investigation of quasi-self-adjoint operators. In this way, we find explicit expressions of metric operators for the case where $S$-matrix has simple nonzero imaginary poles.

The results of the paper were established with the use of expression (2.9) for $S$-matrices which comes from the Lax–Phillips scattering theory and is close to the concept of characteristic function of quasi-self-adjoint operators [19]. Using the equivalent representation (2.28) of the $S$-matrix we can reformulate the obtained results in terms of reflection and transmission coefficients.

The methods used in the paper can be easily generalized to the case of non-symmetric potentials with compact support [9]. It would be very interesting to extend the Lax–Phillips technique for certain long-range potentials and try to clarify the known relations between bound states and poles of an $S$-matrix (see e.g., [21]).

In the paper, the $S$-matrix of a general complex point interaction [11, 12] is studied with the use of non-self-adjoint extension technique for symmetric operators. Due to the specific structure of the perturbation, the model is exactly solvable and the obtained results have the capability to provide some deeper insights into the structural subtleties of scattering theory: the reflectionless potentials [22] and the theory of optical spectral singularities [23].

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