EXTREMAL SPECTRAL FUNCTIONS OF A SYMMETRIC OPERATOR

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1. Introduction. Let $H_1$ be a symmetric operator in a Hilbert space $\mathfrak{H}_1$. If $H$ is a self-adjoint operator in a Hilbert space $\mathfrak{H}$ such that $\mathfrak{H}_1 \subseteq \mathfrak{H}$ and $H_1 \subseteq H$, then $H$ is called a self-adjoint extension of $H_1$. If $\mathfrak{H} \oplus \mathfrak{H}_1$ is finite-dimensional, then $H$ is called a finite-dimensional self-adjoint extension of $H_1$. $H$ is called a minimal self-adjoint extension if neither $\mathfrak{H} \oplus \mathfrak{H}_1$ nor any of its subspaces different from $\{0\}$ reduces $H$.

Suppose $H$ is a self-adjoint extension of $H_1$. If $E(\lambda)$ is the spectral function of $H$ and if $P_1$ is the operator in $\mathfrak{H}$ of orthogonal projection on $\mathfrak{H}_1$, then the operator function $E_1(\lambda) = P_1 E(\lambda)$ restricted to $\mathfrak{H}_1$ is called a spectral function of $H_1$. We shall say that the spectral function $E_1(\lambda)$ is defined by the self-adjoint extension $H$.

The family of spectral functions of $H_1$ is a convex set, i.e., if $E_1'(\lambda)$ and $E_1''(\lambda)$ are spectral functions of $H_1$ and if $a$ and $b$ are non-negative real numbers such that $a + b = 1$, then $aE_1'(\lambda) + bE_1''(\lambda)$ is also a spectral function of $H_1$. A spectral function $E_1(\lambda)$ of $H_1$ is said to be extremal if it is impossible to find two different spectral functions $E_1'(\lambda)$, $E_1''(\lambda)$ and positive real numbers $a$ and $b$, $a + b = 1$, such that $E_1(\lambda) = aE_1'(\lambda) + bE_1''(\lambda)$.

For further information we refer the reader to Achieser and Glasmann [1].

M. A. Naimark [6] has shown that the finite-dimensional extensions of a symmetric operator define extremal spectral functions of the operator. Finite-dimensional extensions exist, however, only for symmetric operators with equal deficiency indices. In §4 of this paper it is shown that self-adjoint extensions defined by the addition of maximal symmetric operators determine extremal spectral functions for a symmetric operator with unequal deficiency indices. The proof uses the proposition of M. A. Naimark [6] that if $E_1(\lambda)$ is defined by the minimal self-adjoint extension $H$, then $E_1(\lambda)$ is extremal if and only if every bounded self-adjoint operator $A$ which commutes with $H$ and satisfies the condition $(Af, g) = (f, g)$ for all $f, g \in \mathfrak{H}_1$ is reduced by $\mathfrak{H}_1$. Section 2 is devoted to a description of the self-adjoint extensions of a symmetric operator, and section 3 identifies some extremal spectral functions of a symmetric operator with infinite equal deficiency indices other than the ones defined by finite-dimensional extensions.

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The proof is based on the proposition of M. A. Naimark mentioned above.

2. Self-adjoint extensions of a symmetric operator. The linear operator $H$ in the Hilbert space $\mathcal{H}$ is said to be Hermitian if $(Hf, g) = (f, Hg)$ for all $f, g \in \mathcal{D}(H)$. $H$ is symmetric if it is Hermitian and $\mathcal{D}(H) = \mathcal{H}$. If $H$ is a closed Hermitian operator and $\lambda$ is a nonreal number, we define the subspaces $\mathcal{M}(\lambda)$ and $\mathcal{S}(\lambda)$ by the equations $\mathcal{S}(\lambda) = \mathcal{H}(H - \lambda E)$ and $\mathcal{M}(\lambda) = \mathcal{H} \ominus \mathcal{S}(\lambda)$. ($E$ stands for the identity operator.) $\mathcal{M}(\lambda)$ is called a deficiency subspace of $H$ and has the same dimensions for all $\lambda$ in the same half-plane (upper or lower.) If $m = \dim \mathcal{M}(\lambda)$, $n = \dim \mathcal{S}(\lambda)$, then $(m, n)$ are called the deficiency indices of $H$ (with respect to $\lambda$). (We add "with respect to $\lambda$" because the ordered pair $(m, n)$ depends on the half-plane $\lambda$ is in.) The operator $U(\lambda) = (H - \lambda E)(H - \lambda E)^{-1}$ is an isometry mapping $\mathcal{S}(\lambda)$ onto $\mathcal{S}(\lambda)$. It is called the Cayley transform of $H$. We have that $H = (\lambda U(\lambda) - \lambda E)(U(\lambda) - E)^{-1}$. Since $\lambda$ is a fixed non-real number in the following, we shall write $U$ in place of $U(\lambda)$. For fixed $\lambda$ the correspondence between a Hermitian operator and its Cayley transform is a one-to-one inclusion-preserving correspondence between the set of closed Hermitian operators $H$ and the set of closed isometric operators $U$ for which $(U - E)^{-1}$ exists. We note, finally, that a subspace $\mathcal{S}_1$ reduces $H$ if and only if $\mathcal{S}_1$ reduces $U$. In this circumstance, if $\mathcal{S}_2 = \mathcal{H} \ominus \mathcal{S}_1$, and if $H_i$ and $U_i$ are $H$ and $U$ respectively restricted to $\mathcal{S}_i$, then $U_i$ is the Cayley transform of $H_i$ and $H = H_1 \oplus H_2$, $U = U_1 \oplus U_2$.

M. A. Naimark [5] has proved the following theorem which describes all self-adjoint extensions of a symmetric operator.

**Theorem 1.** Let $\lambda$ be any fixed nonreal number. Let $H_1$ be a closed symmetric operator with deficiency indices $(m_1, n_1)$ (with respect to $\lambda$). Then every self-adjoint extension $H$ of $H_1$ is obtained as follows:

1. Let $H_2$ be a closed Hermitian operator in $\mathcal{S}_2$ with deficiency indices $(m_2, n_2)$ (with respect to $\lambda$) satisfying $m_1 + m_2 = n_1 + n_2,$ $m_2 \leq n_2$.

2. Let $H_0 = H_1 \oplus H_2$ in $\mathcal{S} = \mathcal{S}_1 \oplus \mathcal{S}_2$. ($H_0$ is therefore a closed Hermitian operator with equal deficiency indices $(m_1 + m_2, n_1 + n_2)$, and if $U_i$ is the Cayley transform of $H_i$, $i = 0, 1, 2$, then $U_0 = U_1 \oplus U_2$. Further, $\mathcal{M}_0(\lambda) = \mathcal{M}_1(\lambda) \oplus \mathcal{M}_2(\lambda)$, $\mathcal{M}_0(\lambda) = \mathcal{M}_1(\lambda) \oplus \mathcal{M}_2(\lambda)$).

3. Let $V$ be an arbitrary isometric operator mapping $\mathcal{M}_0(\lambda)$ onto $\mathcal{M}_0(\lambda)$ satisfying the condition $\varphi \in \mathcal{M}_0(\lambda)$, $V\varphi \in \mathcal{M}_0(\lambda)$ implies $\varphi = 0$.

4. Let $\mathcal{D}(H)$ be defined as all $g = f + V\varphi - \varphi$, where $f \in \mathcal{D}(H_0)$, $\varphi \in \mathcal{M}_0(\lambda)$. 

If \( g \in \mathcal{D}(H) \), let \( H_g = H_f + \lambda V \phi - X \phi \).

Then, \( H \) is self-adjoint extension in \( \mathcal{D} \) of \( H_f \), and every self-adjoint extension of \( H_f \) is obtained in this way. We have that \( \mathcal{D}(H) = \mathcal{D}(H) \cap \mathcal{D}_{2} \).

We say that \( H \) and \( V \) of Theorem 1 define the self-adjoint extension \( H \) of \( H_f \).

We can put the operator \( V \) into correspondence with a matrix \( (V_{ik}) \) of operators such that \( F_{12} : \mathcal{M}_{2}(\lambda) \rightarrow \mathcal{M}_{2}(\lambda) \), \( F_{21} : \mathcal{M}_{1}(\lambda) \rightarrow \mathcal{M}_{1}(\lambda) \), \( F_{22} : \mathcal{M}_{2}(\lambda) \rightarrow \mathcal{M}_{2}(\lambda) \). Then condition on \( F \) in (3) of theorem 1 then becomes \( V_{12} = 0 \) implies \( \phi = 0 \).

We now give a theorem which gives a more detailed analysis of the structure of \( V \).

**Theorem 2.** Suppose that \( \mathcal{M}_{1}(\lambda), \mathcal{M}_{1}(\lambda), \mathcal{M}_{2}(\lambda), \mathcal{M}_{2}(\lambda) \) are Hilbert spaces and that \( V \) is an isometry which maps \( \mathcal{M}_{1}(\lambda) \oplus \mathcal{M}_{2}(\lambda) \) onto \( \mathcal{M}_{2}(\lambda) \oplus \mathcal{M}_{2}(\lambda) \). (\( \lambda \) here has nothing to do with the theorem and is retained only as a notational convenience.) If \( V = (V_{ik}) \) in matrix form, suppose that \( V_{12} = 0 \) implies that \( \phi = 0 \). Then the following conclusions are true:

1. If \( \mathcal{M}_{2}(\lambda) \) is defined by the equation \( \mathcal{M}_{2}(\lambda) = \text{closure of \( \{ V_{12} \mathcal{M}_{2}(\lambda) \} \}) \) (\( c \) indicates closure of a set) and if \( \mathcal{N}_{1}(\lambda) \) is defined by \( \mathcal{N}_{1}(\lambda) = \mathcal{M}_{1}(\lambda) \oplus \mathcal{M}_{1}(\lambda) \), then \( \mathcal{N}_{1}(\lambda) \) is the null space of \( V_{12}^{*} \). Thus, \( V_{12}^{*} \) is one-to-one on \( \mathcal{M}_{1}(\lambda) \). Further, \( \mathcal{M}_{2}(\lambda) = \text{closure of \( \{ V_{12}^{*} \mathcal{M}_{2}(\lambda) \} \}) \).
2. \( V^{*} = V^{-1} \) maps \( \mathcal{N}_{1}(\lambda) \) onto a subspaces of \( \mathcal{M}_{1}(\lambda) \), which we denote by \( \mathcal{N}_{1}(\lambda) \). Thus, \( \mathcal{N}_{1}(\lambda) = V^{*} \mathcal{N}_{1}(\lambda) \). \( \mathcal{N}_{1}(\lambda) = V^{*} \mathcal{N}_{1}(\lambda) \).
3. If \( \mathcal{M}_{2}(\lambda) \) is defined by the equation \( \mathcal{M}_{2}(\lambda) = \mathcal{M}_{2}(\lambda) \), then \( V \) maps \( \mathcal{M}_{2}(\lambda) \oplus \mathcal{M}_{2}(\lambda) \) isometrically onto \( \mathcal{M}_{2}(\lambda) \oplus \mathcal{M}_{2}(\lambda) \).
4. \( V_{21} \) is one-to-one on \( \mathcal{M}_{1}(\lambda) \), and \( \mathcal{N}_{1}(\lambda) \) is the null space of \( V_{21} \). \( \mathcal{M}_{2}(\lambda) = \text{closure of \( \{ V_{21} \mathcal{M}_{2}(\lambda) \} \}) \).
5. \( V_{21}^{*} \) is one-to-one on \( \mathcal{M}_{2}(\lambda) \) and \( \mathcal{M}_{2}(\lambda) = \text{closure of \( \{ V_{21}^{*} \mathcal{M}_{2}(\lambda) \} \}) \).
6. If \( m_{1} = \dim \mathcal{M}_{1}(\lambda), n_{1} = \dim \mathcal{M}_{1}(\lambda), m_{2} = \dim \mathcal{M}_{2}(\lambda), n_{2} = \dim \mathcal{M}_{2}(\lambda) \), then \( m_{1} + m_{2} = n_{1} + n_{2}, m_{2} = \dim \mathcal{M}_{2}(\lambda) = \dim \mathcal{M}_{1}(\lambda) \leq n_{1}, n_{2} = \dim \mathcal{M}_{2}(\lambda) = \dim \mathcal{M}_{2}(\lambda) \leq m_{1} \).
7. If \( m_{2} = n_{2}, m_{1} = n_{1} \).

**Proof.** (1) Since \( \mathcal{N}_{1}(\lambda) \) is the orthogonal complement of the closure of the range of \( V_{12} \), \( \mathcal{N}_{1}(\lambda) \) is the null space of \( V_{12}^{*} \), and \( V_{12}^{*} \) is one-to-one on \( \mathcal{M}_{1}(\lambda) \).

Suppose \( g \in \mathcal{M}_{1}(\lambda) \) and \( g \) is perpendicular to \( V_{12}^{*} \mathcal{M}_{1}(\lambda) \). Then \( 0 = (g, V_{12}^{*}f) = (V_{12}g, f) \) for all \( f \in \mathcal{M}_{1}(\lambda) \). Therefore, \( V_{12}g = 0 \), and, since \( V_{12} \) is one-to-one, \( g = 0 \). Thus, \( \mathcal{M}_{2}(\lambda) = \text{closure of \( \{ V_{21}^{*} \mathcal{M}_{2}(\lambda) \} \}) \).
(2) Since
\[ V^* = \begin{pmatrix} V_{11}^* & V_{12}^* \\ V_{21}^* & V_{22}^* \end{pmatrix}, \]
\[ V^* \mathcal{H}_1(\lambda) = V_{11}^* \mathcal{H}_1(\lambda) \subset \mathcal{M}_1(\lambda). \] Thus, \( V^* = V^{-1} \) maps \( \mathcal{H}_1(\lambda) \) onto a subspace of \( \mathcal{M}_1(\lambda) \).

(3) Clear, since \( \mathcal{H}_1(\lambda) = V \mathcal{H}_1(\lambda) \).

(4) We first show that \( f \in \mathcal{H}_1(\lambda) \), \( V_{21}f = 0 \). Then, \( Vf = V_{11}f + V_{21}f = V_{11}f \in \mathcal{M}_1(\lambda) \). Let \( g = V_{11}f = Vf \), so that \( f = V^*g = V_{11}^*g + V_{21}^*g \). Since \( f \in \mathcal{M}_1(\lambda) \), \( V_{11}^*g \in \mathcal{M}_1(\lambda) \), \( V_{21}^*g \in \mathcal{M}_2(\lambda) \), we have that \( V_{11}^*g = 0 \). By (1) and the fact that \( g \in \mathcal{M}_1(\lambda) \), \( g = 0 \). Thus, \( f = V^*g = 0 \), and our contention is proved.

Since \( \mathcal{H}_1(\lambda) = V \mathcal{H}_1(\lambda) \), \( V_{21}f = 0 \) for all \( f \in \mathcal{H}_1(\lambda) \). On the other hand, we have just shown that \( V_{21} \) is one-to-one on \( \mathcal{M}_1(\lambda) \). It follows that \( \mathcal{H}_1(\lambda) \) is the null space of \( V_{21} \).

Because \( (V_{21}^*)^* = V_{21} \) and the null space of \( (V_{21}^*)^* \) is the orthogonal complement of the closure of the range of \( V_{21}^* \), we see that \( \mathcal{M}_1(\lambda) = [V_{21} \mathcal{M}_2(\lambda)]^\perp \).

We claim finally that \( \mathcal{M}_2(\lambda) = [V_{21} \mathcal{M}_2(\lambda)]^\perp \). Suppose \( g \in \mathcal{M}_2(\lambda) \) and that \( g \) is perpendicular to \( V_{21} \mathcal{M}_1(\lambda) \). Therefore, \( 0 = (V_{21}f, g) = (f, V_{21}^*g) \) for all \( f \in \mathcal{M}_1(\lambda) \). Since \( V_{21}^*g \in \mathcal{M}_1(\lambda) \), it follows that \( V_{21}^*g = 0 \). Thus, \( V^*g = V_{21}^*g \in \mathcal{M}_2(\lambda) \). Let \( f = V^*g \). Then, \( g = Vf = V_{12}f + V_{22}f \), where \( g \in \mathcal{M}_2(\lambda) \), \( V_{12}f \in \mathcal{M}_1(\lambda) \), \( V_{22}f \in \mathcal{M}_2(\lambda) \). Hence, \( V_{12}f = 0 \) and \( f = 0 \). Whence, \( g = Vf = 0 \). This proves our claim and completes the proof of (4).

(5) We have already shown in (4) that \( \mathcal{M}_1(\lambda) = [V_{21} \mathcal{M}_2(\lambda)] \). Since we also showed in (4) that \( \mathcal{M}_2(\lambda) = [V_{21} \mathcal{M}_1(\lambda)] \), it follows that the null space of \( V_{21}^* \) is empty and therefore \( V_{21}^* \) is one-to-one on \( \mathcal{M}_2(\lambda) \).

(6) \( m_1 + m_2 = n_1 + n_2 \) follows from the fact that \( V \) maps \( \mathcal{M}_1(\lambda) \oplus \mathcal{M}_2(\lambda) \) isometrically onto \( \mathcal{M}_1(\lambda) \oplus \mathcal{M}_2(\lambda) \).

We claim now that \( \dim \mathcal{M}_2(\lambda) = \dim \mathcal{M}_1(\lambda) \). Let \( \{\phi_a\} \) be a complete orthonormal system in \( \mathcal{M}_1(\lambda) \). Then \( \{V_{12}\phi_a\} \) is a fundamental set in \( \mathcal{M}_2(\lambda) \). (See Nagy [4] for definitions.) Therefore \( \dim \mathcal{M}_2(\lambda) = P\{\phi_a\} = P\{V_{12}\phi_a\} \geq \dim \mathcal{M}_1(\lambda) \), where \( P \) stands for cardinality. Using \( V_{22} \) and an analogous argument, we obtain that \( \dim \mathcal{M}_1(\lambda) \leq \dim \mathcal{M}_2(\lambda) \). Thus, \( \dim \mathcal{M}_2(\lambda) = \dim \mathcal{M}_1(\lambda) \), and \( m_2 = \dim \mathcal{M}_2(\lambda) = \dim \mathcal{M}_1(\lambda) \leq n_1 \). Similarly, \( n_2 = \dim \mathcal{M}_2(\lambda) = \dim \mathcal{M}_1(\lambda) \leq m_1 \).

(7) The proof is clear from the inequalities in (6).

Theorem 2 is therefore completely proved.

Theorem 3. (M. A. Naimark [5]). For each self-adjoint extension \( H \) in \( \mathbb{S} \) of a symmetric operator \( H_1 \) in \( \mathbb{S}_1 \) there exists a minimal self-adjoint extension \( H_0 \) in \( \mathbb{S}_0 \) such that

(1) \( \mathbb{S}_1 \subset \mathbb{S}_0 \subset \mathbb{S} \);
(2) \( H_1 \subset H_0 \subset H \);
(3) \( H_0 \) and \( H \) define the same spectral function of \( H_1 \).

**Theorem 4.** Suppose that \( H_1 \) is a closed symmetric operator and that \( H_2 \) and \( V \) define a self-adjoint extension \( H \) of \( H_1 \). Let \( H_0 \) be a self-adjoint extension of \( H_1 \) having the properties that \( \mathcal{D}_1 \subset \mathcal{D}_0 \subset \mathcal{D} \) and \( H_1 \subset H_0 \subset H \). Then the following statements are true:

1. If we write \( \mathcal{D}_0 = \mathcal{D}_1 \oplus \mathcal{D}_2 \), \( \mathcal{D} = \mathcal{D}_0 \oplus \mathcal{D}_4 = \mathcal{D}_1 \oplus \mathcal{D}_3 \oplus \mathcal{D}_4 \), \( \mathcal{D}_2 = \mathcal{D}_3 \oplus \mathcal{D}_4 \), then \( H \) is reduced by \( \mathcal{D}_4 \) and \( H = H_0 \oplus H_1 \), where \( H_4 \) is a self-adjoint operator in \( \mathcal{D}_4 \).
2. \( \mathcal{D}_4 \subset L_2(\lambda) \cap L_2(\lambda) \), \( \mathcal{M}_2(\lambda) \subset \mathcal{D}_3 \), \( \mathcal{M}_4(\lambda) \subset \mathcal{D}_4 \).
3. \( H_2 \) is reduced by \( \mathcal{D}_4 \) and \( H_2 = H_3 \oplus H_4 \), where \( H_3 \) is a closed Hermitian operator in \( \mathcal{D}_3 \) with the same deficiency subspaces \( M_2(\lambda) \), \( M_4(\lambda) \) as \( H_2 \).
4. \( H_0 \) is defined by \( H_3 \) and \( V \).
5. \( H \) and \( H_0 \) define the same spectral function of \( H_1 \).

**Proof.** (1) Since \( H_1 \subset H_0 \subset H \), we have that \( U_1 \subset U_0 \subset U \). Because \( U_0 \) maps \( \mathcal{D}_0 \) isometrically onto \( \mathcal{D}_0 \) and \( U \) maps \( \mathcal{D}_0 \) isometrically onto \( \mathcal{D} \), we have that \( U \) maps \( \mathcal{D}_4 \) isometrically onto \( \mathcal{D}_4 \). Thus, \( \mathcal{D}_4 \) reduces \( U \), and hence \( U = U_0 \oplus U_1 \), \( H = H_0 \oplus H_1 \), where \( H_1 \) is a self-adjoint operator in \( \mathcal{D}_4 \) with Cayley transform \( U_1 \). This proves (1).

(2) We claim first that \( \mathcal{D}_4 \subset L_2(\lambda) \). Let \( f \in \mathcal{D}_4 \). Since \( H_4 \subset \mathcal{D}_4 = M_2(\lambda) \oplus L_2(\lambda) \), \( f = f' + f'' \), where \( f' \in M_2(\lambda) \), \( f'' \in L_2(\lambda) \). Hence, \( Uf = UF' + UF'' = VF' + U_2f'' = V_2f' + U_2f'' \), where \( Uf \in \mathcal{D}_4 \subset \mathcal{D}_2 \), \( V_2f' \in M_2(\lambda) \subset \mathcal{D}_1 \), \( V_2f'' \in M_2(\lambda) \subset \mathcal{D}_3 \), \( U_2f'' \in L_2(\lambda) \subset \mathcal{D}_4 \). Thus, \( V_2f'' = 0 \), and therefore \( f' = 0 \). It follows that \( f = f'' \in L_2(\lambda) \) and that \( \mathcal{D}_4 \subset L_2(\lambda) \).

Since \( \mathcal{D}_4 \subset L_2(\lambda) \), and since \( U \) maps \( \mathcal{D}_4 \) isometrically onto \( \mathcal{D}_4 \) and \( L_2(\lambda) \) isometrically onto \( L_2(\lambda) \), we conclude that \( \mathcal{D}_4 \subset L_2(\lambda) \). Hence, \( \mathcal{D}_4 \subset L_2(\lambda) \cap L_2(\lambda) \). It follows immediately that \( M_4(\lambda) \subset \mathcal{D}_3 \), \( M_4(\lambda) \subset \mathcal{D}_4 \). (2) is therefore completely proved.

(3) Because \( U_2 = U \) on \( L_2(\lambda) \), we see that \( U_2 \) maps \( \mathcal{D}_4 \) isometrically onto \( \mathcal{D}_4 \). We know, however, that \( U_2 \) maps \( L_2(\lambda) \) isometrically onto \( L_2(\lambda) \). It follows that \( \mathcal{D}_4 \) reduces \( U_2 \). Thus, \( U_2 = U_3 \oplus U_4 \), where \( U_3 \) maps \( L_2(\lambda) \ominus \mathcal{D}_4 \) isometrically onto \( L_2(\lambda) \ominus \mathcal{D}_4 \), and \( H_3 = H_2 \oplus H_4 \), where \( H_3 \) is a closed Hermitian operator in \( \mathcal{D}_3 \) with Cayley transform \( U_3 \). Noting that \( \mathcal{D}_3 = M_2(\lambda) \oplus [L_2(\lambda) \ominus \mathcal{D}_3] = M_4(\lambda) \oplus [L_2(\lambda) \ominus \mathcal{D}_4] \), we see that \( H_3 \) has deficiency subspaces \( M_2(\lambda), M_4(\lambda) \). This proves (3).

(4) By Theorem 1, \( H_3 \) and \( V \) define a self-adjoint extension \( H'_3 \) of \( H_1 \) in \( \mathcal{D}_3 = \mathcal{D}_1 \oplus \mathcal{D}_3 \). If \( U'_3 \) is the Cayley transform of \( H'_3 \), then \( U'_3 = U_3 = U \) on \( L_2(\lambda) \), \( U'_3 = V = U \) on \( M_2(\lambda) \oplus L_2(\lambda) \), \( U'_3 = U_3 = U \) on \( L_2(\lambda) \ominus \mathcal{D}_4 \). It follows that \( U'_3 = U \) on \( \mathcal{D}_1 \oplus \mathcal{D}_3 = \mathcal{D}_0 \). But since \( U_0 \subset U \), \( U_0 = U \) on \( \mathcal{D}_0 \), hence, \( U_0 = U'_3 \), and therefore \( H_0 = H'_3 \). This
proves (4).

(5) As we have shown, \( H = H_0 \oplus H_4 \). Thus, \( E(\lambda) = E_0(\lambda) \oplus E_4(\lambda) \), and therefore \( E(\lambda)f = E_0(\lambda)f \) for all \( f \in \mathcal{S}_1 \). If \( P \) is the operator of orthogonal projection of \( \mathcal{S} \) onto \( \mathcal{S}_1 \) and if \( P_0 \) is the operator of orthogonal projection of \( \mathcal{S}_0 \) onto \( \mathcal{S}_1 \), \( PE(\lambda)f = PE_0(\lambda)f = P_0E_0(\lambda)f \) for all \( f \in \mathcal{S}_1 \), so that \( H \) and \( H_0 \) define the same spectral function of \( H_1 \). This proves (5), and the proof of theorem 4 is completed.

3. Extremal spectral functions of a symmetric operator with equal deficiency indices.

THEOREM 5. Let \( H \) be a self-adjoint extension of the closed symmetric operator \( H_1 \). Suppose that \( H \) is defined by \( H_2 \) and \( V \). Then the following statements are equivalent:

1. \( \mathcal{D}(H_2) = \{0\} \).
2. \( \mathcal{M}_4(\lambda) = \mathcal{M}_5(\lambda) = \mathcal{S}_2 \).
3. \( \mathcal{D}(H) \cap \mathcal{S}_2 = \{0\} \).

Proof. That (1) implies (2) is clear from the definition of \( \mathcal{M}_4(\lambda) \) and \( \mathcal{M}_5(\lambda) \). Suppose, on the other hand, that \( \mathcal{M}_4(\lambda) = \mathcal{M}_5(\lambda) = \mathcal{S}_2 \). Then, \( \mathcal{M}(H_2 - \lambda E) = \mathcal{M}(H_3 - \lambda E) = \{0\} \). If \( f \in \mathcal{D}(H_2) \), \( H_2f - \lambda f = 0 \) and \( H_3f - \lambda f = 0 \). Subtracting the first equation from the second, \( (\lambda - \lambda)f = 0 \), and therefore \( f = 0 \). Thus, \( \mathcal{D}(H_2) = \{0\} \), and we have proved that (2) implies (1).

By Theorem 1, \( \mathcal{D}(H_2) = \mathcal{D}(H) \cap \mathcal{S}_2 \), so that (1) and (3) are clearly equivalent.

THEOREM 6. Let \( H_1 \) be a closed symmetric operator. Suppose that \( H \) is a self-adjoint extension of \( H_1 \) defined by \( H_2 \) and \( V \). If \( \mathcal{D}(H_2) = \{0\} \), the following statements are true:

1. \( m_1 = n_1 \), i.e., the deficiency indices of \( H_1 \) are equal.
2. \( H \) is minimal.
3. The spectral function \( E_1(\lambda) \) of \( H_1 \) defined by \( H \) is extremal.

Proof. (1) By Theorem 5, \( \mathcal{D}(H_2) = \{0\} \) implies that \( m_2 = n_2 \). By theorem 2, (7), \( m_1 = n_1 \).

(2) By Theorem 5, \( \mathcal{D}(H_2) = \{0\} \) implies that \( \mathcal{M}_4(\lambda) = \mathcal{M}_5(\lambda) = \mathcal{S}_2 \). Hence, \( \mathcal{S}_2(\lambda) = \mathcal{S}_2(\lambda) = \{0\} \). It follows from Theorem 3 and Theorem 4, (2), that \( H \) is minimal.

(3) Let \( A \) be any bounded operator in \( \mathcal{S} \) having a matrix representation,

\[ A \sim \begin{pmatrix} E & B \\ B^* & C \end{pmatrix}, \]
where $E$ is the identity in $\mathcal{B}$, $B$ maps $\mathcal{D}_2$ into $\mathcal{E}_2$, $C$ maps $\mathcal{D}_2$ into $\mathcal{E}_3$, and $C$ is self-adjoint. Suppose that $A$ commutes with $H$. We shall show that this implies that $B \equiv 0$. By the proposition of M. A. Naimark [6] mentioned in the introduction, then, it follows that the spectral function $E_2(\lambda)$ defined by $H$ is extremal.

Since $A$ commutes with $H$, it commutes with the Cayley transform $U$ of $H$. If we represent $U$ as a matrix, $U \sim (U_{jk})$, where $U_{jk}$ maps $\mathcal{D}_k$ into $\mathcal{D}_j$, then the fact that $A$ commutes with $U$ implies that $BU_{21} = U_{12}B^*$. Taking adjoints, we also have that $U_{21}B^* = BU_{12}^*$. We observe, further, that $U = V$ on $\mathcal{M}_i(\lambda) \oplus \mathcal{M}_4(\lambda)$ and that $U^* = U^{-1} = V^* = V^{-1}$ on $\mathcal{M}_i(\lambda) \oplus \mathcal{M}_4(\lambda)$.

Using the equation $BU_{12}^* = U_{21}^*B^*$, the fact that $\mathcal{M}_4(\lambda) = 0$, and Theorem 2, we obtain that $BV_{12}^*\mathcal{M}_i(\lambda) = BU_{12}^*\mathcal{M}_i(\lambda) \subset U_{21}^*\mathcal{D}_2 = U_{21}^*\mathcal{M}_4(\lambda) = V_{21}^*\mathcal{M}_4(\lambda) \subset \mathcal{M}_4(\lambda)$. Since by Theorem 2 $V_{12}^*\mathcal{M}_i(\lambda)$ is dense in $\mathcal{M}_4(\lambda) = 0$, and since $B$ is bounded, it follows that $B\mathcal{D}_2 \subset \mathcal{M}_4(\lambda)$.

Similarly, using the equation $BU_{21} = U_{12}B^*$, we obtain that $BV_{21}\mathcal{M}_i(\lambda) = BU_{21}\mathcal{M}_i(\lambda) \subset U_{12}\mathcal{D}_2 = U_{12}\mathcal{M}_4(\lambda) = V_{12}\mathcal{M}_4(\lambda) \subset \mathcal{M}_4(\lambda)$, and therefore $B\mathcal{D}_2 \subset \mathcal{M}_4(\lambda)$.

Thus, $B\mathcal{D}_2 \subset \mathcal{M}_i(\lambda) \cap \mathcal{M}_4(\lambda)$. But $\mathcal{M}_i(\lambda) \cap \mathcal{M}_4(\lambda) = \{0\}$, because $\mathcal{M}_i(\lambda)$ and $\mathcal{M}_4(\lambda)$ are the deficiency subspaces of a symmetric operator. Hence, $B \equiv 0$. This completes the proof of Theorem 6.

By use of a somewhat less general form of Theorem 6, M. A. Naimark [6] has shown that every finite-dimensional extension $H$ of a closed symmetric operator $H_1$ defines an extremal spectral function of $H_1$.

**Theorem 7.** If $H$ is a finite-dimensional extension of a closed symmetric operator $H_1$, then $H_1$ must have equal deficiency indices.

**Proof.** Suppose that $H$ is defined by $H_2$ and $V$. Then $H_1$ is a Hermitian operator in the finite-dimensional space $\mathcal{S}_2$. Since $U_2$ maps $\mathcal{S}_4(\lambda)$ isometrically onto $\mathcal{S}_4(\lambda)$, it follows that $\dim \mathcal{S}_4(\lambda) = \dim \mathcal{S}_4(\lambda)$. Hence $\dim \mathcal{M}_4(\lambda) = \dim \mathcal{M}_4(\lambda)$, i.e., $m_2 = n_2$. By Theorem 2, (7), $m_1 = n_1$. This proves Theorem 7.

4. **Extremal spectral functions of a symmetric operator with unequal deficiency indices.** We first introduce the notion of a partial isometry and some of the properties thereof. (See Murray and von Neumann [3].) A bounded linear operator $W$ in a Hilbert space $\mathcal{H}$ is called a **partial isometry** if it maps a subspace $\mathcal{E}$ isometrically onto another subspace $\mathcal{F}$, while it maps $\mathcal{H} \ominus \mathcal{E}$ onto $\{0\}$. $\mathcal{E}$ is called the **initial set** of $W$, and $\mathcal{F}$ is called the **final set** of $W$. If $W$ is a partial isometry, then the following statements hold:

1. If $P(\mathcal{E})$ is the operator of orthogonal projection on $\mathcal{E}$ and if $P(\mathcal{F})$ is the operator of orthogonal projection on $\mathcal{F}$, then $P(\mathcal{E}) = W^*W$, 

THEOREM 8. Suppose that $W$ is a partial isometry with initial set $\mathcal{H}$ and final set $\mathcal{G}$. Let $\mathcal{H} = \mathcal{H} \oplus \mathcal{W}$. Then, $\mathcal{W} = \mathcal{W}' \oplus \mathcal{W}''$, where

1. $W$ maps $\mathcal{W}'$ isometrically onto $\mathcal{W}''$;
2. If $f \in \mathcal{H} \oplus \mathcal{W}'$, $\lim_{p \to \infty} W^p f = 0$.

Proof. Let $\mathcal{W}_i = (W^*)^i \mathcal{H}$, $i = 0, 1, 2, \ldots$. Then each $\mathcal{W}_i$ is a subspace (i.e., a closed linear manifold), and the following statements are true:

(a) $\mathcal{W}_i \subset \mathcal{W}$ for $i = 1, 2, \ldots$. This is clear because $W^*$ is a partial isometry with initial set $\mathcal{H}$ and final set $\mathcal{G}$.
(b) If $f \in \mathcal{W}_n$, where $n \geq 0$, then $W^p f \in \mathcal{W}_{n-p}$ for $1 \leq p \leq n$, and $W^p f = 0$ for $p > n$. Proof: If $f \in \mathcal{W}_n$, then $f = (W^*)^n g$ for some $g \in \mathcal{H}$. Since $W^p W^* = E$, $W^p f = (W^*)^n g \in \mathcal{W}_{n-p}$, $1 \leq p \leq n$. If $p > n$, $W^p f = W^{p-n} g = 0$.
(c) If $f \in \mathcal{W}_i$, $i = 0, 1, 2, \ldots$, and if $n$ is a positive integer, then $(W^*)^n f \in \mathcal{W}_{i+n}$. Proof: If $f \in \mathcal{W}_i$, $f = (W^*)^i g$, where $g \in \mathcal{H}$. Therefore, $(W^*)^n f = (W^*)^i g \in \mathcal{W}_{i+n}$.
(d) $\mathcal{W}_i$ is perpendicular to $\mathcal{W}_j$ if $i \neq j$. Proof: Suppose $i < j$, and let $f \in \mathcal{W}_i$, $g \in \mathcal{W}_j$. Then there exists $f_1 \in \mathcal{H}$ and $g_1 \in \mathcal{H}$ such that $f = (W^*)^i f_1$, $g = (W^*)^j g_1$. Hence, $(f, g) = ((W^*)^j f_1, (W^*)^i g_1) = (f_1, (W^*)^j-i g_1) = 0$, since $f_1 \in \mathcal{H}$, $(W^*)^{j-i} g_1 \in \mathcal{W}_{j-i} \subset \mathcal{W}$.

Now let $\mathcal{W}' = \sum_{i=1}^\infty \mathcal{W}_i$. Then $\mathcal{W}'$ is a subspace of $\mathcal{W}$. Let $\mathcal{W}'' = \mathcal{W} \ominus \mathcal{W}'$. We shall show that $\mathcal{W}'$ and $\mathcal{W}''$ satisfy (1) and (2).

Since $\mathcal{W} = \mathcal{W}' \oplus \mathcal{W}''$ and $\mathcal{H} = \mathcal{H} \oplus \mathcal{W}' \oplus \mathcal{W}''$, and since $W$ maps $\mathcal{W}$ isometrically onto $\mathcal{H}$, in order to prove (1) it is sufficient to show that $W$ maps $\mathcal{W}'$ onto $\mathcal{H} \oplus \mathcal{W}'$. Suppose $f \in \mathcal{W}'$. Then, $f = \sum_{i=1}^\infty f_i$, where $f_i \in \mathcal{W}_i$, and $Wf = \sum_{i=1}^\infty Wf_i$. By (b) $Wf_i \in \mathcal{W}_{i-1}$, we see that $Wf \in \mathcal{H} \oplus \mathcal{W}'$. Thus, $W$ maps $\mathcal{W}'$ into $\mathcal{H} \oplus \mathcal{W}'$. To show that the map is onto, let $g \in \mathcal{H} \oplus \mathcal{W}'$. Then, $g = \sum_{i=0}^\infty f_i$, where $f_i \in \mathcal{W}_i$. If $f = W*f = \sum_{i=0}^\infty W^i f_i \in \mathcal{W}'$, by (c). Further, $Wf = WW^* g = g$. Hence, $W$ maps $\mathcal{W}'$ onto $\mathcal{H} \oplus \mathcal{W}'$.

We now prove (2). Let $f \in \mathcal{H} \oplus \mathcal{W}'$. Then, $f = \sum_{i=0}^\infty f_i$, where $f_i \in \mathcal{W}_i$. By (b), $Wf = \sum_{i=0}^\infty W^p f_i = \sum_{i=p}^\infty W^p f_i$. Hence, $||W^p f||^2 = \sum_{i=p}^\infty ||W^p f_i||^2 = \sum_{i=p}^\infty ||f_i||^2$. Thus, $\lim_{p \to \infty} ||W^p f||^2 = 0$. This proves (2) and completes the proof of the theorem.

THEOREM 9. Let $\lambda$ be a fixed nonreal number. Suppose that $H_1$ is a closed symmetric operator in $\mathcal{H}$ with deficiency indices $(m, n)$
(with respect to \( \lambda \)), and suppose that \( m \neq n \). Let \( H \) be a self-adjoint extension of \( H_1 \) defined by \( H_\lambda \) and \( V \), where \( H_\lambda \) is a closed Hermitian operator with deficiency indices \( (0, s) \), \( n + s = m \), if \( m > n \) and \( (s, 0) \), \( m + s = n \), if \( m < n \). Then the spectral function defined by \( H \) is extremal.

**Proof.** Assume that \( m > n \). The case \( m < n \) then follows by interchanging the roles of \( \lambda \) and \( \lambda \) in Theorem 1 and defining \( H \) by \( H_2 \) and \( V^* \).

By Theorem 3 there exists a minimal self-adjoint extension \( H_0 \) of \( H_1 \) such that \( \mathcal{S}_1 \subset \mathcal{S}_0 \subset \mathcal{S}, \ H_1 \subset H_0 \subset H, \) and \( H_0 \) and \( H \) define the same spectral function of \( H_1 \). By Theorem 4, \( H_0 \) is defined by \( V \) and a Hermitian operator \( H_3 \) with the same deficiency subspaces as \( H_2 \).

Since we can always consider \( H_0 \) instead of \( H, \) it follows that without loss of generality we can consider \( H \) to be a minimal self-adjoint extension.

Since \( 2J_2(\lambda) = \{0\} \) and \( S_2(\lambda) = S_2 \), we have that if \( f \in S_2 \), \( Uf \in S_2(\lambda) \subset S_2 \). If we represent \( U \) as a matrix, \( U \sim (U_{jk}) \), where \( U_{jk} \) maps \( S_2 \) into \( S_2 \), then it follows that \( U_{12} = 0 \) on \( S_2 \). Further, \( Uf = U_{22}f \) for all \( f \in S_2 \), so that \( U_{22} \) maps \( S_2 \) isometrically onto \( S_2(\lambda) \). \( U_{22} \) is thus a partial isometry in \( S_2 \) with initial set \( S_2 \) and final set \( S_2(\lambda) \), while \( U_{12}^* \) is a partial isometry with initial set \( S_2(\lambda) \) and final set \( S_2 \). We have that \( E = P(S_2) = U_{22}U_{12} \), while \( P(S_2(\lambda)) = U_{12}U_{22}^* \).

Now let \( A \) be any bounded operator in \( S \) with matrix representation

\[
A \sim \begin{pmatrix} E & B \\ B^* & C \end{pmatrix},
\]

where \( E \) is the identity in \( S_1 \), \( B \) maps \( S_2 \) into \( S_1 \), \( C \) maps \( S_2 \) into \( S_2 \), and \( C \) is self-adjoint. Suppose that \( A \) commutes with \( H \). We shall show that this implies \( B = 0 \). Then by the proposition of M. A. Naimark [6] mentioned in the introduction, it follows that the spectral function \( E_1(\lambda) \) defined by \( H \) is extremal.

Since \( A \) commutes with \( H \), it commutes with the Cayley transform \( U \) of \( H \). This implies that \( BU_{21} = U_{12}B^* \) and \( U_{12} + BU_{22} = U_{12}B + U_{12}C \). Since \( U_{12} = 0 \), these equations become \( BU_{21} = 0 \) and \( BU_{22} = U_{12}B \). On \( \mathcal{M}_2(\lambda) \), \( U_{21} = V_{21} \) and therefore \( BV_{21}\mathcal{M}_2(\lambda) = BU_{21}\mathcal{M}_2(\lambda) = \{0\} \). Because by Theorem 2, \( V_{21}\mathcal{M}_2(\lambda) \) is dense in \( \mathcal{M}_2(\lambda) \), \( B\mathcal{M}_2(\lambda) = \{0\} \), i.e., \( BP(\mathcal{M}_2(\lambda)) = 0 \). From the equation \( BU_{22} = U_{12}B \) we have that \( BP(\mathcal{M}_2(\lambda)) = BU_{22}U_{12}^* = U_{12}BU_{22}^* \). Adding \( BP(\mathcal{M}_2(\lambda)) \) to \( BP(\mathcal{M}_2(\lambda)) = 0 \), we obtain that \( B = U_{12}BU_{22}^* \). By iterating this equation we see that \( B = U_{12}^pB(U_{22}^*)^p \) for every positive integer \( p \).

Since \( \| U_{11} \| \leq 1, \| Bf \| \leq \| B \| \| (U_{22}^*)^p f \| \) for each \( f \in S_2 \) and each positive integer \( p \).
By Theorem 8, \( S_2(\lambda) = W \oplus W' \), where \( U_2^* \) maps \( W' \) isometrically onto \( W'' \), and if \( f \in M_2(\lambda) \oplus W' \), then \( \lim_{p \to \infty} \| (U_2^*)^p f \| = 0 \). But if \( U_2^* \) maps \( W'' \) isometrically onto \( W'' \), then \( U_2 \) and therefore \( U \) maps \( W'' \) isometrically onto \( W'' \). This means that \( U \) and therefore \( H \) is reduced by \( W'' \), a subspace of \( \mathcal{S}_2 \). Since \( H \) is a minimal self-adjoint extension of \( H' \), \( W'' = \{0\} \). Hence, \( \mathcal{S}_2 = M_2(\lambda) \oplus W' \), and thus if \( f \in \mathcal{S}_2 \), \( \lim_{p \to \infty} \| (U_2^*)^p f \| = 0 \). Since \( \| Bf \| \leq \| B \| \| (U_2^*)^p f \| \) for each \( f \in \mathcal{S}_2 \) and for every positive integer \( p \), it follows that \( B \equiv 0 \) on \( \mathcal{S}_2 \). This completes the proof of Theorem 9.

Since the operator \( H_2 \) in Theorem 9 is a Hermitian operator with deficiency indices \((0, s)\) or \((s, 0)\), it may seem that we are dealing with a wider class of operators than the maximal symmetric operators. That this is not so is shown by Theorem 10 below.

**Theorem 10.** If \( H \) is a Hermitian operator with deficiency indices \((0, s)\) or \((s, 0)\), then \( H \) is a maximal symmetric operator. If \( H \) is a Hermitian operator with deficiency indices \((0, 0)\), then \( H \) is a self-adjoint operator.

**Proof.** If \( H \) is a Hermitian operator and \( \mathcal{B} = \mathcal{S} \ominus [\mathcal{S}(H)]^c \), then \( \mathcal{B} \cap \mathcal{S}(\overline{\lambda}) = \{0\} \). (If \( h \in \mathcal{B} \cap \mathcal{S}(\overline{\lambda}) \), then \( h = (H - \lambda E)g \). Hence, \( 0 = (h, g) = (Hg, g) - \lambda(g, g) \). Since \( (Hg, g) \) is real while \( \lambda \) is not, \( g = 0 \). This simple argument is due to M. A. Krasnosel’skii [2, Lemma 2].)

If \( H \) has deficiency indices \((0, s)\), \( M(\overline{\lambda}) = \{0\} \) so that \( \mathcal{B} \subset \mathcal{S}(\overline{\lambda}) \). Thus, \( \mathcal{B} = \{0\} \) and \( H \) is symmetric. Similarly, \( H \) is symmetric if its deficiency indices are \((s, 0)\). It follows immediately that if \( H \) has deficiency indices \((0, 0)\), \( H \) is self-adjoint. Theorem 10 is proved.

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