ALTERNATIVE PROOF OF THE A PRIORI $\tan \Theta$ THEOREM

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Let $A$ be a self-adjoint operator in a separable Hilbert space. We assume that the spectrum of $A$ consists of two isolated components $\sigma_0$ and $\sigma_1$ and the set $\sigma_0$ is in a finite gap of the set $\sigma_1$. It is known that if $V$ is a bounded additive self-adjoint perturbation of $A$ that is off-diagonal with respect to the partition $\text{spec}(A) = \sigma_0 \cup \sigma_1$, then for $\|V\| < \sqrt{2d}$, where $d = \text{dist}(\sigma_0, \sigma_1)$, the spectrum of the perturbed operator $L = A + V$ consists of two isolated parts $\omega_0$ and $\omega_1$, which appear as perturbations of the respective spectral sets $\sigma_0$ and $\sigma_1$. Furthermore, we have the sharp upper bound $\|E_A(\sigma_0) - E_L(\omega_0)\| \leq \sin(\arctan(\|V\|/d))$ on the difference of the spectral projections $E_A(\sigma_0)$ and $E_L(\omega_0)$ corresponding to the spectral sets $\sigma_0$ and $\omega_0$ of the operators $A$ and $L$. We give a new proof of this bound in the case where $\|V\| < d$.

Keywords: perturbation of spectral subspace, operator Riccati equation, $\tan \Theta$ theorem

DOI: 10.1134/S0040577916010074

Dedicated to the memory of Stanislav Petrovich Merkuriev

1. Introduction

Studying variations of invariant and, in particular, spectral subspaces of a linear operator resulting from the action of an additive perturbation (see, e.g., [1]–[3]) is one of fundamental problems of the perturbation theory of linear operators. Classic trigonometric bounds on rotations of spectral subspaces were established by Davis and Kahan [2] in the perturbation theory of self-adjoint operators. Historical remarks and reviews of other known bounds on variations of spectral subspaces in the self-adjoint perturbation problem can be found, for example, in [4]–[6].

Our interest in the perturbation theory of invariant subspaces was aroused by a series of papers written in close contact with S. P. Merkuriev and devoted to constructing three-particle Hamiltonians with a pairwise interaction depending on two-particle energies (see, e.g., [7], [8] and the references therein). Attempts [9], [10] to address the question [11] of the possibility of replacing an energy-dependent potential of the pairwise interaction in a two-particle Schrödinger equation with a spectral-equivalent energy-independent potential (i.e., preserving the spectrum and eigenfunctions) reduced this problem to that of the solvability of an operator Riccati equation. The above question of the possibility of an equivalent replacement of an energy-dependent potential by an energy-independent potential is related to a more general problem of factoring operator-valued functions of a complex variable and of the existence of operator roots of these functions (see [12]–[14]). A Schrödinger operator with the potential depending on energy in a resolvent way is an example of an operator-valued function for which the problem of constructing operator roots is intrinsically related to that of constructing graph representations for invariant subspaces of some block-operator $2 \times 2$ matrix (see [9], [12], [14]–[16]). In turn, the existence problem for graph representations leads to studying...
the mutual geometry of perturbed and unperturbed invariant subspaces and, in particular, to studying spectral properties of operator angles between these subspaces (see [17] and the references therein).

Here, we consider a particular case of a problem of self-adjoint spectral space perturbations. Namely, we assume that the spectrum $\text{spec}(A)$ of the initial self-adjoint operator $A$ acting in a separable Hilbert space $\mathcal{H}$ consists of two nonintersecting parts $\sigma_0$ and $\sigma_1$ such that the first part is located in a finite gap of the second part.\footnote{We recall that a finite gap of a closed set $\sigma \subset \mathbb{R}$ is an open bounded interval in $\mathbb{R}$ that does not intersect with $\sigma$ but both its endpoints belong to $\sigma$.} For convenience of reference, we express our assumptions about the relative location of the spectral components $\sigma_0$ and $\sigma_1$ in the form

$$\text{spec}(A) = \sigma_0 \cup \sigma_1, \quad \overline{\text{conv}(\sigma_0)} \cap \sigma_1 = \emptyset \quad \text{and} \quad \sigma_0 \subset \overline{\text{conv}(\sigma_1)}, \quad (1.1)$$

where the symbol $\text{conv}$ denotes the convex hull and the bar denotes the closure.

We next assume that an (additive) perturbation $V$ is a bounded self-adjoint operator on the space $\mathcal{H}$. We also assume that this perturbation is off-diagonal with respect to the partition $\text{spec}(A) = \sigma_0 \cup \sigma_1$, i.e., that $V$ anticommutes with the difference $E_A(\sigma_0) - E_A(\sigma_1)$ of the spectral projections $E_A(\sigma_0)$ and $E_A(\sigma_1)$ of the operator $A$ corresponding to the respective spectral sets $\sigma_0$ and $\sigma_1$.

Let $d := \text{dist}(\sigma_0, \sigma_1)$ be the distance between the spectral components $\sigma_0$ and $\sigma_1$. For spectral distribution (1.1), it was established in [18] (also see [15]) that gaps between $\sigma_0$ and $\sigma_1$ necessarily stay open under the action of a off-diagonal self-adjoint perturbation $V$ if its norm satisfies the condition

$$\|V\| < \sqrt{2d} \quad (1.2)$$

and this condition is, moreover, optimal. If condition (1.2) is satisfied, then the spectrum of the perturbed operator $L = A + V$ consists of two isolated parts $\omega_0 \subset \Delta$ and $\omega_1 \subset \mathbb{R} \setminus \Delta$. Here and hereafter, we let $\Delta$ denote the finite gap of the set $\sigma_1$ that contains the set $\sigma_0$.

The optimal estimate of variations of spectral subspaces of a self-adjoint operator with spectral set (1.1) under the action of off-diagonal perturbations was established in several steps: in [19] (in the case $\|V\| < d$) and in [20] (for $d \leq \|V\| < \sqrt{2d}$). We express this estimate in terms of the norm of the difference of the corresponding nonperturbed and perturbed spectral projections $E_A(\sigma_0)$ and $E_L(\omega_0)$ and formulate it as a theorem (cf. Theorem 2 in [19] and Theorem 1 in [20]).

**Theorem 1.** Let $A$ be a self-adjoint operator acting in a separable Hilbert space $\mathcal{H}$, and let the spectrum of $A$ consist of two isolated components $\sigma_0$ and $\sigma_1$ satisfying conditions (1.1). We assume that $V$ is a bounded self-adjoint operator on $\mathcal{H}$ off-diagonal with respect to the partition $\text{spec}(A) = \sigma_0 \cup \sigma_1$, and we let $L = A + V$, $\text{Dom}(L) = \text{Dom}(A)$. We also assume that the norm of $V$ satisfies inequality (1.2), and we let $\omega_0 = \text{spec}(L) \cap \Delta$. We then have the estimate

$$\|E_A(\sigma_0) - E_L(\omega_0)\| \leq \sin \left( \arctan \frac{\|V\|}{d} \right). \quad (1.3)$$

We recall that if $P$ and $Q$ are orthogonal projection operators in a Hilbert space, then the quantity

$$\Theta(\mathcal{P}, \mathcal{Q}) := \arcsin |P - Q|, \quad (1.4)$$

where $|P - Q| = \sqrt{(P - Q)^2}$ is the modulus of $P - Q$, is called the operator angle between the subspaces $\mathcal{P} = \text{Ran}(P)$ and $\mathcal{Q} = \text{Ran}(Q)$. A discussion of the term operator angle and relevant references can be found in [21].
found, in particular, in Sec. 2 of [21]. In turn, the norm of the operator angle \( \Theta(\mathfrak{P}, \mathfrak{Q}) \) determines the maximum angle \( \theta(\mathfrak{P}, \mathfrak{Q}) \) between \( \mathfrak{P} \) and \( \mathfrak{Q} \) (see [5]), namely, \( \theta(\mathfrak{P}, \mathfrak{Q}) = \arcsin \|P - Q\| \).

By virtue of (1.4), bound (1.3) is equivalent to the bound

\[
\tan \Theta(\mathfrak{A}_0, \mathfrak{L}_0) \leq \frac{\|V\|}{d} \tag{1.5}
\]
on the tangent of the operator angle \( \Theta(\mathfrak{A}_0, \mathfrak{L}_0) \) between the unperturbed \( \mathfrak{A}_0 = \text{Ran}(E_A(\sigma_0)) \) and the perturbed \( \mathfrak{L}_0 = \text{Ran}(E_L(\omega_0)) \) spectral subspaces. In contrast to the Davis–Kahan tan \( \Theta \) theorem (Theorem 6.3 in [2]) and its extensions in [18] and [22], bound (1.3) contains only the distance between unperturbed spectral components \( \sigma_0 \) and \( \sigma_1 \). This is why we called it the a priori tan \( \Theta \) theorem in [19] and [20].

The proof of Theorem 1 for \( \|V\| < d \) in [19] was based on studying the location of the spectrum of the product \( J'J \) of self-adjoint involutions \( J = E_A(\sigma_0) - E_A(\sigma_1) \) and \( J' = E_L(\omega_0) - E_L(\omega_1) \). This proof requires not only reformulating the problem of perturbations of spectral subspaces in the language of involution pairs but also knowledge of some properties of the polar expansion of maximum accretive operators.

Our aim here is to prove bound (1.3) for \( \|V\| < d \) independently of the approach in [19]. Our proof in Sec. 3 below seems much simpler and more straightforward than the proof in [19]. Our new proof is based on the standard reduction [16] of the problem of perturbations of invariant subspaces to studying the operator Riccati equation

\[
X A_0 - A_1 X + X B X = B^*, \tag{1.6}
\]
where \( A_0 = A|_{\mathfrak{A}_0} \) and \( A_1 = A|_{\mathfrak{A}_1} \) are parts of the operator \( A \) in its spectral subspaces \( \mathfrak{A}_0 = \text{Ran}(E_A(\sigma_0)) \) and \( \mathfrak{A}_1 = \text{Ran}(E_A(\sigma_1)) \) and \( B = V|_{\mathfrak{A}_1} \). As shown in [18], the perturbed spectral subspace \( \mathfrak{L}_0 = \text{Ran}(E_L(\omega_0)) \) is the graph of a solution \( X \in \mathcal{B}(\mathfrak{A}_0, \mathfrak{A}_1) \) of Eq. (1.6). This implies (see, e.g., [17]) that

\[
\|E_A(\sigma_0) - E_L(\omega_0)\| = \sin(\arctan \|X\|). \tag{1.7}
\]
Finding a bound on the norm of the solution \( X \), we thus simultaneously obtain a bound on the norm of the difference of the spectral projections \( E_L(\omega_0) \) and \( E_A(\sigma_0) \).

In our calculations, we use the identities for eigenvalues and eigenvectors of the modulus \( |X| = \sqrt{X^*X} \) of an operator \( X \) that were found in Lemma 2.2 in [20]. Using these identities (in fact, identities (2.6) and (2.7) below), we obtain bound (3.2), more detailed than (1.3), for the quantity \( \|E_A(\sigma_0) - E_L(\omega_0)\| \), which also includes the length \( |\Delta| \) of the gap \( \Delta \) in addition to \( \|V\| \) and \( d \). Bound (3.2) reproduces the main statement of Theorem 5.3 in [19]. Our proof of this bound alternative to the proof in [19] is our main result in this paper. As noted in [19], bound (1.3) is a simple corollary of more detailed bound (3.2).

This paper is structured as follows. In addition to the already mentioned identities (2.6) and (2.7) for eigenvalues and eigenvectors of the modulus of solution (1.6) of the Riccati equation, in Sec. 2, we collect other known results on the location of the spectrum of a perturbed operator \( L = A + V \) and on the solvability of Eq. (1.6) when the finer bound \( \|V\| < \sqrt{d|\Delta|} \), weaker than (1.2), is satisfied. In Sec. 3, we present our main result (see Theorem 3), which is a new proof of the bound on the rotation angle of the spectral subspace \( \mathfrak{A}_0 = \text{Ran}(E_A(\sigma_0)) \) under the action of a off-diagonal perturbation \( V \) subject to the condition \( \|V\| < \sqrt{d(|\Delta| - d)} \). We conclude Sec. 3 with a proof of Theorem 1.

By a subspace, we here understand a closed linear subset of a Hilbert space. We use the notation \( \mathcal{B}(\mathfrak{M}, \mathfrak{N}) \) for the Banach space of bounded linear operators acting from a Hilbert space \( \mathfrak{M} \) to a Hilbert space \( \mathfrak{N} \). We let \( \mathfrak{M} \oplus \mathfrak{N} \) denote the orthogonal sum of two Hilbert spaces (or two orthogonal subspaces) \( \mathfrak{M} \) and \( \mathfrak{N} \). The graph \( \mathcal{G}(K) := \{y \in \mathfrak{M} \oplus \mathfrak{N} \mid y = x \oplus Kx, \ x \in \mathfrak{M}\} \) of an operator \( K \in \mathcal{B}(\mathfrak{M}, \mathfrak{N}) \) is called the graph subspace associated with \( K \). The operator \( K \) itself is then the angular operator associated with the ordered pair \( (\mathfrak{M}, \mathfrak{N}) \) of subspaces \( \mathfrak{M} \) and \( \mathfrak{N} = \mathcal{G}(K) \). We let \( \text{Dom}(Z) \) and \( \text{Ran}(Z) \) denote the respective domain and range of a linear operator \( Z \).
2. Preliminary facts

To use a convenient block-matrix representation of the operators under consideration, we make the following assumption (this assumption does not yet concern the mutual position of spectra of the operators $A_0$ and $A_1$).

Assumption 1. Let $\mathfrak{A}_0$ and $\mathfrak{A}_1$ be mutually complementary orthogonal subspaces of a separable Hilbert space $\mathfrak{H}$, i.e., $\mathfrak{H} = \mathfrak{A}_0 \oplus \mathfrak{A}_1$. We assume that $A$ is a self-adjoint operator in $\mathfrak{H}$ admitting a block-diagonal representation

$$A = \begin{pmatrix} A_0 & 0 \\ 0 & A_1 \end{pmatrix}, \quad \text{Dom}(A) = \mathfrak{A}_0 \oplus \text{Dom}(A_1),$$

(2.1)

where $A_0$ is a bounded self-adjoint operator on $\mathfrak{A}_0$ and $A_1$ is a possibly unbounded self-adjoint operator on $\mathfrak{A}_1$. Let $V$ be a bounded self-adjoint operator in $\mathfrak{H}$ that is off-diagonal with respect to the partition $\mathfrak{H} = \mathfrak{A}_0 \oplus \mathfrak{A}_1$, i.e.,

$$V = \begin{pmatrix} 0 & B \\ B^* & 0 \end{pmatrix},$$

(2.2)

where $0 \neq B \in \mathcal{B}(\mathfrak{A}_1, \mathfrak{A}_0)$, and let $L = A + V$, $\text{Dom}(L) = \text{Dom}(A)$, and hence

$$L = \begin{pmatrix} A_0 & B \\ B^* & A_1 \end{pmatrix}, \quad \text{Dom}(L) = \mathfrak{A}_0 \oplus \text{Dom}(A_1).$$

(2.3)

Under Assumption 1, we call an operator $X \in \mathcal{B}(\mathfrak{A}_0, \mathfrak{A}_1)$ a solution of operator Riccati equation (1.6) if

$$\text{Ran}(X) \subset \text{Dom}(A_1)$$

(2.4)

and equality (1.6) holds as an operator identity (see, e.g., Definition 3.1 in [16] for the definition). A solution $X$, if any exists, obviously must be nonzero, $X \neq 0$. Indeed, the equality $X = 0$ implies $B = 0$, which contradicts the assumption. In what follows, we let $U$ denote a partial isometry in the polar decomposition $X = U|X|$ of the operator $X$. We adopt the convention that the action of $U$ is extended by triviality to the kernel $\text{Ker}(X) = \text{Ker}(|X|)$,

$$U|\text{Ker}(X) = 0.$$  

In this case, the operator $U$ is uniquely defined on the whole subspace $\mathfrak{A}_0$ (see, e.g., Theorem 8.1.2 in [23]). Then

$$U \text{ is an isometry on } \text{Ran}(|X|) = \text{Ran}(X^*).$$

(2.5)

We need two identities on eigenvalues and eigenvectors (if any exist) of the modulus $|X|$. The first among these identities was established in Lemma 2.2 in [20]. The second identity is a trivial corollary of other identities also proved in Lemma 2.2 in [20].

Lemma 1 [20]. Let Assumption 1 hold. We also assume that Riccati equation (1.6) admits a solution $X \in \mathcal{B}(\mathfrak{A}_0, \mathfrak{A}_1)$ and the modulus $|X|$ of this solution has an eigenvalue $\lambda \geq 0$. Let $u$, $u \neq 0$, be an eigenvector corresponding to this eigenvalue, i.e., $|X|u = \lambda u$. If $U$ is an isometry of the polar representation $X = U|X|$ of the solution $X$, then $Uu \in \text{Dom}(A_1)$, and we have the two identities

$$\lambda(\|A_1Uu\|^2 + \|BUu\|^2) = \|A_0u\|^2 - \|B^*u\|^2 = -\lambda(\langle A_0u, BUu \rangle + \langle B^*u, A_1Uu \rangle)$$

(2.6)
and
\[ (A_0u, BUu) + \langle B^*u, A_1 Uu \rangle = -\lambda (\|A_1 Uu\|^2 + \|BUu\|^2 - \|A_0u\|^2), \] (2.7)

where
\[ \Lambda_0 := (I + |X|^2)^{1/2}(A_0 + BX)(I + |X|^2)^{-1/2} \] (2.8)
is a bounded self-adjoint operator on $\mathfrak{A}_0$.

**Remark 1.** Identity (2.6) is identity (2.7) in [20]. We obtain identity (2.7) as a combination of two other identities in Lemma 2.2 in [20] (identities (2.8) and (2.9) in [20]).

Below, we only discuss the case of spectral case (1.1) and need a more detailed description of it.

**Assumption 2.** Let Assumption 1 hold. Let $\sigma_0 = \text{spec}(A_0)$ and $\sigma_1 = \text{spec}(A_1)$. Let an open interval $\Delta = (\gamma_\ell, \gamma_r) \subset \mathbb{R}$, where $\gamma_\ell < \gamma_r$, be a finite gap of the set $\sigma_1$, and let $\sigma_0 \subset \Delta$. Let $d = \text{dist}(\sigma_0, \sigma_1)$.

We now present the known facts concerning the location of the spectrum of the operator $L = A + V$ and the solvability of associated Riccati equation (1.6) for spectral pattern (1.1). All these results were obtained in [18] in the framework of an approach alternative to the methods and technique later used in [19].

**Theorem 2.** Let Assumption 2 hold. We also assume that
\[ \|V\| < \sqrt{d|\Delta|}. \] (2.9)

We have the following statements:

1. The spectrum of the operator matrix $L$ consists of two nonintersecting parts $\omega_0 \subset \Delta$ and $\omega_1 \subset \mathbb{R} \setminus \Delta$. Then
\[ \min(\omega_0) \geq \gamma_\ell + (d - r_V), \quad \max(\omega_0) \leq \gamma_r - (d - r_V), \] (2.10)
where
\[ r_V := \|V\| \tan \left( \frac{1}{2} \arctan \frac{2\|V\|}{|\Delta| - d} \right) < d. \] (2.11)

2. Riccati equation (1.6) admits a unique solution $X \in \mathcal{B}(\mathfrak{A}_0, \mathfrak{A}_1)$ with the properties
\[ \text{spec}(A_0 + BX) = \omega_0, \quad \text{spec}(A_1 - B^*X^*) = \omega_1. \] (2.12)

The spectral subspaces $\mathfrak{L}_0 = \text{Ran}(E_{L}(\omega_0))$ and $\mathfrak{L}_1 = \text{Ran}(E_{L}(\omega_1))$ are then the graph subspaces, $\mathfrak{L}_0 = \mathcal{G}(X)$ and $\mathfrak{L}_1 = \mathcal{G}(-X^*)$, associated with the respective operators $X$ and $-X^*$.

**Remark 2.** The formulations of statements 1 and 2 in Theorem 2 are from Theorem 2.4 in [20]. Statement 1 follows from Theorem 3.2 in [18]. Statement 2 is a combination of statements from Theorem 2.3 in [18] and results for the existence and uniqueness of the solution of operator Riccati equation (1.6) found in Theorem 1(i) in [18].
3. The bound for the rotation angle of the spectral subspace and its new proof

The sharp a priori bound on the norm of the operator angle between the unperturbed and perturbed spectral subspaces \( \mathfrak{A}_0 = \text{Ran}(E_A(\sigma_0)) \) and \( \mathfrak{L}_0 = \text{Ran}(E_L(\omega_0)) \), which in addition to the distance \( d \) includes another parameter, the length \( |\Delta| \) of a spectral gap \( \Delta \), was first found in [19] (see Theorem 5.3 therein). This bound was found under the condition

\[
\|V\| < \sqrt{d(|\Delta| - d)},
\]  

(3.1)

which is stronger than condition (2.9) in Theorem 2. We now reformulate the main statement of Theorem 5.3 in [19] in terms of the norm of the difference \( E_A(\sigma_0) - E_L(\omega_0) \) of the spectral projections \( E_A(\sigma_0) \) and \( E_L(\omega_0) \).

**Theorem 3** [19]. Let Assumption 2 hold. We also assume that condition (3.1) is satisfied. Then

\[
\|E_A(\sigma_0) - E_L(\omega_0)\| \leq \sin \left( \frac{1}{2} \arctan \left( \frac{|\Delta|}{d, \|V\|} \right) \right) \left( < \frac{\sqrt{2}}{2} \right),
\]  

(3.2)

where \( \omega_0 = \text{spec}(L) \cap \Delta \) and we define the quantity \( \kappa(D, d, v) \) at

\[
D > 0, \quad 0 < d \leq \frac{D}{2}, \quad 0 \leq v < \sqrt{d(D - d)}
\]  

(3.3)

by the equalities

\[
\kappa(D, d, v) := \begin{cases} 
\frac{2v}{d} & \text{if } v \leq \frac{1}{2} \sqrt{d(D - 2d)}, \\
\frac{vD + \sqrt{d(D - d)} \sqrt{(D - 2d)^2 + 4v^2}}{2(d(D - d) - v^2)} & \text{if } v > \frac{1}{2} \sqrt{d(D - 2d)}. 
\end{cases}
\]

As mentioned in Sec. 1, our main aim is to prove Theorem 3 independently of the approach in [19] by a method simpler than the method in [19].

We first prove bound (3.2) in the special case where the modulus \( |X| \) of the angular operator \( X \in \mathcal{B}(\mathfrak{A}_0, \mathfrak{A}_1) \) from the graph representation \( \mathfrak{L}_0 = \mathcal{G}(X) \) has an eigenvalue equal to the norm of \( X \). The proof is by a direct estimate of this eigenvalue. We can reduce the general case to this special case using the standard limit procedure including projecting on elements of a sequence of expanding finite-dimensional subspaces of \( \mathfrak{A}_0 \) (see the proof of Theorem 4.1 in [20]; cf. the proof of Theorem 4.2 in [24]). This part of the proof is standard and we omit it.

**Proof of Theorem 3.** Without restricting the generality, we can assume that the interval \( \Delta \) is located symmetrically with respect to the point 0, i.e., that \( \gamma_r = -\gamma_l = \gamma \). Indeed, if this is not the case, we can always replace \( A_0 \) and \( A_1 \) with the respective quantities \( A'_0 = A_0 - cI \) and \( A'_1 = A_1 - cI \), where \( c = (\gamma_l + \gamma_r)/2 \) is the midpoint of the interval \( \Delta \). The operator \( X \) obviously remains a solution of Riccati equation (1.6) under this transformation. We also mention that the assumptions \( \sigma_0 \subset \Delta = (-\gamma, \gamma) \) and \( d = \text{dist}(\sigma_0, \sigma_1) > 0 \) imply that \( \sigma_0 \subset [-a, a] \), where \( a = \gamma - d \). We then have

\[
\|A_0\| = a,
\]  

(3.4)

\( \gamma = a + d \), and we can write condition (3.1) in the form

\[
\|V\| < \sqrt{d(2a + d)}.
\]  

(3.5)
Let $X$ be a (unique) solution of Riccati equation (1.6) noted in statement 2 in Theorem 2. By assumption, $V \neq 0$ (see Assumption 1), and hence $X \neq 0$. We assume that the modulus $|X|$ of the operator $X$ has an eigenvalue $\mu$ coinciding with its norm, i.e.,

$$\mu = ||X|| = ||X|| > 0. \quad (3.6)$$

Let $u$, $||u|| = 1$, be an eigenvector of $|X|$ corresponding to this eigenvalue, $|X|u = \mu u$. Because $\mu \neq 0$ and $u = (1/\mu)|X|u$, we conclude that $u \in \text{Ran}(|X|)$, and by virtue of (2.5), we obtain

$$||Uu|| = ||u|| = 1, \quad (3.7)$$

where $U$ is an isometry from the polar representation $X = U|X|$. Lemma 1 also implies the inclusion $Uu \in \text{Dom}(A_1)$ and satisfaction of the identities

$$\mu(\|A_1Uu\|^2 + \|BUu\|^2 - \|A_0u\|^2 - \|B^*u\|^2) =$$

$$= -(1 - \mu^2)(\langle A_0u, BUu \rangle + \langle B^*u, A_1Uu \rangle), \quad (3.8)$$

$$\langle A_0u, BUu \rangle + \langle B^*u, A_1Uu \rangle = -\mu(\|A_1Uu\|^2 + \|BUu\|^2 - \|A_0u\|^2), \quad (3.9)$$

where $\Lambda_0$ is a bounded self-adjoint operator on $\mathbb{A}_0$ expressed in terms of $A_0$, $B$, and $X$ by relation (2.8).

Similarity relation (2.8) implies that $\text{spec}(\Lambda_0) = \text{spec}(A_0 + BX)$. Statement 2 in Theorem 2 then implies that $\text{spec}(\Lambda_0) = \omega_0$. Statement 1 in Theorem 2 then in turn implies that $\|\Lambda_0u\| \leq \gamma - (d - r_\nu) < \gamma$, i.e.,

$$\|\Lambda_0u\| < a + d. \quad (3.10)$$

Because the spectrum of $A_1$ is located outside the interval $\Delta = (-a - d, a + d)$, from equality (3.7), we obtain

$$\|A_1Uu\| \geq a + d. \quad (3.11)$$

From (3.10) and (3.11), we have

$$\|A_1Uu\|^2 + \|BUu\|^2 - \|\Lambda_0u\|^2 > (a + d)^2 + \|BUu\|^2 - (a + d)^2 \geq 0.$$

Hence, satisfaction of relations (3.6) and (3.9) requires satisfaction of the strict inequality

$$\langle A_0u, BUu \rangle + \langle B^*u, A_1Uu \rangle < 0. \quad (3.12)$$

On the other hand, we find from (3.4) and (3.5) that

$$\|A_1Uu\|^2 + \|BUu\|^2 - \|\Lambda_0u\|^2 \geq (a + d)^2 - a^2 - \|B\|^2 = d(2a + d) - v^2 > 0, \quad (3.13)$$

where we use the notation

$$v = \|B\| \quad (= \|V\|)$$

for brevity. By virtue of (3.12) and (3.13), identity (3.8) implies that

$$\mu < 1. \quad (3.14)$$
Taking (3.13) and (3.14) into account, we can rewrite (3.8) in the form
\[
\frac{\mu}{1-\mu^2} = -\frac{\langle A_0u, BUu \rangle + \langle B^*u, A_1 Uu \rangle}{\|A_1Uu\|^2 + \|BUu\|^2 - \|A_0u\|^2 - \|B^*u\|^2} \quad (> 0)
\]
and conclude that
\[
\frac{\mu}{1-\mu^2} \leq \frac{a\|BUu\| + v\|A_1Uu\|}{\|A_1Uu\|^2 + \|BUu\|^2 - a^2 - v^2}. \tag{3.15}
\]
Let \(x = \|A_1Uu\|\) and \(y = \|BUu\|\). By virtue of (3.11), we have \(x \in [a + d, \infty)\). At the same time, \(y \in [0, v]\), which means that the bound
\[
\frac{\mu}{1-\mu^2} \leq \sup_{(x,y)\in\Omega} \varphi(x, y), \tag{3.16}
\]
where \(\Omega = [a + d, \infty) \times [0, v]\) and
\[
\varphi(x, y) := \frac{vx + ay}{x^2 + y^2 - a^2 - v^2}, \tag{3.17}
\]
is necessarily satisfied. Elementary calculations demonstrate that the maximum of the function \(\varphi\) on the set \(\Omega\) is attained on the part of the boundary of this set corresponding to \(x = a + d\) and \(y \in [0, v]\). Namely, if \(0 < v \leq \sqrt{da/2}\), then the function \(\varphi\) reaches its maximum on the set \(\Omega\) at the point \(x = a + d, y = v\). If \(\sqrt{da/2} < v < \sqrt{d(2a + d)}\), then the function \(\varphi\) reaches its maximum on the set \(\Omega\) when \(x = a + d\) and \(y = a\left(d(2a + d) - v^2\right)/v(a + d) + a\sqrt{d(2a + d)(a^2 + v^2)}\) \((< v)\).

Substituting the corresponding maximum point in (3.17), we obtain
\[
\sup_{(x,y)\in\Omega} \varphi(x, y) = \begin{cases} \frac{v}{d} & \text{if } v \leq \sqrt{\frac{1}{2}da}, \\ \frac{1}{2} \frac{v(a + d) + \sqrt{d(2a + d)}\sqrt{a^2 + v^2}}{d(2a + d) - v^2} & \text{if } v > \sqrt{d(2a + d)}. \end{cases} \tag{3.18}
\]
Noting that
\[
\frac{\mu}{1-\mu^2} = \frac{1}{2} \tan(2\arctan \mu)
\]
and taking the equalities \(\mu = \|X\|\), \(v = \|V\|\), and \(a = |\Delta|/2 - d\) into account, we find that relations (3.14), (3.16), and (3.18) imply the estimate
\[
\|X\| \leq \tan\left(\frac{1}{2} \arctan \kappa(|\Delta|, d, \|V\|)\right). \tag{3.19}
\]
By statement 2 in Theorem 2, the spectral subspace \(\mathcal{L}_0 = \text{Ran}(E_L(\omega_0))\) is the graph of the operator \(X\). We can therefore express the norm of the difference of the orthogonal projection operators \(E_A(\sigma_0)\) and \(E_L(\omega_0)\) via \(\|X\|\) by equality (1.7) (see, e.g., Corollary 3.4 in [17]). By virtue of (1.7), inequality (3.19) is equivalent to bound (3.2). We have thus proved the theorem in the case where the modulus \(|X|\) has an eigenvalue coinciding with its norm.
In the case where $|X|$ has no eigenvalue equal to $\|X\|$, we can reduce the proof to the above case almost literally repeating the arguments used in [20] for proving the corresponding bound for $\|E_A(\sigma_0) - E_L(\omega_0)\|$ at $\sqrt{d(|\Delta| - d)} \leq \|V\| < \sqrt{d|\Delta|}$ (see Theorem 4.1 in [20]). Referring the reader to [20], we conclude the proof of the theorem.

We recall (see the proof of Theorem 2 in [19]) that the statement of Theorem 1 for $\|V\| < d$ is an elementary corollary of the more refined bound (3.2). For the integrity of the presentation, we clarify this statement.

**Proof of Theorem 1 for $\|V\| < d$.** Because $|\Delta| \geq 2d$, the condition $\|V\| < d$ automatically implies the condition $\|V\| < \sqrt{d(|\Delta| - d)}$. Hence, bound (3.2) is satisfied by Theorem 3. We note that at fixed values of $\|V\|$ and $d$ satisfying the inequality $\|V\| < d$, the quantity $\kappa(D, d, \|V\|)$ is a nonincreasing function of the variable $D \in [2d, \infty)$ attaining its maximum

$$\max_{D: D \geq 2d} \kappa(D, d, \|V\|) = \kappa(2d, d, \|V\|) = \frac{2\|V\|d}{d^2 - \|V\|^2} = \tan \left(2\arctan \frac{\|V\|}{d}\right)$$

at $D = 2d$. Therefore, bound (3.2) implies bound (3.1).

**Remark 3.** The optimality of bounds (1.3) at $\|V\| < d$ and (3.2) at $\|V\| < \sqrt{d(|\Delta| - d)}$ is supported by the corresponding actual matrix examples (see Example 5.5 and Remark 5.6 in [19] and Example 4.4 and Remark 4.5 in [20]).

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