

## SCHRÖDINGER OPERATORS WITH NON-SYMMETRIC ZERO-RANGE POTENTIALS

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*Dedicated to Professor V. D. Koshmanenko on the occasion of his seventieth birthday*

ABSTRACT. Non-self-adjoint Schrödinger operators  $A_{\mathbf{T}}$  which correspond to non-symmetric zero-range potentials are investigated. For a given  $A_{\mathbf{T}}$ , a description of non-real eigenvalues, spectral singularities and exceptional points are obtained; the possibility of interpretation of  $A_{\mathbf{T}}$  as a self-adjoint operator in a Krein space is studied, the problem of similarity of  $A_{\mathbf{T}}$  to a self-adjoint operator in a Hilbert space is solved.

### 1. INTRODUCTION

An important class of Schrödinger operators is formed by operators with singular perturbations. For example, this class contains Schrödinger operators with zero-range potentials or point interactions. These operators effectively simulate short range interactions and belong to the class of exactly solvable models. Numerous works are devoted to a study of singularly perturbed Schrödinger operators, in which a series of approaches to the construction and investigation of such operators are developed (see, e.g., [1, 2, 3, 12, 13] and references therein). These studies, in the majority of cases, deal with *symmetric singular perturbations* that lead to *self-adjoint* Schrödinger operators.

In the present paper we study *non-self-adjoint* Schrödinger operators which correspond to non-symmetric zero-range potentials.

Our work was inspired in part by an intensive development of Pseudo-Hermitian ( $\mathcal{PT}$ -Symmetric) Quantum Mechanics PHQM (PTQM) during last decades [7, 8, 16]. The key point of PHQM/PTQM theories is the employing of non-self-adjoint operators with certain properties of symmetry for the description of experimentally observable data. Briefly speaking, in order to interpret a given non-self-adjoint operator  $A$  in a Hilbert space  $\mathfrak{H}$  as a physically meaning Hamiltonian we have to check the reality of its spectrum and to prove the existence of a new inner product that ensures the (hidden) self-adjointness of  $A$ .

The paper is devoted to the implementation of this program for various classes ( $\mathcal{PT}$ -symmetric operators,  $\delta$ - and  $\delta'$ - potentials with complex couplings, see definitions in Examples II-IV of Sec. 2) of non-self-adjoint Schrödinger operators  $A_{\mathbf{T}}$  corresponding to the Schrödinger type differential expression (2.1) with singular zero-range potential

$$a < \delta, \cdot > \delta(x) + b < \delta', \cdot > \delta(x) + c < \delta, \cdot > \delta'(x) + d < \delta', \cdot > \delta'(x),$$

where the parameters  $a, b, c, d$  are complex numbers. The matrix  $\mathbf{T}$  is formed by these parameters and operators  $A_{\mathbf{T}}$  are defined by Lemma 2.1.

In Sec. 2, the necessary and sufficient conditions for the existence of non-real eigenvalues, spectral singularities and exceptional points of  $A_{\mathbf{T}}$  are given.

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Sec. 3 is devoted to an interpretation of  $A_{\mathbf{T}}$  as a self-adjoint operator in a Krein space. Such kind of self-adjointness cannot be considered as completely satisfactory in PHQM/PTQM because it does not guarantee unitarity of the dynamics generated by  $A_{\mathbf{T}}$ . However, possible realization of  $A_{\mathbf{T}}$  as self-adjoint with respect to some indefinite metrics (indefinite inner product) allows us to apply well-developed tools of the Krein spaces theory [6] to solving the problem of similarity of  $A_{\mathbf{T}}$  to a self-adjoint operator in a Hilbert space. The similarity property means that  $A_{\mathbf{T}}$  turns out to be a self-adjoint operator in a Hilbert space with respect to a suitably chosen inner product.

In Sec. 4, we solve the similarity problem for  $A_{\mathbf{T}}$  with the use of a general criterion of similarity [18] and the Krein spaces methods.

The properties of  $A_{\mathbf{T}}$  established in the paper illustrate a typical PHQM/PTQM evolution of spectral properties which can be obtained by changing entries of  $\mathbf{T}$ : complex eigenvalues  $\rightarrow$  spectral singularities / exceptional points  $\rightarrow$  similarity to a self-adjoint operator. For this reason, the operators  $A_{\mathbf{T}}$  considered in the work can be used as exactly solvable models of PHQM/PTQM.

Throughout the paper  $\mathcal{D}(A)$ ,  $\mathcal{R}(A)$ , and  $\ker A$  denote the domain, the range, and the null-space of a linear operator  $A$ , respectively, while  $A \upharpoonright \mathcal{D}$  stands for the restriction of  $A$  to the set  $\mathcal{D}$ . The resolvent set and the spectrum of an operator  $A$  are denoted as  $\rho(A)$  and  $\sigma(A)$ , respectively.

## 2. OPERATOR REALIZATIONS AND THEIR SIMPLEST PROPERTIES

A one-dimensional Schrödinger operator corresponding to a general zero-range potential at the point  $x = 0$  can be defined by the heuristic expression

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

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.

The expression (2.1) gives rise to the symmetric operator

$$(2.2) \quad A_{\text{sym}} = -\frac{d^2}{dx^2}, \quad \mathcal{D}(A_{\text{sym}}) = \{u(x) \in W_2^2(\mathbb{R}) \mid u(0) = u'(0) = 0\}$$

acting in  $L_2(\mathbb{R})$  and, generally speaking, any proper extension  $A$  of  $A_{\text{sym}}$  (i.e.,  $A_{\text{sym}} \subset A \subset A_{\text{sym}}^*$ ) can be considered as an operator realization of (2.1) in  $L_2(\mathbb{R})$ .

In order to specify more exactly which a proper extension  $A$  of  $A_{\text{sym}}$  corresponds to (2.1) we will use an approach suggested in [3]. The idea consists in the construction of some regularization  $\mathbb{A}_{\mathbf{r}}$  of (2.1) that is well defined as an operator from  $\mathcal{D}(A_{\text{sym}}^*) = W_2^2(\mathbb{R} \setminus \{0\})$  to  $W_2^{-2}(\mathbb{R})$ . Then, the corresponding operator realization of (2.1) in  $L_2(\mathbb{R})$  is determined as follows:

$$(2.3) \quad A = \mathbb{A}_{\mathbf{r}} \upharpoonright_{\mathcal{D}(A)}, \quad \mathcal{D}(A) = \{f \in \mathcal{D}(A_{\text{sym}}^*) \mid \mathbb{A}_{\mathbf{r}} f \in L_2(\mathbb{R})\}.$$

To obtain a regularization of (2.1) it suffices to extend the distributions  $\delta$  and  $\delta'$  onto  $W_2^2(\mathbb{R} \setminus \{0\})$ . The most reasonable way (based on preserving of initial homogeneity of  $\delta$  and  $\delta'$  with respect to scaling transformations, see, for details, [3], [9]) leads to the following definition:

$$< \delta_{\text{ex}}, f > = \frac{f(+0) + f(-0)}{2}, \quad < \delta'_{\text{ex}}, f > = -\frac{f'(+0) + f'(-0)}{2}$$

for all  $f(x) \in W_2^2(\mathbb{R} \setminus \{0\})$ . In this case, the regularization of (2.1) onto  $W_2^2(\mathbb{R} \setminus \{0\})$  takes the form

$$\mathbb{A}_{\mathbf{r}} = -\frac{d^2}{dx^2} + a < \delta_{\text{ex}}, \cdot > \delta(x) + b < \delta'_{\text{ex}}, \cdot > \delta(x) + c < \delta_{\text{ex}}, \cdot > \delta'(x) + d < \delta'_{\text{ex}}, \cdot > \delta'(x),$$

where  $-d^2/dx^2$  acts on  $W_2^2(\mathbb{R} \setminus \{0\})$  in the distributional sense.

The definition (2.3) is not always easy to use. Repeating the proof of Theorem 1 in [5] we obtain an equivalent description of operators determined by (2.3).

**Lemma 2.1.** *Let  $A$  be determined by (2.3). Then  $A$  coincides with the restriction of  $A_{\text{sym}}^* = -d^2/dx^2$  onto the domain*

$$(2.4) \quad \mathcal{D}(A) = \{f(x) \in W_2^2(\mathbb{R} \setminus \{0\}) \mid \mathbf{T}\Gamma_0 f = \Gamma_1 f\}, \quad \mathbf{T} = \begin{pmatrix} a & b \\ c & d \end{pmatrix},$$

where

$$(2.5) \quad \Gamma_0 f = \frac{1}{2} \begin{pmatrix} f(+0) + f(-0) \\ -f'(+0) - f'(-0) \end{pmatrix}, \quad \Gamma_1 f = \begin{pmatrix} f'(+0) - f'(-0) \\ f(+0) - f(-0) \end{pmatrix}.$$

**Remark 2.2.** In what follows the notation  $A_{\mathbf{T}}$  will be used for operator realizations of (2.1) defined by (2.4) and (2.5).

It is known that the continuous spectrum of an operator  $A_{\mathbf{T}}$  coincides with  $[0, \infty)$  and the point spectrum of  $A_{\mathbf{T}}$  may appear only in  $\mathbb{C} \setminus \mathbb{R}_+$ .

Denote

$$(2.6) \quad \mathbf{det} \mathbf{T} = ad - bc.$$

**Lemma 2.3.** *An operator  $A_{\mathbf{T}}$  has an eigenvalue  $z = \tau^2$  if and only if the equation*

$$(2.7) \quad 2d\tau^2 + i(\mathbf{det} \mathbf{T} - 4)\tau + 2a = 0$$

has a solution  $\tau \in \mathbb{C}_+ = \{\tau \in \mathbb{C} : \text{Im } \tau > 0\}$ .

*Proof.* Let us denote by  $\tau$  the square root of the energy parameter  $z = \tau^2$  determined uniquely by the condition  $\text{Im } \tau > 0$  and consider the functions

$$(2.8) \quad h_{1\tau}(x) = \begin{cases} e^{i\tau x}, & x > 0 \\ e^{-i\tau x}, & x < 0 \end{cases}, \quad h_{2\tau}(x) = \begin{cases} -e^{i\tau x}, & x > 0 \\ e^{-i\tau x}, & x < 0 \end{cases}$$

that form a basis of  $\ker(A_{\text{sym}}^* - zI)$ , where  $z = \tau^2$  runs  $\mathbb{C} \setminus \mathbb{R}_+$ . It is clear that  $z$  belongs to the point spectrum of  $A$  if and only if there exists a function  $f \in \ker(A_{\text{sym}}^* - zI) \cap \mathcal{D}(A)$ . Representing  $f(x)$  in the form

$$f(x) = c_1 h_{1\tau}(x) + c_2 h_{2\tau}(x), \quad c_i \in \mathbb{C}$$

and substituting this expression into (2.4) we arrive at the conclusion that  $z$  is an eigenvalue of  $A$  if and only if the system of equations

$$\begin{aligned} (a - 2i\tau)c_1 + i\tau c_2 &= 0, \\ cc_1 + (id\tau + 2)c_2 &= 0 \end{aligned}$$

has a nontrivial solution  $c_1, c_2$ . This is possible if the determinant of the coefficient matrix of the system is equal to zero, i.e.,  $2d\tau^2 + i(ad - bc - 4)\tau + 2a = 0$ . Rewriting the obtained equation in the form (2.7) we complete the proof.  $\square$

**Definition 2.4.** *Let  $A_{\mathbf{T}}$  be defined by (2.4), (2.5) and let the spectrum of  $A_{\mathbf{T}}$  do not coincide with  $\mathbb{C}$ . We will say that the operator  $A_{\mathbf{T}}$  has:*

- a nonzero spectral singularity  $z = \tau^2$  if the equation (2.7) has a solution  $\tau \in \mathbb{R} \setminus \{0\}$ ;
- a spectral singularity at point  $z = 0$  if (2.7) has a solution  $\tau = 0$  with multiplicity 2;
- a spectral singularity at point  $z = \infty$  if there are no solutions of (2.7) in  $\mathbb{C}$ .

The non-self-adjoint operator  $A_{\mathbf{T}}$  has an exceptional point  $z = \tau^2$  if the equation (2.7) has a solution  $\tau \in \mathbb{C}_+$  with multiplicity 2.

A spectral singularity (an exception point)  $z$  lies on the continuous spectrum (on the point spectrum) of  $A_{\mathbf{T}}$  and it is a serious defect that rules out the operator as a viable candidate for a physical observable [11, 15].

**Example I.** *Symmetric potential.*

The singular potential

$$(2.9) \quad V = a \langle \delta, \cdot \rangle \delta(x) + b \langle \delta', \cdot \rangle \delta(x) + c \langle \delta, \cdot \rangle \delta'(x) + d \langle \delta', \cdot \rangle \delta'(x)$$

in (2.1) is symmetric (i.e.,  $V^* = V$ ) if and only if

$$(2.10) \quad a, d \in \mathbb{R}, \quad c = \bar{b}.$$

The corresponding operators  $A_{\mathbf{T}}$  turn out to be self-adjoint operators in  $L_2(\mathbb{R})$  with respect to the initial inner product

$$(2.11) \quad (f, g) = \int_{\mathbb{R}} f(x) \overline{g(x)} dx.$$

**Lemma 2.5.** *The spectrum  $\sigma(A_{\mathbf{T}})$  is real and it contains the continuous part  $[0, \infty)$  and possibly, negative eigenvalues. There are no spectral singularities and exceptional points.*

*Proof.* An operator  $A_{\mathbf{T}}$  is a finite dimensional extension of the symmetric operator  $A_{\text{sym}}$  determined by (2.2). This means that the continuous spectrum of  $A_{\mathbf{T}}$  coincides with  $[0, \infty)$ .

Let  $d \neq 0$ . Then the solutions  $\tau_{1,2}$  of (2.7) have the form

$$(2.12) \quad \tau_{1,2} = i \frac{4 - \mathbf{det} \mathbf{T} \pm \sqrt{D}}{4d},$$

where  $\mathbf{det} \mathbf{T}$  and  $D = (4 - \mathbf{det} \mathbf{T})^2 + 16ad$  are real numbers.

Taking (2.6) into account we rewrite

$$(2.13) \quad D = (4 - ad + bc)^2 + 16ad = (4 + ad - bc)^2 + 16bc = (4 + \mathbf{det} \mathbf{T})^2 + 16bc.$$

Moreover, in view of (2.10),  $bc = |b|^2$ . Therefore  $D = (4 + \mathbf{det} \mathbf{T})^2 + 16|b|^2 \geq 0$ . This means that the solutions  $\tau_{1,2}$  determined by (2.12) *always belong to  $i\mathbb{R}$* .

Similarly, if  $d = 0$ , equation (2.7) is reduced to  $-i(|b|^2 + 4)\tau + 2a = 0$ . The solution  $\tau_1 = -2ai/(|b|^2 + 4)$  *belongs to  $i\mathbb{R}$* .

The two cases above and Lemma 2.3 show that  $A_{\mathbf{T}}$  may have negative eigenvalues  $z = \tau^2$  and there are no spectral singularities and exceptional points of  $A_{\mathbf{T}}$ .  $\square$

**Example II.**  *$\mathcal{PT}$ -symmetric potential.*

Denote by  $\mathcal{P}$  and  $\mathcal{T}$  the operators of space parity and complex conjugation, respectively

$$(2.14) \quad \mathcal{P}f(x) = f(-x), \quad \mathcal{T}f(x) = \overline{f(x)}.$$

The potential  $V$  is called  $\mathcal{PT}$ -symmetric if  $\mathcal{PT}V = V\mathcal{PT}$ . Extending  $\mathcal{P}$  onto  $W_2^{-2}(\mathbb{R})$ , one gets  $\mathcal{P}\delta = \delta$  and  $\mathcal{P}\delta' = -\delta'$ . These relations and (2.9) imply that  $V$  is  $\mathcal{PT}$ -symmetric if and only if<sup>1</sup>

$$(2.15) \quad a, d \in \mathbb{R}, \quad b, c \in i\mathbb{R}.$$

The corresponding operators  $A_{\mathbf{T}}$  turn out to be  $\mathcal{PT}$ -symmetric operators, i.e., the relation

$$(2.16) \quad \mathcal{PT}A_{\mathbf{T}} = A_{\mathbf{T}}\mathcal{PT}$$

holds on the domain  $\mathcal{D}(A_{\mathbf{T}})$ .

<sup>1</sup>the cases of symmetric and  $\mathcal{PT}$ -symmetric potentials differs by conditions imposed on parameters  $b, c$ .

**Remark 2.6.** In what follows we will often use operator identities

$$(2.17) \quad XA = BX,$$

where  $A$  and  $B$  are (possible) unbounded operators in  $L_2(\mathbb{R})$  and  $X$  is a bounded operator in  $L_2(\mathbb{R})$ . In that case, we *always assume that (2.17) holds on  $\mathcal{D}(A)$* . This means that  $X : \mathcal{D}(A) \rightarrow \mathcal{D}(B)$  and the identity  $XAu = BXu$  holds for all  $u \in \mathcal{D}(A)$ . If  $A$  is bounded, then (2.17) should hold on the whole  $L_2(\mathbb{R})$ . In particular, relation (2.15) means that the operator  $\mathcal{PT}$  maps  $\mathcal{D}(A_{\mathbf{T}})$  onto  $\mathcal{D}(A_{\mathbf{T}})$  and  $\mathcal{PT}A_{\mathbf{T}}f = A_{\mathbf{T}}\mathcal{PT}f$  for all  $f \in \mathcal{D}(A_{\mathbf{T}})$ .

Comparing the condition of self-adjointness (2.10) and the condition of  $\mathcal{PT}$ -symmetry (2.16) we obtain that  $\mathcal{PT}$ -symmetric operators  $A_{\mathbf{T}}$  are not self-adjoint with respect to the initial inner product (2.11) except the case  $b = -c \in i\mathbb{R}$ . Therefore,  $\mathcal{PT}$ -symmetric operators  $\mathcal{D}(A_{\mathbf{T}})$  may have non-real eigenvalues. In particular, it may happen that the set of complex eigenvalues of  $A_{\mathbf{T}}$  coincide with  $\mathbb{C} \setminus \mathbb{R}_+$ .

**Lemma 2.7.** 1. A  $\mathcal{PT}$ -symmetric operator  $A_{\mathbf{T}}$  has non-real eigenvalues if and only if one of the following conditions are satisfied:

- (i)  $D = (4 - \mathbf{det} \mathbf{T})^2 + 16ad < 0$ ,  $(4 - \mathbf{det} \mathbf{T})d > 0$ ;
- (ii)  $\mathbf{det} \mathbf{T} = 4$ ,  $a = d = 0$ .

Condition (i) corresponds to the case where  $A_{\mathbf{T}}$  has two non-real eigenvalues, which are conjugate to each other. Condition (ii) describes the situation where any point  $z \in \mathbb{C} \setminus \mathbb{R}_+$  is an eigenvalue of  $A_{\mathbf{T}}$ . In that case the spectrum of  $A_{\mathbf{T}}$  coincides with  $\mathbb{C}$ ;

2. A  $\mathcal{PT}$ -symmetric operator  $A_{\mathbf{T}}$  has:

- nonzero spectral singularity if and only if

$$(iii) \quad D < 0, \quad (4 - \mathbf{det} \mathbf{T})d = 0.$$

In that case, the positive number  $z = -\frac{a}{d}$  is the spectral singularity of  $A_{\mathbf{T}}$ ;

- spectral singularity at point  $z = 0$  if and only if

$$(iv) \quad D = 0, \quad (4 - \mathbf{det} \mathbf{T})d = 0, \quad d \neq 0, \quad a = 0;$$

- spectral singularity at point  $z = \infty$  if and only if

$$(v) \quad D = 0, \quad (4 - \mathbf{det} \mathbf{T})d = 0, \quad d = 0, \quad a \neq 0;$$

- exceptional point if and only if

$$(vi) \quad D = 0, \quad (4 - \mathbf{det} \mathbf{T})d > 0.$$

In that case, the negative number  $z = \frac{a}{d}$  is the exceptional point of  $A_{\mathbf{T}}$ .

*Proof.* Let  $A_{\mathbf{T}}$  be a  $\mathcal{PT}$ -symmetric operator. Then, the values of  $\mathbf{det} \mathbf{T}$  and  $D$  are real (it follows from (2.15)).

Using Lemma 2.3 and (2.12), we arrive at the conclusion that condition (i) is necessary and sufficient for the existence of two non-real eigenvalues  $z_{1,2} = \tau_{1,2}^2$  of  $A_{\mathbf{T}}$ , which are conjugate to each other.

The requirement that any point  $z = \tau^2 \in \mathbb{C} \setminus \mathbb{R}_+$  is an eigenvalue of  $A_{\mathbf{T}}$  is equivalent to the condition that any  $\tau \in \mathbb{C}_+$  is a solution of (2.7). This is possible only in the case where the left-hand side of (2.7) vanishes. The latter is equivalent to the condition (ii).

It follows from (2.12) that a nonzero spectral singularity exists in the case where  $D = (4 - \mathbf{det} \mathbf{T})^2 + 16ad < 0$  and  $\mathbf{det} \mathbf{T} = 4$  that is equivalent to (iii). In that case,  $\tau_{1,2} = \pm \sqrt{-\frac{a}{d}}$  and  $z = \tau_{1,2}^2 = -\frac{a}{d}$ .

The descriptions (iv) and (v) of spectral singularities at 0 and at  $\infty$  are obvious due to (2.7).

By Definition 2.4 a point  $z = \tau^2$  ( $\tau \in \mathbb{C}_+$ ) is an exceptional point of  $A_{\mathbf{T}}$  if its multiplicity is 2. Hence,  $d \neq 0$  in (2.7) and  $\tau$  is determined by (2.12) with  $D = 0$ .

Furthermore, the condition  $\tau \in \mathbb{C}_+$  implies  $(4 - \mathbf{det} \mathbf{T})d > 0$ . Thus we show that condition (vi) corresponds to exceptional points. In that case

$$z = \tau^2 = -\frac{(4 - \mathbf{det} \mathbf{T})^2}{16d^2} = \frac{16ad}{16d^2} = \frac{a}{d} < 0$$

(since  $D = 0$ ,  $(4 - \mathbf{det} \mathbf{T}) \neq 0$  and hence,  $ad < 0$ ). Lemma 2.7 is proved.  $\square$

**Example III.**  $\delta$ -potential with a complex coupling [15].

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) gives rise to operators  $A_{\mathbf{T}} \equiv A_a = -\frac{d^2}{dx^2}$  with domains of definition

$$\mathcal{D}(A_a) = \left\{ f(x) \in W_2^2(\mathbb{R} \setminus \{0\}) \mid \begin{array}{l} f(0+) = f(0-) (\equiv f(0)) \\ f'(0+) - f'(0-) = af(0) \end{array} \right\}.$$

By virtue of Lemma 2.3 and Definition 2.4 we conclude:

- if  $\operatorname{Re} a < 0$ , then  $A_a$  has a unique eigenvalue  $z = -a^2/4$ , which is real  $\iff \operatorname{Im} a = 0$ ;
- if  $\operatorname{Re} a \geq 0$ , then the spectrum of  $A_a$  is real, continuous and it coincides with  $[0, \infty)$ ;
- if  $a \in i\mathbb{R} \setminus \{0\}$ , then  $A_a$  has spectral singularity  $z = \frac{|a|^2}{4}$ ;
- there are no exceptional points of  $A_a$ .

**Example IV.**  $\delta'$ -potential with a complex coupling.

Let  $d \in \mathbb{C}$  and  $a = b = c = 0$ . Then (2.1) takes the form

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

and (2.4) gives rise to operators  $A_{\mathbf{T}} \equiv A_d = -\frac{d^2}{dx^2}$  with domains of definition

$$\mathcal{D}(A_d) = \left\{ f(x) \in W_2^2(\mathbb{R} \setminus \{0\}) \mid \begin{array}{l} f'(0+) = f'(0-) (\equiv f'(0)) \\ f(0+) - f(0-) = -df'(0) \end{array} \right\}.$$

By virtue of Lemma 2.3 and Definition 2.4:

- if  $\operatorname{Re} d > 0$ , then  $A_d$  has a unique eigenvalue  $z = -4/d^2$ , which is real  $\iff \operatorname{Im} d = 0$ ;
- if  $\operatorname{Re} d \leq 0$ , then the spectrum of  $A_d$  is real, continuous and it coincides with  $[0, \infty)$ ;
- if  $d \in i\mathbb{R} \setminus \{0\}$ , then  $A_d$  has spectral singularity  $z = \frac{4}{|d|^2}$ ;
- there are no exceptional points of  $A_d$ .

### 3. INTERPRETATION AS SELF-ADJOINT OPERATORS IN KREIN SPACES

Let  $\mathfrak{H}$  be a Hilbert space with inner product  $(\cdot, \cdot)$  and with fundamental symmetry  $J$  (i.e.,  $J = J^*$  and  $J^2 = I$ ). The space  $\mathfrak{H}$  endowed with the indefinite inner product (indefinite metric)  $[f, g]_J := (Jf, g)$ ,  $\forall f, g \in \mathfrak{H}$  is called a Krein space  $(\mathfrak{H}, [\cdot, \cdot]_J)$ .

The difference between the initial inner product  $(\cdot, \cdot)$  and indefinite metric  $[\cdot, \cdot]_J$  consists in the fact that, except the cases  $J = \pm I$ , the sign of the sesquilinear form  $[f, f]_J$  is not determined (i.e, it is possible  $[f, f]_J < 0$ ,  $[f, f]_J = 0$ , or  $[f, f]_J > 0$  for various  $f \neq 0$ ). The Hilbert space  $\mathfrak{H}$  can be considered as a particular case of the Krein space  $(\mathfrak{H}, [\cdot, \cdot]_J)$  with  $J = I$ .

A linear densely defined<sup>2</sup> operator  $A$  acting in  $\mathfrak{H}$  is called self-adjoint in the Krein space  $(\mathfrak{H}, [\cdot, \cdot]_J)$  if  $A$  is self-adjoint with respect to the indefinite metric  $[\cdot, \cdot]_J$ . This condition is equivalent to the relation

$$(3.1) \quad A^* = JAJ.$$

The spectrum of a self-adjoint operator in Krein space is symmetric with respect to the real axis. For an additional information about Krein spaces and operators acting therein we refer to [6].

We recall [16, 17] that a linear densely defined operator  $A$  acting in a Hilbert space  $\mathfrak{H}$  is said to be *pseudo-Hermitian* if there exists a bounded and boundedly invertible self-adjoint operator  $\eta : \mathfrak{H} \rightarrow \mathfrak{H}$  such that

$$(3.2) \quad A^* = \eta A \eta^{-1}.$$

Relation (3.2) means that  $A$  is self-adjoint with respect to the pseudo-metric  $[\cdot, \cdot]_\eta = (\eta \cdot, \cdot)$ .

It follows from (3.1) and (3.2) that self-adjoint operators in Krein spaces are pseudo-Hermitian. The inverse implication is also true. Indeed, let  $A$  be pseudo-Hermitian. Then (3.2) holds for some  $\eta$ . Denote

$$(3.3) \quad |\eta| = \sqrt{\eta^2}, \quad J = \eta|\eta|^{-1}$$

and consider the Hilbert space  $(\mathfrak{H}, (\cdot, \cdot)_{|\eta|})$  endowed with new (equivalent to  $(\cdot, \cdot)$ ) inner product  $(\cdot, \cdot)_{|\eta|} = (|\eta| \cdot, \cdot)$ . Then, the pseudo-metric  $[\cdot, \cdot]_\eta$  coincides with the indefinite metric  $[\cdot, \cdot]_{J|\eta|} = (J \cdot, \cdot)_{|\eta|}$  constructed with the use of fundamental symmetry  $J = \eta|\eta|^{-1}$  and new inner product  $(\cdot, \cdot)_{|\eta|}$ , i.e.,

$$[\cdot, \cdot]_\eta = (\eta \cdot, \cdot) = (J|\eta| \cdot, \cdot) = (J \cdot, \cdot)_{|\eta|} = [\cdot, \cdot]_{J|\eta|}.$$

This means that  $A$  turns out to be a self-adjoint operator in the Krein space  $(\mathfrak{H}, [\cdot, \cdot]_{J|\eta|})$ .

**Example II contd.** It is known [14] that an arbitrary  $\mathcal{PT}$ -symmetric operator  $A_{\mathbf{T}}$  can be interpreted as self-adjoint one in a suitable chosen Krein space  $(L_2(\mathbb{R}), [\cdot, \cdot]_J)$ . Using [14] we can specify the relevant indefinite metrics  $[\cdot, \cdot]_J$ . Denote

$$(3.4) \quad \mathcal{R}f(x) = \text{sign}(x)f(x), \quad f \in L_2(\mathbb{R}).$$

The operator  $\mathcal{R}$  is a fundamental symmetry which anti-commutes with  $\mathcal{P}$ :  $\mathcal{P}\mathcal{R} = -\mathcal{R}\mathcal{P}$ . It is easy to check that the operator  $i\mathcal{P}\mathcal{R}$  is also a fundamental symmetry and, moreover, any operator

$$(3.5) \quad J_{\vec{\alpha}} = \alpha_1 \mathcal{P} + \alpha_2 \mathcal{R} + \alpha_3 i\mathcal{P}\mathcal{R}, \quad \alpha_j \in \mathbb{R}, \quad \alpha_1^2 + \alpha_2^2 + \alpha_3^2 = 1$$

turns out to be a fundamental symmetry in  $L_2(\mathbb{R})$ .

We consider also a subset of the set of fundamental symmetries  $J_{\vec{\alpha}}$  by imposing an additional condition of  $\mathcal{PT}$ -symmetry:  $\mathcal{PT}J_{\vec{\alpha}} = J_{\vec{\alpha}}\mathcal{PT}$ .

The operator  $J_{\vec{\alpha}}$  is  $\mathcal{PT}$ -symmetric if and only if  $\alpha_2 = 0$ . In that case the latter relation in (3.5) takes the form  $\alpha_1^2 + \alpha_3^2 = 1$  and we may set  $\alpha_1 = \cos \phi$  and  $\alpha_3 = \sin \phi$ . Then

$$J_{\vec{\alpha}} = (\cos \phi) \mathcal{P} + i(\sin \phi) \mathcal{P}\mathcal{R} = \mathcal{P}(\cos \phi + i(\sin \phi) \mathcal{R}) = \mathcal{P}e^{i\phi \mathcal{R}}.$$

Thus, fundamental symmetries  $J_{\vec{\alpha}}$  with the additional property of  $\mathcal{PT}$ -symmetry coincide with fundamental symmetries  $\mathcal{P}_\phi = \mathcal{P}e^{i\phi \mathcal{R}}$ ,  $\phi \in [0, 2\pi)$ .

Consider the following collection of indefinite metrics on  $L_2(\mathbb{R})$ :

$$[\cdot, \cdot]_{J_{\vec{\alpha}}} = (J_{\vec{\alpha}} \cdot, \cdot), \quad [\cdot, \cdot]_{\mathcal{P}_\phi} = (\mathcal{P}_\phi \cdot, \cdot).$$

---

<sup>2</sup> with respect to the initial inner product  $(\cdot, \cdot)$

**Proposition 3.1.** ([14]) *Every  $\mathcal{PT}$ -symmetric operator  $A_{\mathbf{T}}$  can be interpreted as a self-adjoint operator in the Krein space  $(L_2(\mathbb{R}), [\cdot, \cdot]_{\mathcal{P}_\phi})$ , where the parameter  $\phi$  is determined by the relation*

$$(3.6) \quad 2(b - c) \cos \phi = i(4 + \det \mathbf{T}) \sin \phi.$$

Proposition 3.1 shows that the collection of Krein spaces  $(L_2(\mathbb{R}), [\cdot, \cdot]_{\mathcal{P}_\phi})$  generated by  $\mathcal{PT}$ -symmetric fundamental symmetries  $\mathcal{P}_\phi$  is sufficient for the interpretation of  $A_{\mathbf{T}}$  as a self-adjoint operator. The possible interpretation of some  $A_{\mathbf{T}}$  as a self-adjoint operator in a Krein space  $(L_2(\mathbb{R}), [\cdot, \cdot]_{J_{\bar{\alpha}}})$ , where  $J_{\bar{\alpha}}$  is not  $\mathcal{PT}$ -symmetric (i.e.  $J_{\bar{\alpha}} \neq \mathcal{P}_\phi$ ) immediately leads to specific spectral properties of  $A_{\mathbf{T}}$ .

**Proposition 3.2.** ([14]) *Let  $A_{\mathbf{T}}$  be a non-self-adjoint  $\mathcal{PT}$ -symmetric operator. Then*

- *if  $A_{\mathbf{T}}$  admits an interpretation as a self-adjoint operator in a Krein space  $(L_2(\mathbb{R}), [\cdot, \cdot]_{J_{\bar{\alpha}}})$ , where  $J_{\bar{\alpha}}$  is not  $\mathcal{PT}$ -symmetric, then  $\sigma(A_{\mathbf{T}}) = \mathbb{C}$ ;*
- *if  $A_{\mathbf{T}}$  admits an interpretation as a self-adjoint operator in two different Krein spaces  $(L_2(\mathbb{R}), [\cdot, \cdot]_{\mathcal{P}_{\phi_1}})$  and  $(L_2(\mathbb{R}), [\cdot, \cdot]_{\mathcal{P}_{\phi_2}})$ , where  $\mathcal{P}_{\phi_1}$  and  $\mathcal{P}_{\phi_2}$  are linearly independent, then the spectrum of  $A_{\mathbf{T}}$  contains a pair of complex conjugated eigenvalues;*
- *if  $A_{\mathbf{T}}$  has a real spectrum, then  $A_{\mathbf{T}}$  has interpretation as self-adjoint operator for the unique choice<sup>3</sup> of the Krein space  $(L_2(\mathbb{R}), [\cdot, \cdot]_{\mathcal{P}_\phi})$ .*

**Examples III. VI contd.** It follows from (2.10) and (2.15) that operators  $A_a$  ( $A_d$ ) with real  $a$  (real  $d$ ) are self-adjoint in the initial Hilbert space  $L_2(\mathbb{R})$ . Moreover, taking [5] into account, we decide that these operators are self-adjoint in the Krein space  $(L_2(\mathbb{R}), [\cdot, \cdot]_{\mathcal{P}})$ , where

$$(3.7) \quad [f, g]_{\mathcal{P}} = (\mathcal{P}f, g) = \int_{\mathbb{R}} f(-x) \overline{g(x)} dx.$$

If  $a$  is non-real and  $\operatorname{Re} a < 0$  (if  $d$  is non-real and  $\operatorname{Re} d > 0$ ), then  $A_a$  ( $A_d$ ) cannot be interpreted as pseudo-Hermitian operator, or that is equivalent, cannot be interpreted as a self-adjoint operator in a Krein space. Indeed, if we assume that such an interpretation is possible, then the spectrum of  $A_a$  (of  $A_d$ ) must be symmetric with respect to the real axis that contradicts to the fact that the spectrum of  $A_a$  (of  $A_d$ ) contains a unique complex eigenvalue  $z = -a^2/4$  ( $d = -4/d^2$ ).

If  $a \in i\mathbb{R} \setminus \{0\}$ , ( $d \in i\mathbb{R} \setminus \{0\}$ ) the operator  $A_a$  ( $A_d$ ) has a spectral singularity. Hence,  $A_a$  ( $A_d$ ) cannot be interpreted as a self-adjoint in a Hilbert space (see Theorem 4.6). The problem of interpretation of  $A_a$  ( $A_d$ ) as a self-adjoint operator in a Krein space is still open.

If  $\operatorname{Re} a > 0$  ( $\operatorname{Re} d < 0$ ), then the operator  $A_a$  ( $A_d$ ) turns out to be self-adjoint in  $L_2(\mathbb{R})$  for a certain choice of inner product equivalent to the initial one  $(\cdot, \cdot)$  (it follows from Corollary 4.11).

#### 4. SIMILARITY TO SELF-ADJOINT OPERATORS

An operator  $A$  acting in a Hilbert space  $\mathfrak{H}$  is called *similar* to a self-adjoint operator  $H$  if there exists a bounded and boundedly invertible operator  $Z$  such that

$$(4.1) \quad A = Z^{-1}HZ.$$

The similarity of  $A$  to a self-adjoint operator means that  $A$  turns out to be self-adjoint for a certain choice of inner product of  $\mathfrak{H}$ , which is equivalent to the initial inner product  $(\cdot, \cdot)$ . Indeed, let (4.1) hold. By analogy with (3.3) we denote

$$(4.2) \quad |Z| = \sqrt{Z^*Z}, \quad U = Z|Z|^{-1}$$

<sup>3</sup> up to linearly dependent fundamental symmetries  $\mathcal{P}_\phi$



and rewrite (4.1) as follows:

$$H = ZAZ^{-1} = U|Z|A|Z|^{-1}U^{-1} = UKU^{-1}, \quad K = |Z|A|Z|^{-1}.$$

The operator  $U$  is unitary but, in general,  $U$  is not self-adjoint.<sup>4</sup> Taking into account that  $H$  is self-adjoint, we obtain

$$H^* = (UKU^{-1})^* = UK^*U^{-1} = H = UKU^{-1}.$$

Therefore,  $K^* = K$ . Then

$$(|Z|A|Z|^{-1})^* = |Z|^{-1}A^*|Z| = |Z|A|Z|^{-1}$$

or, that is equivalent  $A^*|Z|^2 = |Z|^2A$ . The obtained relation allows us to prove the self-adjointness of  $A$  in the Hilbert space  $(\mathfrak{H}, (\cdot, \cdot)_{|Z|^2})$  endowed with new (equivalent to  $(\cdot, \cdot)$ ) inner product  $(\cdot, \cdot)_{|Z|^2} = (|Z|^2\cdot, \cdot)$ . Indeed,

$$(Af, g)_{|Z|^2} = (|Z|^2Af, g) = (f, A^*|Z|^2g) = (f, |Z|^2Ag) = (f, Ag)_{|Z|^2}, \quad f, g \in \mathcal{D}(A).$$

Thus  $A$  is self-adjoint in the Hilbert space  $(\mathfrak{H}, (\cdot, \cdot)_{|Z|^2})$ .

If  $A$  is a self-adjoint operator in Krein space, then similarity of  $A$  to a self-adjoint operator in a Hilbert space admits an equivalent characterization. Indeed, a characteristic property of a Krein space  $(\mathfrak{H}, [\cdot, \cdot]_J)$  is the possibility of its decomposition onto the direct sum of maximal uniformly positive  $\mathfrak{L}_+$  and maximal uniformly negative  $\mathfrak{L}_-$  subspaces, which are orthogonal with respect to the indefinite metric  $[\cdot, \cdot]_J$ :

$$(4.3) \quad \mathfrak{H} = \mathfrak{L}_+[\dot{+}]\mathfrak{L}_-$$

(here  $[\dot{+}]$  means the orthogonality with respect to the indefinite metric  $[\cdot, \cdot]_J$ ).

The pair of subspaces  $\mathfrak{L}_\pm$  in the decomposition (4.3) is not determined uniquely.

Let  $A$  be an operator in  $\mathfrak{H}$ . We say that the decomposition (4.3) is *invariant with respect to  $A$*  if

$$\mathcal{D}(A) = \mathcal{D}_+[\dot{+}]\mathcal{D}_-, \quad \mathcal{D}_\pm = \mathcal{D}(A) \cap \mathfrak{L}_\pm$$

and  $A = A_+[\dot{+}]A_-$ , where the operators  $A_\pm = A|_{\mathcal{D}_\pm}$  acts in the subspaces  $\mathfrak{L}_\pm$ , respectively.

**Proposition 4.1.** ([4]) *A pseudo-Hermitian operator  $A$  is similar to a self-adjoint operator if and only if there exists decomposition (4.3) of the Krein space<sup>5</sup>  $(\mathfrak{H}, [\cdot, \cdot]_{J|\eta|})$  which is invariant with respect to  $A$ .*

The decomposition (4.3) can be easily characterized with the use of the following operator  $\mathcal{C}$ :

$$(4.4) \quad \mathcal{C}f = \mathcal{C}(f_+ + f_-) = f_+ - f_-, \quad f = f_+ + f_-, \quad f_\pm \in \mathfrak{L}_\pm$$

(since  $\mathfrak{L}_+ = (I + \mathcal{C})\mathfrak{H}$  and  $\mathfrak{L}_- = (I - \mathcal{C})\mathfrak{H}$ ). Therefore, *the invariance of a given decomposition (4.3) with respect to a linear operator  $A$  is equivalent to the relation  $\mathcal{A}\mathcal{C} = \mathcal{C}A$ .*

Assume additionally that  $A$  is self-adjoint in a Krein space  $(\mathfrak{H}, [\cdot, \cdot]_J)$ , then the operators  $A_\pm$  in the decomposition  $A = A_+[\dot{+}]A_-$  are self-adjoint in the Hilbert spaces  $\mathfrak{L}_\pm$  endowed with the inner products  $\pm[\cdot, \cdot]_J$ , respectively. Therefore,  $A$  is self-adjoint in the Hilbert space  $\mathfrak{H}$  with the inner product

$$(f, g)_1 = [f_+, g_+]_J - [f_-, g_-]_J, \quad f = f_+ + f_-, \quad g = g_+ + g_-, \quad f_\pm \in \mathfrak{L}_\pm, \quad g_\pm \in \mathfrak{L}_\pm.$$

Taking the definition of  $\mathcal{C}$  into account, we get  $(\cdot, \cdot)_1 = [\mathcal{C}\cdot, \cdot]_J$ . Moreover, it is known (see, for example, [10]) that every operator  $\mathcal{C}$  defined by (4.4) has the form  $\mathcal{C} = Je^Q$ , where  $Q$  is a *bounded self-adjoint operator in  $\mathfrak{H}$  which anticommutes with  $J$ :  $QJ = -JQ$ .* Therefore,

$$(\cdot, \cdot)_1 = [\mathcal{C}\cdot, \cdot]_J = (JJe^Q\cdot, \cdot) = (e^Q\cdot, \cdot)$$

<sup>4</sup> this is a difference with the operator  $J$  in (3.3).

<sup>5</sup> see Sec. 3 for the definition of the Krein space  $(\mathfrak{H}, [\cdot, \cdot]_{J|\eta|})$ .

and, finally we conclude that  $A$  is self-adjoint in the Hilbert space  $(\mathfrak{H}, (e^Q \cdot, \cdot))$ .

**Proposition 4.2.** *A pseudo-Hermitian operator  $A$  is similar to a self-adjoint operator if and only there exists an operator  $\mathcal{C} = Je^Q$  such that  $J = \eta|\eta|^{-1}$ , the operator  $Q$  satisfies the relations*

$$(4.5) \quad Q^*|\eta| = |\eta|Q, \quad -Q^*\eta = \eta Q$$

and  $AC = CA$ . In that case, the operator  $A$  turns out to be self-adjoint in the Hilbert space  $\mathfrak{H}$  endowed with inner product  $(|\eta|e^Q \cdot, \cdot)$ .

*Proof.* According to Proposition 4.1 the similarity of  $A$  to a self-adjoint operator is equivalent to the existence of decomposition (4.3) of the Krein space  $(\mathfrak{H}, [\cdot, \cdot]_{J|\eta|})$  that is invariant with respect to  $A$ . This condition is equivalent to the relation  $AC = CA$ , where  $\mathcal{C} = Je^Q$  corresponds to the mentioned decomposition of  $(\mathfrak{H}, [\cdot, \cdot]_{J|\eta|})$ . Taking (3.3) into account, we conclude that  $J = \eta|\eta|^{-1}$ . Then the relation  $QJ = -JQ$  and the condition of self-adjointness of  $Q$  with respect to the inner product  $(\cdot, \cdot)_{|\eta|}$  take the form

$$Q\eta|\eta|^{-1} = -\eta|\eta|^{-1}Q, \quad Q^*|\eta| = |\eta|Q$$

that is equivalent to (4.5).

The operator  $A$  is self-adjoint in the Krein space  $(\mathfrak{H}, [\cdot, \cdot]_{J|\eta|})$  and it commutes with operator  $\mathcal{C} = Je^Q$ . In that case, as was established above, the operator  $A$  is self-adjoint with respect to the inner product  $[\mathcal{C} \cdot, \cdot]_{\eta} = (e^Q \cdot, \cdot)_{|\eta|} = (|\eta|e^Q \cdot, \cdot)$ . The proof is completed.  $\square$

For the case, where  $A$  cannot be interpreted as self-adjoint operator in Krein space, the following general integral-resolvent criterion of similarity can be used:

**Lemma 4.3.** ([18]) *A closed densely defined operator  $A$  acting in  $\mathfrak{H}$  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*

$$(4.6) \quad \begin{aligned} \sup_{\varepsilon > 0} \varepsilon \int_{-\infty}^{\infty} \|(A - zI)^{-1}g\|^2 d\xi &\leq M\|g\|^2, \\ \sup_{\varepsilon > 0} \varepsilon \int_{-\infty}^{\infty} \|(A^* - zI)^{-1}g\|^2 d\xi &\leq M\|g\|^2, \quad \forall g \in \mathfrak{H}, \end{aligned}$$

where the integrals are taken along the line  $z = \xi + i\varepsilon$  ( $\varepsilon > 0$  is fixed) of upper half-plane  $\mathbb{C}_+$ .

In order to apply Lemma 4.3 to Examples II-IV, we need an explicit form of the resolvent  $(A_{\mathbf{T}} - zI)^{-1}$ . Repeating the proof of Lemma 2 in [5], we obtain

**Lemma 4.4.** *Let  $A_{\mathbf{T}}$  be defined by (2.4), (2.5) and let  $A_0 = -d^2/dx^2$ ,  $\mathcal{D}(A_0) = W_2^2(\mathbb{R})$  be the free Schrödinger operator in  $L_2(\mathbb{R})$ . Then, for all  $g_{\pm} \in L_2(\mathbb{R}_{\pm})$  and for all  $z = \tau^2$  from the resolvent set of  $A_{\mathbf{T}}$ ,*

$$(4.7) \quad [(A_{\mathbf{T}} - zI)^{-1} - (A_0 - zI)^{-1}]g_{\pm} = c_{1\pm}(\tau)h_{1\tau} + c_{2\pm}(\tau)h_{2\tau},$$

where  $h_{j\tau}(x)$  are defined by (2.8) and

$$\begin{aligned} c_{1\pm}(\tau) &= \frac{iF_{\pm}(\tau)}{\tau} \left( -1 + \frac{2d\tau^2 - 2i\tau(2 \pm b)}{p(\tau)} \right), \\ c_{2\pm}(\tau) &= \pm \frac{iF_{\pm}(\tau)}{\tau} \left( -1 + \frac{-2i\tau(2 \mp c) + 2a}{p(\tau)} \right), \end{aligned}$$

where  $F_{\pm}(\tau) = \frac{1}{2} \int_{\mathbb{R}} e^{\pm i\tau s} g_{\pm}(s) ds$  and  $p_{\mathbf{T}}(\tau) = 2d\tau^2 + i(\det \mathbf{T} - 4)\tau + 2a$ .

It is known that the resolvent of an arbitrary self-adjoint operator  $H$  satisfies the inequality  $\|(H - zI)^{-1}\| \leq \frac{1}{|\operatorname{Im} z|}$  for all  $z \in \mathbb{C} \setminus \mathbb{R}$ . If  $A$  is similar to a self-adjoint operator  $H$  (i.e., (4.1) holds), then the inequality above takes the form

$$(4.8) \quad \|(A - zI)^{-1}\| \leq \frac{C}{|\operatorname{Im} z|}, \quad C = \|Z^{-1}\| \|Z\|, \quad z \in \mathbb{C} \setminus \mathbb{R}.$$

**Lemma 4.5.** *If an operator  $A_{\mathbf{T}}$  is similar to a self-adjoint operator in  $L_2(\mathbb{R})$ , then the functions*

$$(4.9) \quad \Phi_{\pm}(\tau) = \frac{(\operatorname{Re} \tau)^2}{|\tau|^2} \cdot \frac{|2d\tau^2 + i\tau(\det \mathbf{T} \mp 2c)|^2 + |i\tau(\det \mathbf{T} \pm 2b) + 2a|^2}{|p_{\mathbf{T}}(\tau)|^2}$$

are uniformly bounded on  $\mathbb{C}_{++} = \{\tau \in \mathbb{C}_+ : \operatorname{Re} \tau > 0\}$  (i.e., there exists  $K > 0$  such that  $\Phi_{\pm}(\tau) < K$  for all  $\tau \in \mathbb{C}_{++}$ ).

*Proof.* Let  $A_{\mathbf{T}}$  be similar to self-adjoint. Since  $A_0$  is self-adjoint, the inequalities (4.8) hold for  $A_{\mathbf{T}}$  and for  $A_0$ . Therefore, for all  $g \in L_2(\mathbb{R})$  and  $z = \tau^2 \in \mathbb{C}_+$ ,

$$(4.10) \quad \|[(A_{\mathbf{T}} - zI)^{-1} - (A_0 - zI)^{-1}]g\|^2 \leq \frac{M}{(\operatorname{Im} z)^2} \|g\|^2,$$

where  $M$  is a constant independent of  $g$  and  $z$ . In particular, the inequality (4.10) holds if we put  $g = g_+$  or  $g = g_-$ , where

$$g_+(x) = \begin{cases} e^{-i\bar{\tau}x}, & x > 0 \\ 0, & x < 0 \end{cases}, \quad g_-(x) = \begin{cases} 0, & x > 0 \\ e^{i\bar{\tau}x}, & x < 0 \end{cases}, \quad \tau \in \mathbb{C}_{++}.$$

In these cases, using (4.7) and taking into account that: the functions  $h_{j\tau}$  in (4.7) are orthogonal in  $L_2(\mathbb{R})$ ,

$$(4.11) \quad \|g_{\pm}\|^2 = \frac{1}{2(\operatorname{Im} \tau)}, \quad \|h_{j\tau}\|^2 = \frac{1}{\operatorname{Im} \tau}, \quad F_{\pm}(\tau) = \frac{1}{4(\operatorname{Im} \tau)},$$

and  $(\operatorname{Im} z)^2 = 4(\operatorname{Im} z)^2(\operatorname{Re} \tau)^2$  we can rewrite (4.10) as follows

$$\Phi_{\pm}(\tau) = \frac{(\operatorname{Re} \tau)^2}{|\tau|^2} M_{\pm}(\tau) \leq 2M, \quad \forall \tau \in \mathbb{C}',$$

where

$$M_{\pm}(\tau) = \left| 1 - \frac{2d\tau^2 - 2i\tau(2 \pm b)}{p_{\mathbf{T}}(\tau)} \right|^2 + \left| 1 - \frac{-2i\tau(2 \mp c) + 2a}{p_{\mathbf{T}}(\tau)} \right|^2.$$

Finally, remembering that  $p_{\mathbf{T}}(\tau) = 2d\tau^2 + i\tau(\det \mathbf{T} - 4) + 2a$  we rewrite  $M_{\pm}(\cdot)$  as

$$(4.12) \quad M_{\pm}(\tau) = \frac{|2d\tau^2 + i\tau(\det \mathbf{T} \mp 2c)|^2 + |i\tau(\det \mathbf{T} \pm 2b) + 2a|^2}{|p_{\mathbf{T}}(\tau)|^2}$$

that gives (4.9). Lemma 4.5 is proved.  $\square$

The proof of Lemma 4.8 is close to the part of the proof of Theorem 4 in [5], where the particular case of operators  $A_{\mathbf{T}}$  was considered.

**Theorem 4.6.** *Let  $A \in \{A_{\mathbf{T}}, A_a, A_d\}$  be an operator considered in Examples II-IV. If the spectrum of  $A$  contains the spectral singularity (the exceptional point), then  $A$  cannot be similar to a self-adjoint operator.*

*Proof.* Assume that  $A = A_{\mathbf{T}}$  is a  $\mathcal{PT}$ -symmetric operator from Example II. It follows from the proof of Lemma 2.7 that  $A_{\mathbf{T}}$  has a nonzero spectral singularity if the positive number  $\tau = \sqrt{-\frac{a}{d}}$  is the root of  $p_{\mathbf{T}}(\tau)$ ; and  $A_{\mathbf{T}}$  has an exceptional point if the imaginary number  $\tau = i\sqrt{-\frac{a}{d}} \in \mathbb{C}_+$  is the root of  $p_{\mathbf{T}}(\tau)$  with multiplicity 2.

Let us suppose that  $A_{\mathbf{T}}$  is similar to self-adjoint. Then, by virtue of Lemma 4.5, the functions  $\Phi_{\pm}(\cdot)$  have to be uniformly bounded on  $\mathbb{C}_{++}$ . This is impossible since  $\Phi_{\pm}(\tau)$  tend to infinity in neighborhood of  $\tau$ .

Consider now the case of spectral singularity at point 0. Then, in view of relations (iv) of Lemma 2.7,

$$\Phi_{\pm}(\tau) = \frac{(\operatorname{Re} \tau)^2}{|\tau|^2} \cdot \frac{|d\tau + i(2 \mp c)|^2 + |i(2 \pm b)|^2}{d^2|\tau|^2}.$$

Here  $|bc| \neq 0$  because  $4 = \mathbf{det} \mathbf{T} = -bc$ . Hence, at least one of functions  $\Phi_{\pm}(\cdot)$  tends to infinity when  $\tau \rightarrow 0$ .

Finally, if  $A_{\mathbf{T}}$  has spectral singularity at  $\infty$ , then relations (v) of Lemma 2.7 hold and

$$\Phi_{\pm}(\tau) = \frac{(\operatorname{Re} \tau)^2}{|\tau|^2} \cdot \frac{|i\tau(2 \mp c)|^2 + |i\tau(2 \pm b) + a|^2}{|a|^2}.$$

It follows from relations (v) that  $4 = \mathbf{det} \mathbf{T} = -bc$ . Hence,  $|bc| \neq 0$  and at least one of functions  $\Phi_{\pm}(\cdot)$  tends to infinity when  $\tau \rightarrow \infty$ .

Summing the cases above we conclude that  $A_{\mathbf{T}}$  cannot be similar to a self-adjoint operator.

The cases  $A = A_a$  and  $A = A_d$  can be considered similarly (it suffices to consider the case of spectral singularity only). Theorem 4.6 is proved.  $\square$

The functions  $M_{\pm}(\tau)$  in (4.12) corresponds to the operator  $A_{\mathbf{T}}$  defined by (2.4), (2.5). The adjoint operator  $A_{\mathbf{T}}^*$  coincides with  $A_{\overline{\mathbf{T}}}$ . Hence, the following functions:

$$(4.13) \quad M'_{\pm}(\tau) = \frac{|2\bar{d}\tau^2 + i\tau(\mathbf{det} \overline{\mathbf{T}} \mp 2\bar{b})|^2 + |i\tau(\mathbf{det} \overline{\mathbf{T}} \pm 2\bar{c}) + 2\bar{a}|^2}{|p_{\overline{\mathbf{T}}}(\tau)|^2}$$

correspond to  $A_{\mathbf{T}}^*$ .

**Theorem 4.7.** *Let  $A_{\mathbf{T}}$  be an operator defined by (2.4), (2.5) with real spectrum. If the functions  $M_{\pm}(\tau), M'_{\pm}(\tau)$  are uniformly bounded in  $\mathbb{C}_{++} = \{\tau \in \mathbb{C}_+ : \operatorname{Re} \tau > 0\}$ , then  $A_{\mathbf{T}}$  is similar to self-adjoint.*

*Proof.* The operator  $A_0$  satisfies relations (4.6) as a self-adjoint operator. Hence, the inequalities

$$(4.14) \quad \begin{aligned} \sup_{\varepsilon > 0} \varepsilon \int_{-\infty}^{\infty} \|[(A_{\mathbf{T}} - zI)^{-1} - (A_0 - zI)^{-1}]g\|^2 d\xi &\leq M\|g\|^2, \\ \sup_{\varepsilon > 0} \varepsilon \int_{-\infty}^{\infty} \|[(A_{\mathbf{T}}^* - zI)^{-1} - (A_0 - zI)^{-1}]g\|^2 d\xi &\leq M\|g\|^2, \quad \forall g \in L_2(\mathbb{R}), \end{aligned}$$

are necessarily and sufficient condition for the similarity of  $A_{\mathbf{T}}$  to a self-adjoint operator.

Let  $g = g_+$  be an arbitrary function from  $L_2(\mathbb{R}_+)$ . Using Lemma 4.4 and the relation  $\|h_{j\tau}(x)\|^2 = \frac{1}{\operatorname{Im} \tau}$  (see (4.11)), we get

$$(4.15) \quad \|[(A_{\mathbf{T}} - zI)^{-1} - (A_0 - zI)^{-1}]g_+\|^2 = \frac{|F_+(\tau)|^2}{|\tau|^2(\operatorname{Im} \tau)} M_+(\tau),$$

where  $F_+(\tau)$  is the Fourier transform of  $g_+$  and  $z = \tau^2$  ( $\tau \in \mathbb{C}_{++}$ ).

Since  $M_+(\tau)$  is uniformly bounded on  $\mathbb{C}_{++}$ , there is a constant  $K_1 > 0$  such that  $|M_+(\tau)| \leq K_1$ . Then

$$(4.16) \quad \varepsilon \int_{-\infty}^{\infty} \|[(A_{\mathbf{T}} - zI)^{-1} - (A_0 - zI)^{-1}]g_+\|^2 d\xi \leq K_1 \int_{-\infty}^{\infty} \frac{\varepsilon |F_+(\tau)|^2}{|\tau|^2(\operatorname{Im} \tau)} d\xi.$$

Let us consider an auxiliary self-adjoint operator  $\tilde{A}_{\mathbf{T}}$  with  $b = c = 0$ ,  $a = 1$ , and  $d = 4$ . Then  $\det \mathbf{T} = 4$  and

$$\tilde{M}_+(\tau) = \frac{|\gamma^2 + i\gamma|^2 + |i\gamma + 1|^2}{|\gamma^2 + 1|^2} = \frac{|\gamma|^2}{|\gamma - i|^2} + \frac{1}{|\gamma + i|^2}, \quad \gamma = 2\tau \in \mathbb{C}_{++}.$$

The obtained expression leads to the conclusion that  $\tilde{M}_+(\tau) \geq \frac{1}{4}$  for all  $\tau \in \mathbb{C}_{++}$ . Taking this inequality into account and using (4.14) and (4.15) for the pair of self-adjoint operators  $\tilde{A}_{\mathbf{T}}$ ,  $A_0$ , we obtain

$$\begin{aligned} \frac{1}{4} \int_{-\infty}^{\infty} \frac{\varepsilon |F_+(\tau)|^2}{|\tau|^2 (\operatorname{Im} \tau)} d\xi &\leq \int_{-\infty}^{\infty} \frac{\varepsilon |F_+(\tau)|^2}{|\tau|^2 (\operatorname{Im} \tau)} \tilde{M}_+(\tau) d\xi \\ &= \varepsilon \int_{-\infty}^{\infty} \|[(\tilde{A}_{\mathbf{T}} - zI)^{-1} - (A_0 - zI)^{-1}]g_+\|^2 d\xi < M \|g_+\|^2, \end{aligned}$$

where  $M$  is a constant independent of  $\varepsilon > 0$  and  $g_+$ .

Combining the obtained evaluation with (4.16), we obtain

$$\varepsilon \int_{-\infty}^{\infty} \|[(A_{\mathbf{T}} - zI)^{-1} - (A_0 - zI)^{-1}]g_+\|^2 d\xi < 4K_1 M \|g_+\|^2,$$

where  $4K_1 M$  does not depend on  $\varepsilon > 0$  and  $g_+$ .

Considering similarly the case  $g = g_-(x) \in L_2(\mathbb{R}_-)$  (here the uniform boundedness of  $M_-(\tau)$  has to be used) and, consequently, the case of operator  $A_{\mathbf{T}}^*$ , we arrive at the conclusion that (4.14) hold for all functions from  $L_2(\mathbb{R})$ . Hence,  $A$  is similar to a self-adjoint operator. Theorem 4.7 is proved.  $\square$

**Corollary 4.8.** *Let  $A_{\mathbf{T}}$  satisfy conditions of Theorem 4.7. If, in addition,  $A_{\mathbf{T}}$  can be interpreted as a self-adjoint operator in a Krein space, then the property of  $M_{\pm}(\tau)$  to be uniformly bounded in  $\mathbb{C}_{++}$  implies the similarity of  $A_{\mathbf{T}}$  to a self-adjoint operator.*

*Proof.* If  $A_{\mathbf{T}}$  can be interpreted as self-adjoint in a Krein space, then, for a certain choice of fundamental symmetry  $J$ , the equality (3.1) holds for  $A_{\mathbf{T}}$  and  $A_{\mathbf{T}}^*$ . In that case, the first and the second inequalities in (4.6) are equivalent. Obviously, the same remains true for the inequalities (4.14). Thus, for the similarity of  $A_{\mathbf{T}}$  to a self-adjoint operator it suffices to establish the first inequality in (4.14). The latter is ensured by uniform boundedness property of  $M_{\pm}(\tau)$  in  $\mathbb{C}_{++}$  (see the proof of Theorem 4.7).  $\square$

### Example II contd.

**Corollary 4.9.** *Let  $A_{\mathbf{T}}$  be a  $\mathcal{PT}$ -symmetric operator considered in Example II. If one of the following conditions is satisfied, then  $A_{\mathbf{T}}$  is similar to a self-adjoint operator:*

- (i)  $D = (4 - \det \mathbf{T})^2 + 16ad < 0$ ,  $(4 - \det \mathbf{T})d < 0$ ;
- (ii)  $D = 0$ ,  $(4 - \det \mathbf{T})d < 0$ .

*Proof.* Every condition (i), (ii) guarantees that  $d \neq 0$  and the roots  $\tau_{1,2}$  of the polynomial  $p_{\mathbf{T}}(\tau)$  (see (2.12)) belong to  $\mathbb{C}_-$ . Then the functions  $M_{\pm}(\tau)$  (see (4.12)) are uniformly bounded in  $\mathbb{C}_{++}$ . By Proposition 3.1,  $A_{\mathbf{T}}$  can be realized as self-adjoint in a Krein space. Hence, we can apply Corollary 4.8 that completes the proof.  $\square$

The conditions of Corollary 4.9 ensure the uniform boundedness of  $M_{\pm}(\tau)$ . This property is *sufficient* for the similarity of  $A_{\mathbf{T}}$  to a self-adjoint operator. If  $D > 0$  the corresponding roots  $\tau_{1,2}$  in (2.12) lie on imaginary axes  $i\mathbb{R}$  and may happen that at least one of them (let, for definiteness,  $\tau_1$ ) belongs to  $\mathbb{C}_+$ . In that case the functions  $M_{\pm}(\tau)$  may tend to infinity as  $\tau \rightarrow \tau_1$ . However, as we show below, the corresponding operator  $A_{\mathbf{T}}$  remains similar to a self-adjoint operator.

**Theorem 4.10.** *Let  $A_{\mathbf{T}}$  be a  $\mathcal{PT}$ -symmetric operator considered in Example II and let  $D = (4 - \det \mathbf{T})^2 + 16ad > 0$ . Then  $A_{\mathbf{T}}$  is similar to a self-adjoint operator.*

*Proof.* By virtue of Proposition 3.1,  $A_{\mathbf{T}}$  is self-adjoint in the Krein space  $(L_2(\mathbb{R}), [\cdot, \cdot]_{\mathcal{P}_\phi})$ . Using Proposition 4.2 with  $\eta = J = \mathcal{P}_\phi$  we conclude that the similarity of  $A_{\mathbf{T}}$  to a self-adjoint operator in a Hilbert space is equivalent to the existence of an operator  $\mathcal{C} = \mathcal{P}_\phi e^Q$  which satisfies the following conditions:

$$(4.17) \quad Q^* = Q, \quad \mathcal{P}_\phi Q = -Q\mathcal{P}_\phi, \quad \mathcal{A}\mathcal{C} = \mathcal{C}\mathcal{A}.$$

Let  $Q = \chi i\mathcal{R}\mathcal{P}_\phi$ , where  $\chi \in \mathbb{R}$  and  $\mathcal{R}$  be defined by (3.4). The fundamental symmetry  $\mathcal{R}$  anti-commutes with  $\mathcal{P}$  and hence,  $\mathcal{R}$  anti-commutes with the fundamental symmetry  $\mathcal{P}_\phi = \mathcal{P}e^{i\phi\mathcal{R}}$ . This means that  $Q$  satisfies the first two conditions of (4.17). The third condition is equivalent to the relation

$$(4.18) \quad A_{\mathbf{T}}^* e^Q = e^Q A_{\mathbf{T}}$$

since  $A_{\mathbf{T}}\mathcal{P}_\phi = \mathcal{P}_\phi A_{\mathbf{T}}^*$  and  $\mathcal{C} = \mathcal{P}_\phi e^Q$ .

The operator  $i\mathcal{R}\mathcal{P}_\phi$  is a fundamental symmetry in  $L_2(\mathbb{R})$  because  $\mathcal{R}$  anti-commutes with  $\mathcal{P}_\phi$ . This property allows us to rewrite  $e^Q$  as

$$(4.19) \quad e^Q = e^{\chi i\mathcal{R}\mathcal{P}_\phi} = [\cosh \chi]I + [\sinh \chi]i\mathcal{R}\mathcal{P}_\phi.$$

The obtained expression shows that  $e^Q$  commutes with the symmetric operator  $A_{\text{sym}}$  defined by (2.2) and commutes with the adjoint operator  $A_{\text{sym}}^*$ . Hence, (4.18) holds if  $e^Q : \mathcal{D}(A_{\mathbf{T}}) \rightarrow \mathcal{D}(A_{\mathbf{T}}^*)$ . The latter relation is equivalent to the following implication:

$$(4.20) \quad \text{if } \mathbf{T}\Gamma_0 f = \Gamma_1 f, \quad \text{then } \overline{\mathbf{T}}^t \Gamma_0 e^{\chi i\mathcal{R}\mathcal{P}_\phi} f = \Gamma_1 e^{\chi i\mathcal{R}\mathcal{P}_\phi} f,$$

where  $\Gamma_j$  are boundary operators from Lemma 2.1 and  $f$  is an arbitrary element of  $\mathcal{D}(A_{\mathbf{T}})$ .

Thus if (4.20) holds for a certain  $\chi \in \mathbb{R}$ , then  $A_{\mathbf{T}}$  is similar to a self-adjoint operator in a Hilbert space.

Denote

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Using (2.5), (2.14), (3.4), and (4.19) it is easy to verify that

$$\Gamma_0 e^Q f = \cosh \chi \Gamma_0 f + \sinh \chi \left[ -\frac{i}{2} \cos \phi \sigma_1 \Gamma_1 f + \sin \phi \sigma_3 \Gamma_0 f \right],$$

and

$$\Gamma_1 e^Q f = \cosh \chi \Gamma_1 f + \sinh \chi [2i \cos \phi \sigma_1 \Gamma_0 f + \sin \phi \sigma_3 \Gamma_1 f]$$

for all  $f \in \mathcal{D}(A_{\text{sym}}^*) = W_2^2(\mathbb{R} \setminus \{0\})$ .

Substituting these expressions into (4.20), we obtain that (4.20) is equivalent to the matrix equality

$$(4.21) \quad \cosh \chi (\mathbf{T} - \overline{\mathbf{T}}^t) = -\sinh \chi \left( \frac{i}{2} \cos \phi [\overline{\mathbf{T}}^t \sigma_1 \mathbf{T} + 4\sigma_1] + \sin \phi [\sigma_3 \mathbf{T} - \overline{\mathbf{T}}^t \sigma_3] \right).$$

Since  $A_{\mathbf{T}}$  is  $\mathcal{PT}$ -symmetric, the entries of  $\mathbf{T}$  satisfy (2.15) and we can set  $b = ix$ ,  $c = iy$ , where  $x, y$  are arbitrary real numbers.

Simple calculations give

$$\mathbf{T} - \overline{\mathbf{T}}^t = i(x+y)\sigma_1, \quad \overline{\mathbf{T}}^t \sigma_1 \mathbf{T} + 4\sigma_1 = (\det \mathbf{T} + 4)\sigma_1, \quad \sigma_3 \mathbf{T} - \overline{\mathbf{T}}^t \sigma_3 = i(x-y)\sigma_1.$$

Hence, the matrix relation (4.21) can be reduced to the equality

$$x + y = -\frac{\sinh \chi}{\cosh \chi} \left[ \frac{1}{2} (\det \mathbf{T} + 4) \cos \phi + (x - y) \sin \phi \right],$$

which, obviously, has a solution  $\chi$  if and only if

$$(4.22) \quad \left[ \frac{1}{2}(\det \mathbf{T} + 4) \cos \phi + (x - y) \sin \phi \right]^2 > (x + y)^2.$$

Using the identity  $2(x - y) \cos \phi = (\det \mathbf{T} + 4) \sin \phi$ , which follows directly from (3.6), and making elementary transformations, we reduce (4.22) to the inequality

$$(4.23) \quad (\det \mathbf{T} + 4)^2 - 16xy > 0.$$

To complete the proof it is sufficient to observe that the inequality (4.23) coincides with the condition  $D > 0$  (since (2.13) and  $b = ix, c = iy$ ). Theorem 4.10 is proved.  $\square$

Summing the results above we obtain the following relationship between properties of  $A_{\mathbf{T}}$  and the parameters  $D = (4 - \det \mathbf{T})^2 + 16ad$ ,  $K = (4 - \det \mathbf{T})d$ .

	$K > 0$	$K = 0$	$K < 0$
$D > 0$	similarity	similarity	similarity
$D = 0$	exceptional point	spectral singularity at 0 spectral singularity at $\infty$ $\sigma(A_{\mathbf{T}}) = \mathbb{C}$	similarity
$D < 0$	pair of complex eigenvalues	nonzero spectral singularity	similarity

### Examples III. VI contd.

**Corollary 4.11.** *Let  $A_a$  ( $A_d$ ) be an operator considered in Example III (IV). If  $\operatorname{Re} a > 0$  ( $\operatorname{Re} d < 0$ ), then  $A_a$  ( $A_d$ ) is similar to a self-adjoint operator.*

*Proof.* Let  $\operatorname{Re} a > 0$ . Then the spectrum of  $A_a$  is real. The adjoint  $A_a^*$  coincides with  $A_{\bar{a}}$ . The functions  $M_{\pm}(\tau), M'_{\pm}(\tau)$  have the form

$$M_+(\tau) = M_-(\tau) = \frac{|a|^2}{|-2i\tau + a|^2}, \quad M'_+(\tau) = M'_-(\tau) = \frac{|\bar{a}|^2}{|-2i\tau + \bar{a}|^2}.$$

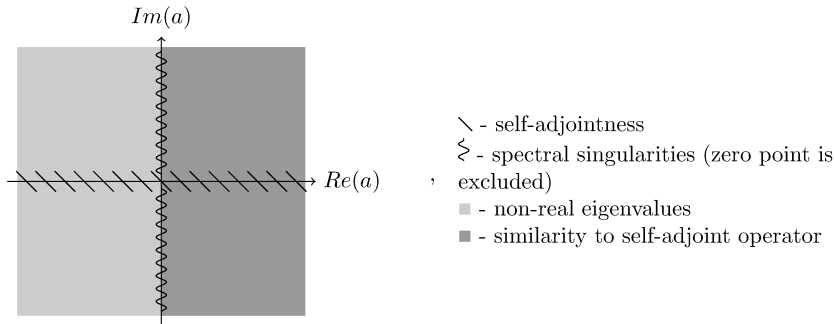
If  $\operatorname{Re} a > 0$ , then the roots  $\tau_1 = -\frac{ia}{2}$ ,  $\tau_2 = -\frac{i\bar{a}}{2}$  of the denominators belong to  $\mathbb{C}_-$ . In these cases,  $M_{\pm}(\tau), M'_{\pm}(\tau)$  are uniformly bounded in  $\mathbb{C}_{++}$ . By Theorem 4.7, the operator  $A_a$  is similar to self-adjoint.

The operators  $A_d$  have real spectrum when  $\operatorname{Re} d < 0$  and  $A_d^* = A_{\bar{d}}$ . The functions

$$M_+(\tau) = M_-(\tau) = \frac{|d\tau|^2}{|d\tau - 2i|^2}, \quad M'_+(\tau) = M'_-(\tau) = \frac{|\bar{d}\tau|^2}{|\bar{d}\tau - 2i|^2}.$$

are uniformly bounded in  $\mathbb{C}_{++}$ . Using again Theorem 4.7 we complete the proof.  $\square$

The following picture illustrates the change of properties of  $A_a$  (complex eigenvalue  $\rightarrow$  spectral singularity  $\rightarrow$  similarity to a self-adjoint operator):



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