AN ADDENDUM TO KREIN'S FORMULA

FRITZ GESZTESY, KONSTANTIN A. MAKAROV, EDUARD TSEKANOVSKII

ABSTRACT. We provide additional results in connection with Krein's formula, which describes the resolvent difference of two self-adjoint extensions A_1 and A_2 of a densely defined closed symmetric linear operator $\dot{A}$ with deficiency indices (n,n), $n \in \mathbb{N} \cup \{\infty\}$. In particular, we explicitly derive the linear fractional transformation relating the operator-valued Weyl-Titchmarsh M-functions $M_1(z)$ and $M_2(z)$ corresponding to A_1 and A_2.

The purpose of this note is to derive some elementary but useful consequences of Krein's formula, which appear to have escaped notice in the literature thus far.

We start with the basic setup following a short note of Saakjan [20]. This paper is virtually unknown in the western hemisphere, and to the best of our knowledge, no English translation of it seems to exist. Since the paper contains few details, we provide some proofs of the basic facts used in [20].

Let $\mathcal{H}$ be a complex separable Hilbert space with scalar product $(\,\cdot\,,\,\cdot\,)$ (linear in the second factor), denote the identity operator in $\mathcal{H}$ by I, abbreviate the restriction $I\big|_{\mathcal{N}}$ of I to a closed subspace $\mathcal{N}$ of $\mathcal{H}$ by $I_{\mathcal{N}}$, and let $\mathcal{B}(\mathcal{H})$ be the Banach space of bounded linear operators on $\mathcal{H}$. Let $\dot{A} : \mathcal{D}(\dot{A}) \to \mathcal{H}$, $\overline{\mathcal{D}(\dot{A})} = \mathcal{H}$ be a densely defined closed symmetric linear operator in $\mathcal{H}$ with equal deficiency indices def $(\dot{A}) = (n,n)$, $n \in \mathbb{N} \cup \{\infty\}$. We denote by $\mathcal{N}_\pm$ the deficiency subspaces of $\dot{A}$, that is,

$$\mathcal{N}_\pm = \ker(\dot{A}^* \mp i). \tag{1}$$

For any self-adjoint extension A of $\dot{A}$ we introduce its unitary Cayley transform C_A by

$$C_A = (A+i)(A-i)^{-1}. \tag{2}$$

In addition, we call two self-adjoint self-adjoint extensions A_1 and A_2 of $\dot{A}$ relatively prime if $\mathcal{D}(A_1) \cap \mathcal{D}(A_2) = \mathcal{D}(\dot{A})$. (In this case we shall also write that A_1 and A_2 are relatively prime w.r.t. $\dot{A}$). The point spectrum (i.e., the set of eigenvalues) and the resolvent set of a linear operator T in $\mathcal{H}$ are abbreviated by $\sigma_p(T)$ and $\rho(T)$, respectively, and the direct sum of two linear subspaces $\mathcal{V}$ and $\mathcal{W}$ of $\mathcal{H}$ is denoted by $\mathcal{V} \dot{+} \mathcal{W}$ in the following.

Lemma 1. *Let A, A_1, and A_2 be self-adjoint extensions of $\dot{A}$. Then*
(i). The Cayley transform of A maps $\mathcal{N}_-$ onto $\mathcal{N}_+$

$$C_A \mathcal{N}_- = \mathcal{N}_+. \tag{3}$$

(ii). $\mathcal{D}(A) = \mathcal{D}(\dot{A}) \dot{+} (I - C_A^{-1})\mathcal{N}_+$.
(iii). For $f_+ \in \mathcal{N}_+$, $(A-i)^{-1} C_A^{-1} f_+ = (i/2)(C_A^{-1} - I) f_+$.

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(iv). $\mathcal{N}_+$ is an invariant subspace for $C_{A_1}C_{A_2}^{-1}$ and $C_{A_2}C_{A_1}^{-1}$. In addition, A_1 and A_2 are relatively prime if and only if

$$1 \notin \sigma_p(C_{A_1}C_{A_2}^{-1}\big|_{\mathcal{N}_+}). \tag{4}$$

(v). Suppose A_1 and A_2 are relatively prime w.r.t. $\dot{A}$. Then

$$\overline{\operatorname{ran}((A_2-i)^{-1}-(A_1-i)^{-1})} = \mathcal{N}_+, \tag{5}$$

$$\ker(((A_2-i)^{-1}-(A_1-i)^{-1})\big|_{\mathcal{N}_-}) = \{0\}. \tag{6}$$

Proof. Since the facts are standard we only sketch the main steps.
(i). Pick $g \in \mathcal{D}(\dot{A})$, $f = (\dot{A}-i)g$, then $C_A f = (\dot{A}+i)g \in \operatorname{ran}(\dot{A}+i)$ yields $C_A\operatorname{ran}(\dot{A}-i) \subseteq \operatorname{ran}(\dot{A}+i)$. Similarly one infers $C_A^{-1}\operatorname{ran}(\dot{A}+i) \subseteq \operatorname{ran}(\dot{A}-i)$ and hence $C_A\operatorname{ran}(\dot{A}-i) = \operatorname{ran}(\dot{A}+i)$. Since $C_A \in \mathcal{B}(\mathcal{H})$ (in fact, C_A is unitary), $C_A\overline{\operatorname{ran}(\dot{A}-i)} = \overline{\operatorname{ran}(\dot{A}+i)}$. $\mathcal{H} = \ker(\dot{A}^*-i)\oplus\overline{\operatorname{ran}(\dot{A}+i)}$ then yields $C_A\mathcal{N}_- = \mathcal{N}_+$.
(ii). By von Neumann's formula [18],

$$\mathcal{D}(A) = \mathcal{D}(\dot{A})\dot{+}\mathcal{N}_+\dot{+}\mathcal{U}_A\mathcal{N}_+ \tag{7}$$

for some linear isometric isomorphism $\mathcal{U}_A : \mathcal{N}_+ \to \mathcal{N}_-$. Since $I - C_A^{-1} = 2i(A+i)^{-1}$, $(I-C_A^{-1})\mathcal{N}_+ = 2i(A+i)^{-1}\mathcal{N}_+ \subseteq \mathcal{D}(A)$, one concludes

$$\mathcal{U}_A = -C_A^{-1}\big|_{\mathcal{N}_+}. \tag{8}$$

(iii). $(i/2)(I-C_A^{-1})f_+ \in \mathcal{D}(A)$ and

$$\begin{aligned}(i/2)(A-i)(I-C_A^{-1})f_+ &= (i/2)(A-i)2i(A+i)^{-1}f_+ = -(A-i)(A+i)^{-1}f_+\\ &= -C_A^{-1}f_+.\end{aligned} \tag{9}$$

(iv). By (i), $\mathcal{N}_+$ is an invariant subspace for the unitary operators $C_{A_1}C_{A_2}^{-1}$ and $C_{A_2}C_{A_1}^{-1}$. To complete the proof of (4) it suffices to note that

$$\begin{aligned}1 \in \sigma_p(C_{A_1}C_{A_2}^{-1}|\mathcal{N}_+) &\iff \exists\, 0 \neq f_+ \in \mathcal{N}_+ :\ C_{A_1}^{-1}f_+ = C_{A_2}^{-1}f_+\\ &\iff (I-C_{A_1}^{-1})f_+ = (I-C_{A_2}^{-1})f_+ \in \mathcal{D}(A_1)\cap\mathcal{D}(A_2)\end{aligned} \tag{10}$$

(by the proof of (ii)) and $(I-C_{A_1}^{-1})f_+ \notin \mathcal{D}(\dot{A})$ (by (ii)) yields a contradiction to A_1 and A_2 being relatively prime w.r.t. $\dot{A}$.
(v). Let $g \in \mathcal{D}(\dot{A})$, $f = (\dot{A}+i)g$, then

$$(f,((A_2-i)^{-1}-(A_1-i)^{-1})h) = (((A_2+i)^{-1}-(A_1+i)^{-1})(\dot{A}+i)g,h) = 0, \quad h \in \mathcal{H} \tag{11}$$

yields

$$\operatorname{ran}((A_2-i)^{-1}-(A_1-i)^{-1}) \subseteq \operatorname{ran}(\dot{A}+i)^{\perp} = \ker(\dot{A}^*-i) = \mathcal{N}_+. \tag{12}$$

Next, let $0 \neq f_+ \in \mathcal{N}_+$ and $f_+ \perp \operatorname{ran}((A_2-i)^{-1}-(A_1-i)^{-1})$. In particular, $f_+ \perp ((A_2-i)^{-1}-(A_1-i)^{-1})C_{A_1}^{-1}f_+$. By (iii), $(A_1-i)^{-1}C_{A_1}^{-1}f_+ = -(i/2)(I-C_{A_1}^{-1})f_+$ and

$$\begin{aligned}(A_2-i)^{-1}C_{A_1}^{-1}f_+ &= (A_2-i)^{-1}C_{A_2}^{-1}(C_{A_2}C_{A_1}^{-1}f_+) = -(i/2)(I-C_{A_2}^{-1})(C_{A_2}C_{A_1}^{-1}f_+)\\ &= -(i/2)(C_{A_2}C_{A_1}^{-1}-C_{A_1}^{-1})f_+,\end{aligned} \tag{13}$$

and hence

$$((A_2-i)^{-1}-(A_1-i)^{-1})C_{A_1}^{-1}f_+ = -(i/2)(C_{A_2}C_{A_1}^{-1}-I)f_+. \tag{14}$$

Thus, $f_+ \perp (C_{A_2}C_{A_1}^{-1} - I)f_+$, that is,

$$(f_+, C_{A_2}C_{A_1}^{-1}f_+) = ||f_+||^2. \tag{15}$$

Since $C_{A_2}C_{A_1}^{-1}\big|_{\mathcal{N}_+}$ is unitary, one concludes $C_{A_2}C_{A_1}^{-1}f_+ = f_+ = C_{A_1}C_{A_2}^{-1}f_+$ and hence

$$1 \in \sigma_p(C_{A_1}C_{A_2}^{-1}|\mathcal{N}_+). \tag{16}$$

But (16) contradicts the hypothesis that A_1 and A_2 are relatively prime w.r.t. $\dot{A}$. Consequently, $\overline{\operatorname{ran}((A_2 - i)^{-1} - \operatorname{ran}((A_1 - i)^{-1}))} = \mathcal{N}_+$, which is (5).

To prove (6) we note that every $f_- \in \mathcal{N}_-$ is of the form $f_- = C_{A_1}^{-1}f_+$ for some $f_+ \in \mathcal{N}_+$ using (i). Suppose $((A_2-i)^{-1}-(A_1-i)^{-1})C_{A_1}^{-1}f_+ = 0$. By (14), this yields $C_{A_1}C_{A_2}^{-1}f_+ = f_+$ and hence $1 \in \sigma_p(C_{A_1}C_{A_2}^{-1}\big|_{\mathcal{N}_+})$. Since A_1 and A_2 are relatively prime w.r.t. $\dot{A}$ one concludes $f_- = C_{A_1}^{-1}f_+ = 0$. $\square$

Next, assuming $A_\ell, \ell = 1, 2$ to be self-adjoint extensions of $\dot{A}$, define

$$P_{1,2}(z) = (A_1 - z)(A_1 - i)^{-1}((A_2 - z)^{-1} - (A_1 - z)^{-1})(A_1 - z)(A_1 + i)^{-1}, \quad z \in \rho(A_1) \cap \rho(A_2). \tag{17}$$

We collect the following properties of $P_{1,2}(z)$.

Lemma 2. [20] *Let $z, z' \in \rho(A_1) \cap \rho(A_2)$.*
(i). $P_{1,2} : \rho(A_1) \cap \rho(A_2) \to \mathcal{B}(\mathcal{H})$ is analytic and

$$P_{1,2}(z)^* = P_{1,2}(\bar{z}). \tag{18}$$

(ii).

$$P_{1,2}(z)\big|_{\mathcal{N}_+^\perp} = 0, \quad P_{1,2}(z)\mathcal{N}_+ \subseteq \mathcal{N}_+. \tag{19}$$

(iii).

$$P_{1,2}(z) = P_{1,2}(z') + (z - z')P_{1,2}(z')(A_1 + i)(A_1 - z')^{-1}(A_1 - i)(A_1 - z)^{-1}P_{1,2}(z). \tag{20}$$

(iv). $\operatorname{ran}(P_{1,2}(z)\big|_{\mathcal{N}_+})$ *is independent of $z \in \rho(A_1) \cap \rho(A_2)$.*
(v). Assume A_1 and A_2 are relatively prime self-adjoint extensions of $\dot{A}$. Then $P_{1,2}(z)\big|_{\mathcal{N}_+} : \mathcal{N}_+ \to \mathcal{N}_+$ is invertible (i.e., one-to-one).
(vi). Assume A_1 and A_2 are relatively prime self-adjoint extensions of $\dot{A}$. Then

$$\overline{\operatorname{ran}(P_{1,2}(i))} = \mathcal{N}_+. \tag{21}$$

(vii).

$$P_{1,2}(i)\big|_{\mathcal{N}_+} = (i/2)(I - C_{A_2}C_{A_1}^{-1})\big|_{\mathcal{N}_+}. \tag{22}$$

Next, let

$$C_{A_2}C_{A_1}^{-1}\big|_{\mathcal{N}_+} = -e^{-2i\alpha_{1,2}} \tag{23}$$

for some self-adjoint (possibly unbounded) operator $\alpha_{1,2}$ in $\mathcal{N}_+$. If A_1 and A_2 are relatively prime, then

$$\{(m + \tfrac{1}{2})\pi\}_{m\in\mathbb{Z}} \cap \sigma_p(\alpha_{1,2}) = \emptyset \tag{24}$$

and

$$(P_{1,2}(i)\big|_{\mathcal{N}_+})^{-1} = \tan(\alpha_{1,2}) - iI_{\mathcal{N}_+}. \tag{25}$$

In addition, $\tan(\alpha_{1,2}) \in \mathcal{B}(\mathcal{N}_+)$ *if and only if* $\operatorname{ran}(P_{1,2}(i)) = \mathcal{N}_+$.

Proof. (i) is clear from (17).
(ii). Let $f \in \mathcal{D}(\dot{A})$, $g = (\dot{A} + i)f$. Then

$$P_{1,2}(z)g = (A_1 - z)(A_1 - i)^{-1}((A_2 - z)^{-1} - (A_1 - z)^{-1})(\dot{A} - z)f = 0 \tag{26}$$

yields $P_{1,2}(z)\big|_{\operatorname{ran}(\dot{A}+i)} = 0$ and hence $P_{1,2}(z)\big|_{\overline{\operatorname{ran}(\dot{A}+i)}} = P_{1,2}(z)\big|_{\mathcal{N}_+^\perp} = 0$ since $P_{1,2}(z) \in \mathcal{B}(\mathcal{H})$. Moreover, by (17)

$$\operatorname{ran}(P_{1,2}(z)) \subseteq (A_1 - z)(A_1 - i)^{-1} \ker(\dot{A}^* - z) \subseteq \ker(\dot{A}^* - i) = \mathcal{N}_+ \tag{27}$$

since

$$\begin{aligned}
&(\dot{A}^* - i)(A_1 - z)(A_1 - i)^{-1}\big|_{\ker(\dot{A}^* - z)} \\
&= (\dot{A}^* - i)(I - (z - i)(A_1 - i)^{-1})\big|_{\ker(\dot{A}^* - z)} \\
&= ((z - i)I - (z - i)(\dot{A}^* - i)(A_1 - i)^{-1})\big|_{\ker(\dot{A}^* - z)} = 0.
\end{aligned} \tag{28}$$

This proves (19).
(iii). (20) is a straightforward (though tedious) computation using (17).
(iv). By (20), $\operatorname{ran}(P_{1,2}(z)\big|_{\mathcal{N}_+}) \subseteq \operatorname{ran}(P_{1,2}(z')\big|_{\mathcal{N}_+})$. By symmetry in z and z',

$$\operatorname{ran}(P_{1,2}(z)\big|_{\mathcal{N}_+}) = \operatorname{ran}(P_{1,2}(z')\big|_{\mathcal{N}_+}) \tag{29}$$

is independent of $z \in \rho(A_1) \cap \rho(A_2)$.
(v). Since

$$P_{1,2}(i) = ((A_2 - i)^{-1} - (A_1 - i)^{-1})C_{A_1}^{-1}, \tag{30}$$

$C_{A_1}^{-1} : \mathcal{N}_+ \to \mathcal{N}_-$ is isometric, $\ker((A_2 - i)^{-1} - (A_1 - i)^{-1}))\big|_{\mathcal{N}_-}) = \{0\}$ by (6), one infers $\ker((P_{1,2}(i)\big|_{\mathcal{N}_+}) = \{0\}$. Taking $z' = i$ in (20) yields $\ker(P_{1,2}(z)\big|_{\mathcal{N}_+}) = \{0\}$, that is, $P_{1,2}(z)\big|_{\mathcal{N}_+}$ is invertible.
(vi). Since $\overline{\operatorname{ran}((A_2 - i)^{-1} - (A_1 - i)^{-1})} = \mathcal{N}_+$ by (5) and $C_{A_1}^{-1} : \mathcal{H} \to \mathcal{H}$ is unitary, (29) implies (21).
(vii). (22) follows from (14) and (30). (24) is a consequence of (4), and (25) follows from the elementary trigonometric identity $(i/2)(1 + e^{-2ix}) = (\tan(x) - i)^{-1}$. By (25) and (21) $\operatorname{ran}(P_{1,2}(i)) = \mathcal{D}(\tan(\alpha_{1,2}))$ is dense in $\mathcal{N}_+$ and hence $\tan(\alpha_{1,2}) \in \mathcal{B}(\mathcal{N}_+)$ if and only if $\operatorname{ran}(P_{1,2}(i)) = \mathcal{N}_+$. □

Next, we turn to the definition of Weyl-Titchmarsh operators associated with self-adjoint extensions of $\dot{A}$.

Definition 3.
Let A be a self-adjoint extension of $\dot{A}$, $\mathcal{N} \subseteq \mathcal{N}_+$ a closed linear subspace of $\mathcal{N}_+ = \ker(\dot{A}^* - i)$, and $z \in \rho(A)$. Then the Weyl-Titchmarsh operator $M_{A,\mathcal{N}}(z) \in \mathcal{B}(\mathcal{N})$ associated with the pair $(A, \mathcal{N})$ is defined by

$$M_{A,\mathcal{N}}(z) = P_{\mathcal{N}}(zA + I)(A - z)^{-1}P_{\mathcal{N}}\big|_{\mathcal{N}} = zI_{\mathcal{N}} + (1 + z^2)P_{\mathcal{N}}(A - z)^{-1}P_{\mathcal{N}}\big|_{\mathcal{N}}, \tag{31}$$

with $P_{\mathcal{N}}$ the orthogonal projection in $\mathcal{H}$ onto $\mathcal{N}$.

Weyl-Titchmarsh m-functions of the type (31) have attracted a lot of interest since their introduction by Weyl [26] in the context of second-order ordinary differential operators and their function-theoretic study initiated by Titchmarsh [24]. Subsequently, Krein introduced the concept of Q-functions, the appropriate generalization of the scalar Weyl-Titchmarsh m-function, and he and his school launched a systematic investigation of Q. The literature on Q-functions is too extensive to be discussed exhaustively in this note. We refer, for instance, to [10], [11], [12], [13], [14], [15], [25] and the literature therein. Saakjan [20] considers a Q-function of the type (31) in the general case where $\operatorname{def}(\dot{A}) = (n, n)$, $n \in \mathbb{N} \cup \{\infty\}$. The special case $\operatorname{def}(\dot{A}) = (1, 1)$ was also discussed by Donoghue [6], who apparently was unaware of Krein's work in this context. For a recent treatment of operator-valued m-functions we also refer to Derkach and Malamud [4], [5] and the extensive bibliography therein.

Lemma 4. [20] *Let A_ℓ, $\ell = 1, 2$ be relatively prime self-adjoint extensions of $\dot{A}$. Then*

$$(P_{1,2}(z)\big|_{\mathcal{N}_+})^{-1} = (P_{1,2}(i)\big|_{\mathcal{N}_+})^{-1} - (z - i)P_{\mathcal{N}_+}(A_1 + i)(A_1 - z)^{-1}P_{\mathcal{N}_+} \tag{32}$$

$$= \tan(\alpha_{1,2}) - M_{A_1,\mathcal{N}_+}(z), \ z \in \rho(A_1). \tag{33}$$

Proof. By Lemma 2 (v), $P_{1,2}(z)\big|_{\mathcal{N}_+}$ is invertible for $z \in \rho(A_1) \cap \rho(A_2)$ and hence (32) follows from (30) (and extends by continuity to all $z \in \rho(A_1)$). Equation (33) is then clear from (25) and (31). □

Given Lemmas 1,2, and 4 we can summarize Saakjans's results on Krein's formula as follows.

Theorem 5. [20] *Let A_1 and A_2 be self-adjoint extensions of $\dot{A}$ and $z \in \rho(A_1) \cap \rho(A_2)$. Then*

$$(A_2 - z)^{-1} = (A_1 - z)^{-1} + (A_1 - i)(A_1 - z)^{-1}P_{1,2}(z)(A_1 + i)^{-1}(A_1 - z)^{-1} \tag{34}$$

$$\begin{aligned} &= (A_1 - z)^{-1} + (A_1 - i)(A_1 - z)^{-1}P_{\mathcal{N}_{1,2,+}} \\ &\quad \times (\tan(\alpha_{\mathcal{N}_{1,2,+}}) - M_{A_1,\mathcal{N}_{1,2,+}}(z))^{-1}P_{\mathcal{N}_{1,2,+}}(A_1 + i)(A_1 - z)^{-1}, \end{aligned} \tag{35}$$

where

$$\mathcal{N}_{1,2,+} = \ker((A_1\big|_{\mathcal{D}(A_1)\cap\mathcal{D}(A_2)})^* - i) \tag{36}$$

and

$$e^{-2i\alpha_{\mathcal{N}_{1,2,+}}} = -C_{A_2}C_{A_1}^{-1}\big|_{\mathcal{N}_{1,2,+}}. \tag{37}$$

Proof. If A_1 and A_2 are relatively prime w.r.t. $\dot{A}$, Lemmas 1, 2, and 4 prove (34)–(37). If A_1 and A_2 are arbitrary self-adjoint extensions of $\dot{A}$ one replaces $\dot{A}$ by the largest common symmetric part of A_1 and A_2 given by $A_1\big|_{\mathcal{D}(A_1)\cap\mathcal{D}(A_2)}$. □

Apparently, Krein's formula (34), (35) was first derived independently by Krein [10] and Naimark [17] in the special case $\operatorname{def}(\dot{A}) = (1, 1)$. The case $\operatorname{def}(\dot{A}) = (n, n)$, $n \in \mathbb{N}$ is due to Krein [11]. A proof for this case can also be found in the classic monograph by Akhiezer and Glazman [1], Sect. 84. Saakjan [20] extended Krein's formula to the general case $\operatorname{def}(\dot{A}) = (n, n)$, $n \in \mathbb{N} \cup \{\infty\}$. In another form, the generalized resolvent formula for symmetric operators (including the case of non-densely defined operators) has been obtained by Straus [21], [22]. For a variety of further results and extensions of Krein's formula we refer, for instance, to [8], [9], [14], [15], [16], [23], and the literature therein.

Saakjan [20] makes no explicit attempt to relate Krein's formula and von Neumann's parametrization [18] of self-adjoint extensions of $\dot{A}$ (or $A_1|_{\mathcal{D}(A_1)\cap\mathcal{D}(A_2)}$). This connection, however, easily follows from the preceding formalism:

Corollary 6.

$$P_{1,2}(i)\big|_{\mathcal{N}_{1,2,+}} = (i/2)(I - \mathcal{U}_{A_2}^{-1}\mathcal{U}_{A_1})\big|_{\mathcal{N}_{1,2,+}}, \tag{38}$$

where

$$\mathcal{U}_{A_\ell} = -C_{A_\ell}^{-1}\big|_{\mathcal{N}_+}, \ \ell = 1,2 \tag{39}$$

denotes the linear isometric isomorphism from $\mathcal{N}_+$ onto $\mathcal{N}_-$ parametrizing the self-adjoint extensions A_ℓ of $\dot{A}$.

Proof. Combine (7), (8), and (22). □

Krein's formula has been used in a large variety of problems in mathematical physics as can be inferred from the extensive number of references provided, for instance, in [2]. (A complete bibliography on Krein's formula is beyond the scope of this short note.)

Next, we observe that $M_{A,\mathcal{N}}(z)$ and hence $-(P_{1,2}(z)\big|_{\mathcal{N}_+})^{-1}$ and $P_{1,2}(z)\big|_{\mathcal{N}_+}$ (cf. (33)) are operator-valued Herglotz functions. More precisely, denoting $\mathrm{Re}(T) = (T+T^*)/2$, $\mathrm{Im}(T) = (T-T^*)/2i$ for linear operators T with $\mathcal{D}(T) = \mathcal{D}(T^*)$ in some Hilbert space $\mathcal{K}$, one can prove the following result.

Lemma 7. *Let A be a self-adjoint extension of $\dot{A}$, $\mathcal{N}$ a closed subspace of $\mathcal{N}_+$. Then the Weyl-Titchmarsh operator $M_{A,\mathcal{N}}(z)$ is analytic for $z \in \mathbb{C}\backslash\mathbb{R}$ and*

$$\mathrm{Im}(z)\mathrm{Im}(M_{A,\mathcal{N}}(z)) \geq (\max(1,|z|^2) + |\mathrm{Re}(z)|)^{-1}, \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{40}$$

In particular, $M_{A,\mathcal{N}}(z)$ is a $\mathcal{B}(\mathcal{N})$-valued Herglotz function.

Proof. Using (31), an explicit computation yields

$$\begin{aligned}\mathrm{Im}(z)\mathrm{Im}(M_{A,\mathcal{N}}(z)) &= P_{\mathcal{N}}(I+A^2)^{1/2}((A-\mathrm{Re}(z))^2 + (\mathrm{Im}(z))^2)^{-1} \\ &\quad \times (I+A^2)^{1/2}P_{\mathcal{N}}\big|_{\mathcal{N}}.\end{aligned} \tag{41}$$

Next we note that for $z \in \mathbb{C}\backslash\mathbb{R}$,

$$\frac{1+\lambda^2}{(\lambda-\mathrm{Re}(z))^2 + (\mathrm{Im}(z))^2} \geq \frac{1}{\max(1,|z|^2)+|\mathrm{Re}(z)|}, \quad \lambda \in \mathbb{R}. \tag{42}$$

Since by the Rayleigh-Ritz technique, projection onto a subspace contained in the domain of a self-adjoint operator bounded from below can only rise the lower bound of the spectrum (cf. [19], Sect. XIII.1), (41) and (42) prove (40). □

In the remainder of this note we shall explicitly derive the linear fractional transformation relating the Weyl-Titchmarsh operators $M_{A_\ell,\mathcal{N}_{1,2,+}}$ associated with two self-adjoint extensions A_ℓ, $\ell = 1,2$, of $\dot{A}$. For simplicity we first consider the case where A_1 and A_2 are relatively prime w.r.t. $\dot{A}$.

Lemma 8. *Suppose A_1 and A_2 are relatively prime self-adjoint extensions of $\dot{A}$ and $z \in \rho(A_1) \cap \rho(a_2)$. Then*

$$\begin{aligned} M_{A_2,\mathcal{N}_+}(z) &= (P_{1,2}(i)\big|_{\mathcal{N}_+} + (I_{\mathcal{N}_+} + iP_{1,2}(i)\big|_{\mathcal{N}_+})M_{A_1,\mathcal{N}_+}(z)) \\ &\qquad \times ((I_{\mathcal{N}_+} + iP_{1,2}(i)\big|_{\mathcal{N}_+}) - P_{1,2}(i)\big|_{\mathcal{N}_+} M_{A_1,\mathcal{N}_+}(z))^{-1} \qquad (43) \\ &= e^{-i\alpha_{1,2}}(\cos(\alpha_{1,2}) + \sin(\alpha_{1,2})M_{A_1,\mathcal{N}_+}(z)) \\ &\qquad \times (\sin(\alpha_{1,2}) - \cos(\alpha_{1,2})M_{A_1,\mathcal{N}_+}(z))^{-1} e^{i\alpha_{1,2}}, \qquad (44) \end{aligned}$$

where

$$e^{-2i\alpha_{1,2}} = -C_{A_2}C_{A_1}^{-1}\big|_{\mathcal{N}_+}. \qquad (45)$$

Proof. Using (33) and (35) one computes

$$\begin{aligned} &M_{A_2,\mathcal{N}_+}(z) = (zI + (1+z^2)P_{\mathcal{N}_+}(A_2 - z)^{-1}P_{\mathcal{N}_+})\big|_{\mathcal{N}_+} \\ &= M_{A_1,\mathcal{N}_+}(z) + (1+z^2)P_{\mathcal{N}_+}(A_1 - i)(A_1 - z)^{-1}P_{\mathcal{N}_+}(\tan(\alpha_{1,2}) - M_{A_1,\mathcal{N}_+}(z))^{-1} \\ &\qquad\qquad \times P_{\mathcal{N}_+}(A_1 + i)(A_1 - z)^{-1}P_{\mathcal{N}_+} \\ &= M_{A_1,\mathcal{N}_+}(z) + (iI_{\mathcal{N}_+} + M_{A_1,\mathcal{N}_+}(z))(\tan(\alpha_{1,2}) - M_{A_1,\mathcal{N}_+}(z))^{-1} \\ &\qquad\qquad \times (-iI_{\mathcal{N}_+} + M_{A_1,\mathcal{N}_+}(z)) \\ &= M_{A_1,\mathcal{N}_+}(z) + (iI_{\mathcal{N}_+} + M_{A_1,\mathcal{N}_+}(z))(\tan(\alpha_{1,2}) - M_{A_1,\mathcal{N}_+}(z))^{-1} \\ &\qquad \times (-iI_{\mathcal{N}_+} + M_{A_1,\mathcal{N}_+}(z) - \tan(\alpha_{1,2}) + \tan(\alpha_{1,2})) \\ &= -iI_{\mathcal{N}_+} + (iI_{\mathcal{N}_+} + M_{A_1,\mathcal{N}_+}(z))(\tan(\alpha_{1,2}) - M_{A_1,\mathcal{N}_+}(z))^{-1}(-iI_{\mathcal{N}_+} + \tan(\alpha_{1,2})) \\ &= -i(-iI_{\mathcal{N}_+} + \tan(\alpha_{1,2}))^{-1}(\tan(\alpha_{1,2}) - M_{A_1,\mathcal{N}_+}(z))(\tan(\alpha_{1,2}) - M_{A_1,\mathcal{N}_+}(z))^{-1} \\ &\qquad\qquad \times (-iI_{\mathcal{N}_+} + \tan(\alpha_{1,2})) \\ &\quad + (iI_{\mathcal{N}_+} + M_{A_1,\mathcal{N}_+}(z))(\tan(\alpha_{1,2}) - M_{A_1,\mathcal{N}_+}(z))^{-1}(-iI_{\mathcal{N}_+} + \tan(\alpha_{1,2})) \\ &= (-iI_{\mathcal{N}_+} + \tan(\alpha_{1,2}))^{-1}[-i\tan(\alpha_{1,2}) + iM_{A_1,\mathcal{N}_+}(z) \\ &\quad + (-iI_{\mathcal{N}_+} + \tan(\alpha_{1,2}))(iI_{\mathcal{N}_+} + M_{A_1,\mathcal{N}_+}(z))](\tan(\alpha_{1,2}) - M_{A_1,\mathcal{N}_+}(z))^{-1} \\ &\qquad\qquad \times ((-iI_{\mathcal{N}_+} + \tan(\alpha_{1,2})) \\ &= (-iI_{\mathcal{N}_+} + \tan(\alpha_{1,2}))^{-1}(I_{\mathcal{N}_+} + \tan(\alpha_{1,2})M_{A_1,\mathcal{N}_+}(z))(\tan(\alpha_{1,2}) - M_{A_1,\mathcal{N}_+}(z))^{-1} \\ &\qquad\qquad \times ((-iI_{\mathcal{N}_+} + \tan(\alpha_{1,2})) = (44). \qquad (46) \end{aligned}$$

Equation (43) then immediately follows from (46) since $P_{1,2}(i)\big|_{\mathcal{N}_+} = (\tan(\alpha_{1,2}) - iI_{\mathcal{N}_+})^{-1}$ by (25). ☐

Finally, we treat the case of general self-adjoint extensions of $\dot{A}$ and state the principal result of this note.

Theorem 9. *Suppose A_1 and A_2 are self-adjoint extensions of $\dot{A}$ and $z \in \rho(A_1) \cap \rho(A_2)$. Then (43) still holds, that is,*

$$\begin{aligned} M_{A_2,\mathcal{N}_+}(z) &= (P_{1,2}(i)\big|_{\mathcal{N}_+} + (I_{\mathcal{N}_+} + iP_{1,2}(i)\big|_{\mathcal{N}_+})M_{A_1,\mathcal{N}_+}(z)) \\ &\qquad \times ((I_{\mathcal{N}_+} + iP_{1,2}(i)\big|_{\mathcal{N}_+}) - P_{1,2}(i)\big|_{\mathcal{N}_+} M_{A_1,\mathcal{N}_+}(z))^{-1}, \qquad (47) \end{aligned}$$

where

$$P_{1,2}(i)\big|_{\mathcal{N}_+} = (i/2)(I - C_{A_2}C_{A_1}^{-1})\big|_{\mathcal{N}_+}, \ I_{\mathcal{N}_+} + P_{1,2}(i)\big|_{\mathcal{N}_+} = (1/2)(I + C_{A_2}C_{A_1}^{-1})\big|_{\mathcal{N}_+}. \qquad (48)$$

Proof. Choose a self-adjoint extension A_3 of $\dot{A}$ such that (A_1, A_3) and (A_2, A_3) are relatively prime w.r.t. $\dot{A}$. (Existence of A_3 is easily confirmed using the criterion (4)). Then express $M_{A_1,\mathcal{N}_+}(z)$ in terms of $M_{A_3,\mathcal{N}_+}(z)$ and an associated $\alpha_{3,1}$ according to (44) and (45) and similarly, express $M_{A_2,\mathcal{N}_+}(z)$ in terms of $M_{A_3,\mathcal{N}_+}(z)$ and some $\alpha_{3,2}$. One obtains,

$$\begin{aligned} M_{A_1,\mathcal{N}_+}(z) &= e^{-i\alpha_{3,1}}(\cos(\alpha_{3,1}) + \sin(\alpha_{3,1})M_{A_3,\mathcal{N}_+}(z)) \\ &\qquad \times (\sin(\alpha_{3,1}) - \cos(\alpha_{3,1})M_{A_3,\mathcal{N}_+}(z))^{-1}e^{i\alpha_{3,1}}, \qquad (49) \\ M_{A_2,\mathcal{N}_+}(z) &= e^{-i\alpha_{3,2}}(\cos(\alpha_{3,2}) + \sin(\alpha_{3,2})M_{A_3,\mathcal{N}_+}(z)) \\ &\qquad \times (\sin(\alpha_{3,2}) - \cos(\alpha_{3,2})M_{A_3,\mathcal{N}_+}(z))^{-1}e^{i\alpha_{3,2}}. \qquad (50) \end{aligned}$$

Computing $M_{A_3,\mathcal{N}_+}(z)$ from (49) yields

$$\begin{aligned} M_{A_3,\mathcal{N}_+}(z) &= -e^{i\alpha_{3,1}}(\cos(\alpha_{3,1}) - \sin(\alpha_{3,1})M_{A_1,\mathcal{N}_+}(z)) \\ &\qquad \times (\sin(\alpha_{3,1}) + \cos(\alpha_{3,1})M_{A_1,\mathcal{N}_+}(z))^{-1}e^{-i\alpha_{3,1}}. \qquad (51) \end{aligned}$$

Insertion of (51) into (50) yields (47) taking into account (48). □

Since the boundary values $\lim_{\varepsilon\downarrow 0}(f, M_{A_1,\mathcal{N}_+}(\lambda + i\varepsilon)g)$ for $f, g \in \mathcal{N}_+$ and a.e. $\lambda \in \mathbb{R}$ contain spectral information on the self-adjoint extension A_1 of $\dot{A}$, relations of the type (47) entail important connections between the spectra of A_1 and A_2. In particular, the well-known unitary equivalence of the absolutely continuous parts $A_{1,ac}$ and $A_{2,ac}$ of A_1 and A_2 in the case $\operatorname{def}(\dot{A}) = (n, n)$, $n \in \mathbb{N}$, can be inferred from (47) as discussed in detail in [7]. Moreover, in concrete applications to ordinary differential operators with matrix-valued coefficients, the choice of different self-adjoint boundary conditions associated with a given formally symmetric differential expression τ yields self-adjoint realizations of τ whose corresponding M-functions are related via linear fractional transformations of the type considered in Theorem 9.

Although it appears very unlikely that the explicit formula (47) has been missed in the extensive literature on self-adjoint extensions of symmetric operators of equal deficiency indices, we were not able to locate a pertinent reference. In the special case $\operatorname{def}(\dot{A}) = (1, 1)$, equations (44) and (47) are of course well-known and were studied in great detail by Aronszajn [3] and Donoghue [6].

We conclude with a simple illustration.

Example 10. $\mathcal{H} = L^2((0,\infty); dx)$,

$$\begin{aligned} &\dot{A} = -\frac{d^2}{dx^2}, \\ &\mathcal{D}(\dot{A}) = \{g \in L^2((0,\infty); dx) \,|\, g, g' \in AC_{\mathrm{loc}}((0,\infty)),\ g(+0) = g'(+0) = 0\}, \\ &\dot{A}^* = -\frac{d^2}{dx^2}, \\ &\mathcal{D}(\dot{A}^*) = \{g \in L^2((0,\infty); dx) \,|\, g, g' \in AC_{\mathrm{loc}}((0,\infty)),\ g'' \in L^2((0,\infty); dx)\}, \\ &A_1 = A_F = -\frac{d^2}{dx^2}, \quad \mathcal{D}(A_1) = \{g \in \mathcal{D}(\dot{A}^*) \,|\, g(+0) = 0\}, \\ &A_2 = -\frac{d^2}{dx^2}, \quad \mathcal{D}(A_2) = \{g \in \mathcal{D}(\dot{A}^*) \,|\, g'(+0) + 2^{-1/2}(1 - \tan(\alpha_2))g(+0) = 0\}, \end{aligned}$$

$$\alpha_2 \in [0,\pi)\backslash\{\pi/2\},$$

where A_F denotes the Friedrichs extension of $\dot{A}$ (corresponding to $\alpha_2 = \pi/2$). One verifies,

$$\ker(\dot{A}^* - z) = \{ce^{i\sqrt{z}x}, c \in \mathbb{C}\},\ \operatorname{Im}(\sqrt{z}) > 0,\ z \in \mathbb{C}\backslash[0,\infty), \quad \operatorname{def}(\dot{A}) = (1,1),$$

$$(A_2 - z)^{-1} = (A_1 - z)^{-1} - (2^{-1/2}(1 - \tan(\alpha_2)) + i\sqrt{z})^{-1}(\overline{e^{i\sqrt{z}\cdot}}, \cdot)e^{i\sqrt{z}\cdot},$$

$$z \in \rho(A_2),\ \operatorname{Im}(\sqrt{z}) > 0,$$

$$\mathcal{U}_2^{-1}\mathcal{U}_1 = -e^{-2i\alpha_2},$$

$$P_{1,2}(z) = -(1 - \tan(\alpha_2) + i\sqrt{2z})^{-1},\ z \in \rho(A_2), \quad P_{1,2}(i)^{-1} = \tan(\alpha_2) - i,$$

$$M_{A_1,\mathcal{N}_+}(z) = i\sqrt{2z} + 1, \quad M_{A_2,\mathcal{N}_+}(z) = \frac{\cos(\alpha_2) + \sin(\alpha_2)(i\sqrt{2z} + 1)}{\sin(\alpha_2) - \cos(\alpha_2)(i\sqrt{2z} + 1)}.$$

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Department of Mathematics, University of Missouri, Columbia, MO 65211, USA
E-mail address: fritz@math.missouri.edu
URL: http://www.math.missouri.edu/people/faculty/fgesztesy.html

Department of Mathematics, University of Missouri, Columbia, MO 65211, USA
E-mail address: makarov@azure.math.missouri.edu

Department of Mathematics, University of Missouri, Columbia, MO 65211, USA
E-mail address: tsekanov@leibniz.cs.missouri.edu