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Extensions of symmetric operators I: The inner characteristic function case

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Abstract: Given a symmetric linear transformation on a Hilbert space, a natural problem to consider is the characterization of its set of symmetric extensions. This problem is equivalent to the study of the partial isometric extensions of a fixed partial isometry. We provide a new function theoretic characterization of the set of all self-adjoint extensions of any symmetric linear transformation B with finite equal indices and inner Livšic characteristic function Θ_B by constructing a bijection between the quotient of this set by a certain natural equivalence relation and the set of all contractive analytic functions Φ which are greater or equal to Θ_B.

Keywords: symmetric operators; partial isometries; self-adjoint and unitary extensions; reproducing kernel Hilbert spaces of analytic functions; Hardy and deBranges Rovnyak spaces; Livšic characteristic function

1 Introduction

The purpose of this paper is to study of the family of all self-adjoint extensions of a given closed simple symmetric linear transformation B with equal deficiency indices (n, n), $1 \leq n < \infty$ defined on a domain in a separable Hilbert space in the case where the Livšic characteristic function of B is an inner function. For $n \in \mathbf{N} \cup \{\infty\}$, $\mathcal{S}_n(\mathcal{H})$ will denote the set of all closed simple symmetric linear transformations with indices (n, n) defined in a separable Hilbert space $\mathcal{H}$. More generally $\mathcal{S}_n$ will denote the family of all closed simple symmetric linear transformations with indices (n, n) defined in some separable Hilbert space, and $\mathcal{S}$ the set of all closed simple symmetric linear transformations with equal indices defined in some separable Hilbert space.

If A is a self-adjoint linear operator which extends $B \in \mathcal{S}_n(\mathcal{H})$, *i.e.* $A|_{\mathrm{Dom}(B)} = B$, and $\mathrm{Dom}(A)$ is also contained in $\mathcal{H}$ then we call A a canonical extension of B. If, on the other hand, A is self-adjoint in $\mathcal{K}$ where $\mathcal{K} \supsetneq \mathcal{H}$, then we call A a non-canonical extension of B. The set of all canonical extensions of B can be completely characterized by the set of all surjective isometries between the deficiency subspaces $\mathrm{Ker}(B^* - i)$ and $\mathrm{Ker}(B^* + i)$, see for example [1, Chapter VII].

Our goal is to provide a new characterization of the set, $\mathrm{Ext}(B)$, of both canonical and non-canonical extensions in the case where the characteristic function Θ_B is inner (Recall that in this case B is unitarily equivalent to multiplication by z in a model subspace $K^2_{\Theta_B} = H^2(\mathbb{C}_+) \ominus \Theta_B H^2(\mathbb{C}_+)$ of Hardy space [2–4].) Namely, given any $A \in \mathrm{Ext}(B)$, we construct a contractive analytic (matrix) function Φ_A which obeys:

$$\Phi_A \geq \Theta_B,$$

see Theorem 8.8. Here, given contractive analytic matrix functions Φ, Θ on $\mathbb{C}_+$, we say that $\Theta \leq \Phi$ provided that $\Theta^{-1}\Phi$ is contractive and analytic on $\mathbb{C}_+$. We then define a natural equivalence relation on $\mathrm{Ext}(B)$ by defining $A_1 \sim A_2$ for $A_1, A_2 \in \mathrm{Ext}(B)$ if $\Phi_{A_1} = \Phi_{A_2}$ and in Theorem 8.11 we show that $A_1 \sim A_2$ if and only if A_1 is unitarily equivalent to A_2 via a unitary whose restriction to $\mathcal{H}$ is the identity. Finally Theorem 8.13 shows that

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if $\mathrm{ext}(B)$ is the set of $\sim$ equivalence classes of $\mathrm{Ext}(B)$ that the map $[A] \in \mathrm{ext}(B) \mapsto \Phi_A$ is a bijection. This provides an alternative to the classical results of M.G. Krein (see *e.g* [29, Theorem 6.5] for the $(1, 1)$ case) which are formulated in terms of generalized resolvents and Nevanlinna-Herglotz functions. Our characterization has the advantage of providing a natural function-theoretic connection between the Livšic characteristic function of $B \in \mathcal{S}$ and the set of its self-adjoint extensions.

These results will be achieved using the concept of a generalized model. This is a reproducing kernel Hilbert space theory approach which generalizes the concept of a model for a symmetric operator as defined in [4, 5].

1.1 Motivation

The study of symmetric, non-selfadjoint operators $B \in \mathcal{S}$ and, in particular, this problem of characterizing the set of all self-adjoint extensions, $\mathrm{Ext}(B)$, of a given symmetric linear transformation $B \in \mathcal{S}$, arises naturally in many important areas of mathematical physics.

Examples of symmetric linear transformations from mathematical physics include many differential operators: hermitian Sturm-Liouville ordinary differential operators of arbitrary even order on intervals of $\mathbb{R}$ such as Schrödinger Hamiltonians from quantum mechanics [6–10], hermitian partial differential operators such as the Laplacian of a compact Riemannian manifold with boundary or the d'Alembertian of a pseudo-Riemannian manifold, discrete Laplacians on graphs [11–18], and Jacobi matrices (which arise, for example, in the study of Schrödinger Hamiltonians on graphs, and in the study of systems of orthogonal polynomials) [19–21]. The references listed above are, of course, just a small sample of the current literature on these subjects.

The study of formally hermitian Sturm-Liouville differential expressions on (subsets of) the real line is an important branch of modern analysis with many applications to mathematical physics and engineering. It is well known that under mild assumptions on the coefficient functions any such differential expression of even order $2m$ can be used to construct a densely defined symmetric operator $H(I) \in \mathcal{S}_n(L^2(a, b))$, where $I = (a, b) \subset \mathbb{R}$ is an arbitrary interval and $n \leq 2m$. If $J \supset I$ is any larger interval (or collection of intervals), it is easy to verify that $H(I) \subset H(J)$ so that any canonical self-adjoint extension H' of $H(J)$ on $L^2(J)$ is a self-adjoint extension of $H(I)$ to a strictly larger Hilbert space, see Example 4.8 for details. Here for linear transformations A, B, the subset notation $B \subset A$ means that A extends B: $\mathrm{Dom}(B) \subset \mathrm{Dom}(A)$ and $A|_{\mathrm{Dom}(B)} = B$. Recall here that all canonical self-adjoint extensions of $H(I)$ can be obtained by enlarging the domain of $H(I)$ to include elements in the domain of its adjoint obeying certain boundary conditions [6]. This provides a large and interesting class of examples of the problem we are considering in this paper, and it is an open question as to whether every $A \in \mathrm{Ext}(H(I))$ can be realized as the canonical self-adjoint extension of some $H(J)$ for $J \supset I$. In this class of examples, $H(I)$ always has finite and equal deficiency indices, and under mild assumptions on the coefficient functions of the differential expression, the characteristic function of $H(I)$ is inner so that the results of this paper apply (see Example 4.8).

Similarly let M be a smooth and complete Riemannian manifold. It is known that the Laplacian, $-\Delta$, can be defined as an essentially self-adjoint operator on the domain of all infinitely differentiable functions with compact support in M [22, 23]. If $M_0 \subset M$ is a smooth compact submanifold with smooth boundary, then as in [24, Section 2.2] (for example), it is easy to check that the restriction, $-\Delta_0$ of $-\Delta$ to $C_0^\infty(M_0)$, the domain of all smooth functions with compact support in M_0 defines a symmetric, non-selfadjoint operator in $L^2(M_0)$ with infinite deficiency indices. Again, all canonical extensions of $-\Delta_0$ are obtained by enlarging the domain of $-\Delta_0$ to include functions obeying more relaxed boundary conditions. It follows that $-\Delta$ is a non-canonical self-adjoint extension of $-\Delta_0$, and if $M_1 \supset M_0$ is another, larger smooth compact submanifold of M with smooth boundary, then any canonical self-adjoint extension of $-\Delta_1$ will be a a non-canonical extension of $-\Delta_0$ to a strictly larger Hilbert space. This is an important class of examples, however, since the deficiency indices of $-\Delta_0$ are always infinite, one would need to carefully check that our results extend to the case where $n = \infty$ in order to apply them.

For an analogous class of examples with finite deficiency indices, one can consider Jacobi matrices arising from the study of Schrödinger Hamiltonians on graphs [19–21], or one can consider graph Laplacians [17, 18]. In a recent and exciting trend in operator theory, several authors have initiated the study of graph Laplacians on infinite resistance networks, *i.e.* countably infinite, connected graphs equipped with a positive definite 'conductance function', c, on the edges [11–16] (this is again a very small sample of the literature on this subject). This conductance function can be in turn used to define several natural 'resistance' metrics on the graph, and a natural 'energy' Hilbert space $\mathcal{H}_E$ which can be viewed as a reproducing kernel Hilbert space of functions on the graph which vanish at a prescribed base point [16]. Such networks have many concrete applications including modeling electrical resistance networks in engineering, providing mathematical models of the internet, and studying stochastic processes and random walk models on graphs [11] (and hence potential connections to quantum statistical mechanics and the study of fractals [25, 26]). It can be shown that the graph Laplacian, Δ, naturally defines a symmetric semi-bounded operator in the energy Hilbert space $\mathcal{H}_E$, and that in contrast to the graph Laplacian acting in the l^2 Hilbert space over the graph, Δ often has non-zero (and always equal) finite deficiency indices as an operator in $\mathcal{H}_E$ [11, 13, 14]. Moreover, it has been shown that key metric properties of the resistance network can be understood in terms of the energy Hilbert space $\mathcal{H}_E$ and spectral properties of the symmetric Laplacian Δ and its self-adjoint extensions (such as its Friedrich's extension).

As in the previous class of examples arising from nested compact submanifolds of a complete Riemmannian manifold, if one has nested resistance networks $\Gamma_0 \subset \Gamma_1$, it is clear that the Laplacian Δ_1 on Γ_1 is a symmetric extension of Δ_0, so that each self-adjoint extension of Γ_1 defines an element of $\mathrm{Ext}(\Delta_0)$. Since the results of this paper do not require a symmetric linear transformation to be densely defined, they also apply to symmetric non-selfadjoint $B \in \mathcal{S}$ defined in finite dimensional Hilbert space, such as (a suitable restriction of) the graph Laplacian defined in the energy Hilbert space of a finite resistance network. Note here that the graph Laplacian of a finite resistance network is a symmetric, everywhere defined operator in $\mathcal{H}_E$, and hence is self-adjoint. However by the spectral theorem any self-adjoint operator is unitarily equivalent to the operator M^Σ of multiplication by the independent variable in $L^2(\mathbb{R}, \Sigma)$ where Σ is a $\mathbb{C}^{n\times n}$ or operator-valued measure on $\mathbb{R}$ (n is the spectral multiplicity). One can always assume (by rescaling by a measurable function) that the measure Σ obeys the Herglotz condition:

$$\| \int_{-\infty}^{\infty} \frac{1}{1+t^2} \Sigma(dt) \| < \infty,$$

and so [4, Subsection 3.5] shows that one can construct a simple symmetric restriction $M_\Sigma \in \mathcal{S}_n(L^2(\mathbb{R}, \Sigma))$ of M^Σ to a suitable domain which has indices (n, n). In particular it follows that the graph Laplacian on a finite resistance network Γ can be viewed as a self-adjoint extension of a symmetric (non-densely defined) linear transformation $\Delta_\Gamma \in \mathcal{S}_n(\mathcal{H}_E)$. In the theory of [11, 16, 27, 28], an 'exhaustion' of a resistance network Γ is a sequence of finite, nested sub-networks $\Gamma_0 \subset \Gamma_1 \subset \ldots \subset \Gamma = \cup \Gamma_k$. Exhaustions can be used to study properties and obtain inequalities for the resistance metric. It follows that given an exhaustion (Γ_k) of $\Gamma = \Gamma_\infty$, one can construct simple symmetric Laplacians Δ_k with equal indices in the energy Hilbert spaces $\mathcal{H}_E(\Gamma_k) \subset \mathcal{H}_E(\Gamma_{k+1})$ which obey $\Delta_0 \subset \Delta_1 \subset \ldots \subset \Delta_\infty := \Delta_\Gamma$. This suggests one interesting application of our results could be to study exhaustions in terms of sequences of contractive analytic matrix functions Θ_k on $\mathbb{C}_+$ obeying $\Theta_k \leq \Theta_{k+1}$ with $\Theta_0 = \Theta_{\Delta_0}$, the Livšic characteristic function of Δ_0 and $\Theta_k = \Phi_{\Delta_k'}$, the characteristic function of a canonical self-adjoint extension Δ_k' of Δ_k viewed as a non-canonical element of $\mathrm{Ext}(\Delta_0)$.

1.2 Overview

The paper will proceed as follows: In the next section we introduce the basic objects of study, $\mathcal{S}_n(\mathcal{H})$, the set of all simple symmetric linear transformations with deficiency indices (n, n) in $\mathcal{H}$ and $\mathrm{Ext}(B)$, the set of all self-adjoint extensions of a symmetric linear transformation $B \in \mathcal{S}_n(\mathcal{H})$. We also review the construction of the Livšic characteristic function, Θ_B for $B \in \mathcal{S}$ and discuss the fundamental result of Livšic that the characteristic function is a complete unitary invariant for $\mathcal{S}_n(\mathcal{H})$. The subsequent section recalls basic results on symmetric linear relations which apply to the non-densely defined symmetric linear transformations in $\mathcal{S}_n(\mathcal{H})$. Section 4 provides a brief introduction to Nevanlinna-Herglotz functions and constructs an associated family of reproducing kernel Hilbert spaces (Herglotz spaces): given any contractive analytic matrix-valued function Θ on $\mathbb{C}_+$, $G_\Theta := (1+\Theta)(1-\Theta)^{-1}$ is a Herglotz function on $\mathbb{C}_+$, and any such function can be used to define a natural sesqui-analytic reproducing kernel K_Θ, and hence a reproducing kernel Hilbert space of analytic vector-valued functions, $\mathcal{L}(\Theta)$, on $\mathbb{C}\setminus\mathbb{R}$. We show that any $B \in \mathcal{S}_n(\mathcal{H})$ can be represented as multiplication by z on its largest possible domain in the Herglotz space $\mathcal{L}(\Theta_B)$ (Corollary 4.5). This section also contains the key Example 4.6 which shows that if $B_1, B_2 \in \mathcal{S}_n$ have Livšic characteristic functions Θ_k, and $\Theta_1^{-1}\Theta_2$ is a contractive analytic (matrix) function, then B_2 extends B_1 so that any self-adjoint extension of B_2 is a self-adjoint extension of B_1.

In Sections 5 and 6 we develop the concept of a generalized model for a symmetric $B \in \mathcal{S}$. A generalized model for $B \in \mathcal{S}_n(\mathcal{H})$ is a map $\Gamma : \mathbb{C}\setminus\mathbb{R} \to \mathcal{B}(\mathcal{J}, \mathcal{H})$ where $\mathcal{J}$ is any Hilbert space of dimension n, $\Gamma(z) \in \operatorname{Ker}(B^* - \bar{z})$ and

$$\bigvee_{z\in\mathbb{C}\setminus\mathbb{R}} \Gamma(z) = \mathcal{H}.$$

This generalizes the concept of a model for a symmetric operator as introduced in [4]. Any generalized model Γ for $B \in \mathcal{S}$ can be used to construct a reproducing kernel Hilbert space of analytic functions $\mathcal{H}_\Gamma$ on $\mathbb{C}\setminus\mathbb{R}$ such that B is unitarily equivalent to multiplication by z on its maximal domain in $\mathcal{H}_\Gamma$ (Proposition 6.2). Proposition 5.15 shows that if Θ_B is inner, then any $A \in \operatorname{Ext}(B)$ naturally gives rise to a generalized model Γ_A of B. Subsection 6.5 provides a concrete formula for the reproducing kernel of $\mathcal{H}_\Gamma$ which relates it to the Livšic characteristic function Θ_B of B.

Section 7 proves the key fact that Θ_B is inner if and only if $\operatorname{Ker}(B^* - w)$ is cyclic for every $A \in \operatorname{Ext}(B)$ and $w \in \mathbb{C}\setminus\mathbb{R}$. This result also holds for infinite n, and is an important ingredient in our function theoretic characterization of $\operatorname{Ext}(B)$.

Our function theoretic characterization of $\operatorname{Ext}(B)$ and our main results are finally presented in Section 8. Here we show that if $B \in \mathcal{S}_n(\mathcal{H})$ with $n < \infty$ and Θ_B inner is fixed, then for any $A \in \operatorname{Ext}(B)$ with associated generalized model Γ_A, there is a natural reproducing kernel Hilbert space $\mathcal{K}_A \supset \mathcal{H}_A := \mathcal{H}_{\Gamma_A}$, constructed using A. This natural reproducing kernel Hilbert space is actually a Herglotz space, so that $\mathcal{K}_A = \mathcal{L}(\Phi)$ for some contractive analytic function Φ. We call $\Phi_A := \Phi$ the characteristic function of $A \in \operatorname{Ext}(B)$ relative to $B \in \mathcal{S}$ and prove the following key results which completely characterize $\operatorname{Ext}(B)$ in terms of the contractive analytic matrix functions Φ_A:

Theorem. *Let $B \in \mathcal{S}_n$ with $n < \infty$ and inner Livšic characteristic function Θ_B.*

Fix an isometry $J : \mathbb{C}^n \to \operatorname{Ker}(B^* + i)$. Given any self-adjoint extension $A \in \operatorname{Ext}(B)$, let $b(A) := (A-i)(A+i)^{-1}$ be the unitary Cayley transform of A, and let $P_{b(A)}$ be the projection-valued measure of $b(A)$ on the unit circle $\mathbf{T}$. Define the characteristic function Φ_A of A relative to B as:

$$\Phi_A := (G_A - I)(G_A + I)^{-1},$$

where G_A is the $\mathbb{C}^{n\times n}$-valued Herglotz function:

$$G_A(z) := -iJ^* \left(zP_{b(A)}(\{1\}) + (Az+1)(A-z)^{-1} \right) J.$$

Under these assumptions the following assertions hold:

1. *For $A_1, A_2 \in \operatorname{Ext}(B)$ with relative characteristic functions $\Phi_i = \Phi_{A_i}$, $\Phi_1 = \Phi_2$ if and only if $A_1 = U^* A_2 U$ for a unitary U with $U|_{\mathcal{H}} = I$. (Theorem 8.11)*

2. *Define an equivalence relation on $\operatorname{Ext}(B)$ by $A_1 \sim A_2$ if $\Phi_{A_1} = \Phi_{A_2}$. Let $\operatorname{ext}(B) := \operatorname{Ext}(B)/\sim$ be the quotient set. Then the map $\operatorname{ext}(B) \ni [A] \mapsto \Phi_A$ is a bijection onto the set of all contractive, analytic $\mathbb{C}^{n\times n}$-valued functions Φ on $\mathbb{C}_+$ such that $\Phi(i) = 0$ and $\Theta_B \le \Phi$. (Theorem 8.13)*

3. *A is a canonical self-adjoint extension of B if and only if $\Phi_A = V\Theta_B$ for a fixed unitary $V \in \mathbb{C}^{n\times n}$. (Theorem 8.14)*

The above results provide a complete function theoretic characterization of $\mathrm{Ext}(B)$ for $B \in \mathcal{S}_n$ with $n < \infty$ and Θ_B inner which is analogous to the fundamental results of Livšic characterizing $\mathcal{S}$:

Theorem. *(Livšic) Given any $B \in \mathcal{S}_n$ one can construct a contractive analytic $\mathbb{C}^{n\times n}$-valued function Θ_B on $\mathbb{C}_+$, the Livšic characteristic function of B, such that:*
1. *$B_1, B_2 \in \mathcal{S}_n$ with characteristic functions $\Theta_k := \Theta_{B_k}$ are unitarily equivalent if and only if their characteristic functions are equivalent,* i.e. *$\Theta_1 = Q\Theta_2 R$ for fixed unitary matrices $R, Q \in \mathbb{C}^{n\times n}$.*

2. *If $\simeq$ denotes unitary equivalence then the map $\mathcal{S}_n/\simeq\, \ni [B] \mapsto [\Theta_B]$ is a bijection onto the set of all equivalence classes (with respect to relation described above) of contractive analytic $\mathbb{C}^{n\times n}$-valued functions Θ on $\mathbb{C}_+$ which obey $\Theta(i) = 0$.*

We will define the Livšic characteristic function Θ_B of $B \in \mathcal{S}$ in the next section.

2 Preliminaries

Recall that a linear transformation B is simple, symmetric and closed with deficiency indices (n, n) if it is defined on a domain $\mathrm{Dom}(B)$ contained in a separable Hilbert space $\mathcal{H}$ and has the following properties:

$$\langle Bx, y\rangle = \langle x, By\rangle\,, \qquad \forall x, y \in \mathrm{Dom}(B), \qquad B \text{ is } \textit{symmetric}; \tag{2.1}$$

$$\bigcap_{z\in\mathbb{C}\setminus\mathbb{R}} \mathrm{Ran}\,(B - z) = \{0\}, \qquad B \text{ is } \textit{simple}; \tag{2.2}$$

$$\{(x, Bx) |\; x \in \mathrm{Dom}(B)\} \text{ is a closed subset of } \mathcal{H} \oplus \mathcal{H}, \quad B \text{ is } \textit{closed}; \tag{2.3}$$

$$n_- := \dim\left(\mathrm{Ran}\,(B - i)^{\perp}\right) = n = \dim\left(\mathrm{Ran}\,(B + i)^{\perp}\right) =: n_+,$$

$$B \textit{ has equal deficiency indices } (n_+, n_-). \tag{2.4}$$

Condition (2.2) can be restated equivalently as: B is simple if and only if there is no non-trivial subspace reducing for B such that the restriction of B to the intersection of its domain with this subspace is self-adjoint. For many of our results we will need to assume that $n < \infty$ is finite.

A partial isometry V is called simple, or c.n.u. (completely non-unitary) if it has no unitary restriction to a proper (and non-trivial) reducing subspace. The deficiency indices for V are the pair of non-negative integers (n_+, n_-) defined by

$$n_+ := \dim\left(\mathrm{Ker}(V)\right) \quad \text{and} \quad n_- := \dim\left(\mathrm{Ran}\,(V)^{\perp}\right),$$

and it is not difficult to see that these are the same as the defect indices of V as defined in [31].

There is a bijective correspondence between $\mathcal{S}_n(\mathcal{H})$ and $\mathcal{V}_n(\mathcal{H})$ which we now describe: Given a simple symmetric linear transformation $B \in \mathcal{S}_n(\mathcal{H})$ and $z \in \mathbb{C} \setminus \mathbb{R}$, let Q_z denote the projection onto $\mathrm{Ran}\,(B - \overline{z})$. The Cayley transform V_B of B is the partial isometry

$$V_B := b(B)Q_i = (B - i)(B + i)^{-1}Q_i; \qquad b(z) := \frac{z - i}{z + i}, \tag{2.5}$$

where $b(B) = (B - i)(B + i)^{-1}$ is a well-defined isometry from $Q_i\mathcal{H} = \mathrm{Ran}\,(B + iI)$ onto $Q_{-i}\mathcal{H} = \mathrm{Ran}\,(B - i)$. Note that $\mathrm{Ker}(V) = \mathrm{Ran}\,(B + i)^{\perp}$ and $\mathrm{Ran}\,(V)^{\perp} = \mathrm{Ran}\,(B - i)^{\perp}$, and so it follows that the deficiency indices of V_B are the same as those of B.

Conversely suppose that V is a simple partial isometry on $\mathcal{H}$ with defect indices (n_+, n_-). One can construct a symmetric linear transformation B_V by defining

$$\mathrm{Dom}(B_V) := (1 - V)\mathrm{Ker}(V)^\perp,$$

and

$$B_V f = b^{-1}(V)f = i(1+V)(1-V)^{-1}f, \quad f \in \mathrm{Dom}(B_V); \quad b^{-1}(z) := i\frac{1+z}{1-z}.$$

Again it is easy to check that B_V and V have the same deficiency indices. One can further verify that $B_{V_B} = B$ and $V_{B_V} = V$ for any simple symmetric linear transformation B and simple partial isometry V, respectively. This shows that the maps $B \mapsto V_B$ and $V \mapsto B_V$ are inverses of each other so that these maps are bijections between $\mathcal{S}$ and $\mathcal{V}$. We will use this bijection to formulate problems in whichever setting is most convenient, and to obtain equivalent results for both classes of linear transformations.

Given $B \in \mathcal{S}_n(\mathcal{H})$, $n < \infty$, one can construct a complete unitary invariant Θ_B, called the Livšic characteristic function as follows: For each $z \in \mathbb{C} \setminus \mathbb{R}$ let $J_z : \mathbb{C}^n \to \mathrm{Ran}\,(B - \overline{z})^\perp$ be a fixed linear isomorphism such that $J_{\pm i}$ are onto isometries. Define

$$B(z) := J_i^* J_z, \tag{2.6}$$

and

$$A(z) := J_{-i}^* J_z \tag{2.7}$$

The Livšic characteristic function is then [32]:

$$\Theta_B(z) := b(z)B^{-1}(z)A(z), \tag{2.8}$$

and this can be shown to be a contractive $\mathbb{C}^{n\times n}$ matrix-valued analytic function on $\mathbb{C}_+$, the upper half-plane. Note that the characteristic function Θ_B always vanishes at $z = i$. Different choices of $J_z, J_{\pm i}$ in the above definition yield a new characteristic function $\widetilde{\Theta}_B$ which is related to the first by

$$\widetilde{\Theta}_B(z) = R\Theta_B(z)Q,$$

where R, Q are fixed unitary matrices. Two Livšic characteristic functions Θ_1, Θ_2 are said to coincide or to be equivalent if they are related in this way.

For most of this paper we will assume that Θ_B is an inner function, *i.e.* Θ_B has non-tangential boundary values on $\mathbb{R}$ almost everywhere with respect to Lebesgue measure (tensored with the $\mathbb{C}^{n\times n}$ identity matrix), and these non-tangential boundary values are unitary matrix-valued. In this case $B \simeq Z_{\Theta_B}$, where $Z_{\Theta_B} \in \mathcal{S}\left(K^2_{\Theta_B}\right)$ is the symmetric operator of multiplication by z on the domain

$$\mathrm{Dom}(Z_{\Theta_B}) = \{f \in K^2_{\Theta_B} |\, zf \in K^2_{\Theta_B}\},$$

in the model space $K^2_{\Theta_B} = H^2 \ominus \Theta_B H^2$, and here $H^2 = H^2(\mathbb{C}_+)$ is the Hardy space of the upper half-plane (of $\mathbb{C}^n$-vector valued functions).

As shown by M.S. Livšic (see also [4]), the Livšic characteristic function is a complete unitary invariant for $\mathcal{S}_n(\mathcal{H})$:

Theorem. *(Livšic) Linear transformations $B_1 \in \mathcal{S}_n(\mathcal{H}_1)$ and $B_2 \in \mathcal{S}_n(\mathcal{H}_2)$ are unitarily equivalent if and only if their characteristic functions Θ_1, Θ_2 are equivalent.*

Theorem 8.11 of this paper will provide a similar result for all $A \in \mathrm{Ext}(B)$, the family of all self-adjoint extensions of B (extensions to Hilbert spaces which in general contain $\mathcal{H}$ as a proper subspace). Given any $A \in \mathrm{Ext}(B)$, we will define a characteristic function $\Phi_A = \Phi[A; B]$ which has the property that $\Phi_A \geq \Theta_B$. Theorem 8.11 will show that $\Phi_{A_1} = \Phi_{A_2}$ if and only if $A_1 \simeq A_2$ via a unitary which is the identity when restricted to $\mathcal{H}$. Here $\simeq$ denotes unitary equivalence.

Here is our formal definition of $\mathrm{Ext}(B)$:

Definition 2.1. Given $V \in \mathcal{V}_n(\mathcal{H})$, let $\mathrm{Ext}(V)$ denote the set of all unitary operators U such that

1. U is an extension of $V = b(B)$, *i.e.* $V \subseteq U$ $(U|_{\mathrm{Ker}(V)^\perp} = V|_{\mathrm{Ker}(V)^\perp})$ and U is unitary in some Hilbert space $\mathcal{K} \supset \mathcal{H}$.
2. $\mathcal{K}$ is the smallest reducing subspace for vN(U), the von Neumann algebra generated by U, which contains $\mathcal{H}$.

Given $B \in \mathcal{S}_n(\mathcal{H})$, we will define Ext$(B)$ to be a relabeling of the set Ext$(b(B))$. Namely if $U \in$ Ext$(b(B))$, and $1 \notin \sigma_p(U)$, the point spectrum or set of eigenvalues of U, then we define A to be the self-adjoint operator $b^{-1}(U)$. If however $U \in$ Ext$(b(B))$ and $1 \in \sigma_p(U)$, then we formally define A by $b^{-1}(U)$. In this case A is not a well defined linear transformation, it is just a renaming of $U \in$ Ext$(b(B))$ with the understanding that $A_1 = A_2$ for $A_1 = b^{-1}(U_1)$, $A_2 = b^{-1}(U_2)$ and $U_1, U_2 \in$ Ext$(b(B))$ if and only if $U_1 = U_2$. Ext(B) is then defined to be the set of all such A. In this way there is a bijection between Ext$(b(B))$ and Ext(B) by construction.

Recall that the subset notation $B \subset A$ means that A is an extension of B, *i.e.* Dom$(B) \subset$ Dom(A) and $A|_{\mathrm{Dom}(B)} = B$. The subset notation $V \subseteq U$ for partial isometries V, U means that $U|_{\mathrm{Ker}(V)^\perp} = V|_{\mathrm{Ker}(V)^\perp}$. For simple symmetric linear transformations B_1, B_2 we have that $B_1 \subset B_2$ if and only if $b(B_1) \subseteq b(B_2)$ (see [5]).

Remark 2.2. If B is densely defined then every unitary extension U of $b(B)$ does not have 1 as an eigenvalue [2, Lemma 6.1.3],[33], so that every element of Ext(B) is a densely defined self-adjoint operator. Note that if $A \in$ Ext(B) and $A = b^{-1}(U)$ for some $U \in$ Ext$(b(B))$ such that $1 \notin \sigma_p(U)$, then the two conditions of the above definition are equivalent to

1. A is an extension of B, *i.e.* $B \subset A$ and A is self-adjoint in some Hilbert space $\mathcal{K} \supset \mathcal{H}$.
2. $\mathcal{K}$ is the smallest reducing subspace for vN(A), the von Neumann algebra generated by $b(A)$, which contains $\mathcal{H}$.

However if B is not densely defined, then one can find canonical unitary extensions U of $V = b(B)$ which have 1 as an eigenvalue [2, Lemma 6.1.3],[32]. In this exceptional case where U is a unitary extension of $b(B)$ and $1 \in \sigma_p(U)$, then we will always work with the unitary extension U associated with $A = b^{-1}(U)$. If $1 \in \sigma_p(U)$, one could define $A := b^{-1}(U)P_U(\mathbf{T} \setminus \{1\}) = b^{-1}(U)\chi_{\mathbf{T}\setminus\{1\}}(U)$, where χ_Ω is the characteristic function of Ω, $\mathbf{T}$ is the unit circle and $P_U(\mathbf{T} \setminus \{1\}) = \chi_{\mathbf{T}\setminus\{1\}}(U)$ projects onto the orthogonal complement of the eigenspace to eigenvalue 1 of U. However we will have no need for this construction, and in this exceptional case where $1 \in \sigma_p(U)$ for $U \in$ Ext$(b(B))$ we will simply work with $U \in$ Ext$(b(B))$ instead of its inverse Cayley transform $A = b^{-1}(U)$ in Ext(B). In this sense we are really studying unitary extensions of partial isometries, although we choose to work in the setting of self-adjoint extensions of symmetric linear maps as a matter of preference. This choice is motivated by the opinion that many of our results appear more elegant in this formulation.

It will also be convenient to define Ext$_U(B)$ to be the set of all self-adjoint linear transformations A on $\mathcal{K}$ for which $A \in$ Ext(UBU^*) for some isometry $U : \mathcal{H} \to \mathcal{K}$.

The set Ext(B) is called the set of self-adjoint extensions of B. In the case where $\mathcal{K} = \mathcal{H}$, we say that A is a canonical self-adjoint extension of B. It is well known that the canonical self-adjoint extensions A of B can all be obtained by first computing the Cayley transform $V := b(B)$, extending this by a $rank - n$ isometry $U : \mathrm{Dom}(V)^\perp \to \mathrm{Ran}\,(V)^\perp$ to obtain a unitary extension V_U of V, and then taking the inverse Cayley transform to obtain a self-adjoint linear transformation $A := b^{-1}(V_U)$ [1]. Characterizing the set Ext(B) of all self-adjoint extensions of a symmetric linear transformation B, including the non-canonical extensions to larger Hilbert spaces is a much more complicated problem. One of the main goals of this paper is to construct a natural function theoretic characterization of Ext(B) in terms of contractive analytic functions which are greater or equal to the Livšic characteristic function Θ_B of B.

3 Linear relations

In the case where B is not densely defined, its adjoint B^* is not a linear operator. Instead B^* can be realized as a linear relation, and we will dicuss the basic facts about linear relations that will be needed in this section. The material from this section is taken primarily from [34] and [35, Section 1.1]. A *linear relation* L on a separable Hilbert space $\mathcal{H}$ is defined to be a subspace of $\mathcal{H} \oplus \mathcal{H}$. Note that L is the graph, $\mathfrak{G}(T)$, of some closed linear operator T provided that L is closed and $(0, f) \in L$ implies that $f = 0$.

Given a linear relation L, one defines the adjoint linear relation L^* by

$$L^* := \left\{ (g_1, g_2) | \ \langle f_1, g_2 \rangle = \langle f_2, g_1 \rangle \quad \forall (f_1, f_2) \in L \right\}. \tag{3.1}$$

L is called symmetric if $L \subset L^*$ and L is self-adjoint if $L = L^*$. Clearly if B is a closed symmetric linear operator with adjoint B^* then the graph, $\mathfrak{G}(B)$ of B is a closed symmetric linear relation, and the graph, $\mathfrak{G}(B^*)$ of B^* is the adjoint relation to $\mathfrak{G}(B)$.

In this paper we will be considering closed symmetric linear transformations B with deficiency indices (n, n), which are not necessarily densely defined. If this is the case then this means that B does not have a uniquely defined adjoint operator, and it will be convenient to identify B with its graph $\mathfrak{G}(B)$:

$$\mathfrak{G}(B) := \{ (f, Bf) | \ f \in \mathrm{Dom}(B) \},$$

in which case

$$\mathfrak{G}(B)^* = \{ (g_1, g_2) | \ \langle f, g_2 \rangle = \langle Bf, g_1 \rangle \quad \forall f \in \mathrm{Dom}(B) \}$$

is a closed linear relation but not the graph of a linear operator. Indeed, observe that if $g \perp \mathrm{Dom}(B)$ then by equation (3.1), $(0, g) \in \mathfrak{G}(B)^*$ since

$$\langle f, g \rangle = \langle Bf, 0 \rangle,$$

for every $(f, Bf) \in \mathfrak{G}(B)$. For convenience we will simply write B^* for $\mathfrak{G}(B)^*$ in the case where B is not densely defined. Note that

$$B^*(0) := \{ f \in \mathcal{H} | \ (0, f) \in \mathfrak{G}(B)^* = B^* \} = \overline{\mathrm{Dom}(B)}^{\perp}.$$

One can show that if B has deficiency indices (n, n) that the co-dimension of $\mathrm{Dom}(B)$ is at most n:

Lemma 3.1. *If $B \in \mathcal{S}_n(\mathcal{H})$, the orthogonal complement of* $\mathrm{Dom}(B)$ *is at most n–dimensional.*

Proof. If $V = b(B)$ then $\mathrm{Ker}(V)$ is n–dimensional, and $\mathrm{Dom}(B) = (1 - V)\mathrm{Ker}(V)^{\perp}$. If $f \perp \mathrm{Dom}(B)$, then

$$0 = \left\langle f, (1 - V)\mathrm{Ker}(V)^{\perp} \right\rangle = \left\langle (1 - V^*)f, \mathrm{Ker}(V)^{\perp} \right\rangle,$$

and so $(1 - V^*)f \in \mathrm{Ker}(V)$ which is n–dimensional. Now $(1 - V^*)f \neq 0$ as then f would be an eigenfunction to eigenvalue 1 and V would not be simple. It follows that the dimension of $\mathrm{Dom}(B)^{\perp}$ is at most n as otherwise we could find a $g \in \mathrm{Dom}(B)^{\perp}$ such that $(1 - V^*)g = 0$. □

For $z \in \mathbb{C}$ define

$$(B^* - z) := \{ (f, g - zf) | \ (f, g) \in B^* \},$$

and

$$\mathrm{Ker}(B^* - z) := \{ f \in \mathcal{H} | \ (f, 0) \in (B^* - z) \}.$$

Then, as in the case of densely defined B, it follows that

$$\mathrm{Ker}(B^* - z) = \mathrm{Ran}\,(B - \overline{z})^{\perp},$$

so that

$$\mathcal{H} = \mathrm{Ran}\,(B - \overline{z}) \oplus \mathrm{Ker}(B^* - z),$$

for any $z \in \mathbb{C} \setminus \mathbb{R}$.

If B is a symmetric linear transformation then one can show, whether or not B is densely defined, that $\dim \left(\mathrm{Ker}(B^* - z) \right)$ is constant for $z \in \mathbb{C}_{\pm}$, so that the deficiency indices of B obey $n_{\pm} = \dim \left(\mathrm{Ker}(B^* - z) \right)$ for $z \in \mathbb{C}_{\pm}$. For lack of a reference, here is an elementary proof of this fact.

Proposition 3.2. *Let B be a symmetric linear transformation in a separable Hilbert space $\mathcal{H}$. Then* $\dim\left(\operatorname{Ker}(B^* - z)\right)$ *is constant in $\mathbb{C}_+$ and in $\mathbb{C}_-$.*

Proof. Given $w \in \mathbb{C} \setminus \mathbb{R}$ let $P_w :=$ projection onto $\operatorname{Ker}(B^* - w) = \operatorname{Ran}(B - \overline{w})^\perp$, and let $Q_w :=$ projection onto $\operatorname{Ran}(B - w)$ so that $Q_w = 1 - P_{\overline{w}}$.

Now fix $w \in \mathbb{C} \setminus \mathbb{R}$. Choose any $f \in Q_w\mathcal{H}$ of unit norm, $\|f\| = 1$. Since $f \in \operatorname{Ran}(B - w)$, we have that $f = (B - w)g$ for some $g \in \operatorname{Dom}(B)$. Now $B - w$ is bounded below, an easy calculation shows that for any $g \in \operatorname{Dom}(B)$:

$$\|(B - w)g\|^2 = \|(B - \operatorname{Re}(w))g\|^2 + |\operatorname{Im}(w)|^2\|g\|^2 \geq |\operatorname{Im}(w)|^2\|g\|^2.$$

Hence

$$\|g\| \leq \frac{\|(B - w)g\|}{|\operatorname{Im}(w)|} = \frac{\|f\|}{|\operatorname{Im}(w)|} = \frac{1}{|\operatorname{Im}(w)|}.$$

Now choose z in the same half-plane as w and consider:

$$\begin{aligned} Q_zQ_wf &= Q_zf = Q_z(B - w)g = Q_z\left((B - z)g + (z - w)g\right) \\ &= (B - z)g + (z - w)Q_zg. \end{aligned}$$

It follows that

$$\begin{aligned} (Q_w - Q_zQ_w)f &= (B - w)g - (B - z)g - (z - w)Q_zg = (z - w)(1 - Q_z)g \\ &= (z - w)P_{\overline{z}}g. \end{aligned}$$

This implies that

$$\|(Q_w - Q_zQ_w)f\| \leq |z - w|\|g\| \leq \frac{|z - w|}{|\operatorname{Im}(w)|}.$$

Since f was an arbitrary norm one vector in $Q_w\mathcal{H}$ we conclude that

$$\|Q_w - Q_zQ_w\| \leq \frac{|z - w|}{|\operatorname{Im}(w)|}.$$

Taking adjoints it follows that we also have

$$\|Q_w - Q_wQ_z\| \leq \frac{|z - w|}{|\operatorname{Im}(w)|}.$$

Now

$$\begin{aligned} \|Q_w - Q_z\| &= \|Q_w - Q_wQ_z + Q_wQ_z - Q_z\| \\ &\leq \|Q_w - Q_wQ_z\| + \|Q_z - Q_wQ_z\| \\ &\leq \frac{|z - w|}{|\operatorname{Im}(w)|} + \frac{|z - w|}{|\operatorname{Im}(z)|}. \end{aligned}$$

For fixed $w \in \mathbb{C}_+$ or $\mathbb{C}_-$, this is less than one for all z in a small enough neighbourhood of w.

It follows that for z close enough to w we have

$$\|P_{\overline{w}} - P_{\overline{z}}\| = \|(1 - Q_w) - (1 - Q_z)\| = \|Q_w - Q_z\| < 1,$$

so that by [1, Section 34] $P_{\overline{z}}\mathcal{H}$ and $P_{\overline{w}}\mathcal{H}$ have the same dimension. It follows that the dimension of $P_z\mathcal{H} = \operatorname{Ker}(B^* - z) = \operatorname{Ran}(B - \overline{z})^\perp$ is constant for $z \in \mathbb{C}_+$, and for $z \in \mathbb{C}_-$. □

4 Herglotz Spaces

In this section we will show that any $B \in \mathcal{S}_n$ is unitarily equivalent to the operator of multiplication by z in a certain natural reproducing kernel Hilbert space of analytic functions called a Herglotz space. Assume that $n < \infty$.

4.1 Herglotz Functions

It will be convenient to begin with a brief review of the Nevanlinna-Herglotz representation theory of Herglotz functions on both the unit disk $\mathbf{D}$ and the upper half-plane $\mathbb{C}_+$. Let g be a $\mathbb{C}^{n\times n}$-valued Herlglotz function on $\mathbf{D}$, *i.e.* an analytic function with non-negative real part. Here $\mathbb{C}^{n\times n}$ is our notation for the $n \times n$ matrices over $\mathbb{C}$. Then by the Herglotz representation theorem there is a unique positive Borel $\mathbb{C}^{n\times n}$-valued measure σ on the unit circle $\mathbf{T}$ such that

$$\mathrm{Re}\left(g(z)\right) = \int_{\mathbf{T}} \mathrm{Re}\left(\frac{\alpha + z}{\alpha - z}\right) \sigma(d\alpha).$$

The measure σ determines the Herglotz function g up to an imaginary constant so that

$$g(z) = ib + \int_{\mathbf{T}} \frac{\alpha + z}{\alpha - z} \sigma(d\alpha).$$

We will always impose the normalization condition that $b = 0$ in this paper. Observe that with this condition in place, σ is a probability measure, *i.e.* σ is unital, $\sigma(\mathbf{T}) = \mathbf{1}$, if and only if $g(0) = 1$. We will also extend g to a function on $\mathbb{C} \setminus \mathbf{T}$ using the convention that

$$g(1/\overline{z})^* = -g(z).$$

Now let $G := g \circ b$ be the corresponding matrix-valued Herglotz function on $\mathbb{C}_+$ (G has non-negative real part in $\mathbb{C}_+$). Setting $w := b^{-1}(z)$ and $t = b^{-1}(\alpha)$, we obtain that

$$G(w) = -i\sigma(\{1\})w + \int_{-\infty}^{\infty} \frac{wt + 1}{i(t - w)} (\sigma \circ b)(dt).$$

The convention that $g(1/\overline{z})^* = -g(z)$ implies that $G(\overline{w})^* = -G(w)$ and this extends G to a function on $\mathbb{C} \setminus \mathbb{R}$. Again, we have that σ is unital if and only if $g(0) = \mathbf{1}$ which happens if and only if $G(i) = \mathbf{1}$.

Now the Herglotz theorem on the upper half-plane states that

$$\mathrm{Re}\left(G(w)\right) = cy + \int_{-\infty}^{\infty} P_w(t)\Sigma(dt),$$

for unique Borel measure Σ obeying

$$\int_{-\infty}^{\infty} \frac{\Sigma(dt)}{1 + t^2} < \infty,$$

and positive constant matrix $c \geq 0$ where $y = \mathrm{Im}\,(w)$ and

$$P_w(t) = \mathrm{Re}\left(\frac{1}{i\pi}\frac{1}{t - w}\right),$$

is the Poisson kernel for $\mathbb{C}_+$. It will be convenient to determine the relationship between the Herglotz measure σ of g and Σ of $G := g \circ b$. As above we let

$$z(w) = \frac{w - i}{w + i} = b(w) \quad \text{and} \quad w(z) = i\frac{1 + z}{1 - z} = b^{-1}(z).$$

The function $g := G \circ b^{-1}$ obeys

$$\mathrm{Re}\left(g(z)\right) = \int_{\mathbf{T}} p_z(\alpha)\sigma(d\alpha),$$

where

$$p_z(\alpha) = \mathrm{Re}\left(\frac{\alpha + z}{\alpha - z}\right),$$

is the Poisson kernel on the disk. We can write

$$\operatorname{Re}\big(g(z)\big) = p_z(1)\sigma(\{1\}) + \int_{\mathbf{T}\setminus\{1\}} p_z(\alpha)\sigma(d\alpha).$$

Now for $\alpha \in \mathbf{T}\setminus\{1\}$ we can let $\alpha = z(t)$ for $t \in \mathbb{R}$ to write

$$\operatorname{Re}\big(G(w)\big) = \operatorname{Re}\big(g(z(w))\big) = p_{z(w)}(1)\sigma(\{1\}) + \int_{-\infty}^{\infty} p_{z(w)}(z(t))\widetilde{\sigma}(dt),$$

where $\widetilde{\sigma}$ is the measure on $\mathbb{R}$ defined by $\widetilde{\sigma}(\Omega) := \sigma(z(\Omega)) = (\sigma \circ b)(\Omega)$, so that $z(\Omega) = b(\Omega) \in \mathbf{T}\setminus\{1\}$.

A bit of algebra shows that

$$p_z(1) = \frac{1-|z|^2}{|1-z|^2},$$

and that if $w = x + iy \in \mathbb{C}_+$, then

$$p_{z(w)}(1) = y.$$

Some more algebra shows that

$$P_w(t) = \frac{1}{2\pi i}\frac{w-\overline{w}}{|t-w|^2},$$

while

$$p_{z(w)}(z(t)) = \pi(1+t^2)P_w(t).$$

We conclude that

$$\operatorname{Re}\big(G(w)\big) = \operatorname{Re}\big(g(z(w))\big) = y\sigma(\{1\}) + \int_{-\infty}^{\infty} P_w(t)\pi(1+t^2)\widetilde{\sigma}(dt).$$

Finally this shows how the measures $\widetilde{\sigma} = \sigma \circ b$ and Σ are related:

$$\Sigma(\Omega) = \int_{\Omega} \pi(1+t^2)(\sigma \circ b)(dt). \tag{4.1}$$

There is a bijective correspondence between $\mathbb{C}^{n\times n}$-valued Herglotz functions G on $\mathbb{C}\setminus\mathbb{R}$ and $\mathbb{C}^{n\times n}$-valued contractive analytic functions Θ on $\mathbb{C}_+$ defined by

$$\Theta \mapsto G_\Theta := \frac{1+\Theta}{1-\Theta} \quad \text{and} \quad G \mapsto \Theta_G := \frac{G-1}{G+1}.$$

The Nevanlinna-Herglotz representation theory can also be used to define a bijective correspondence between $\mathbb{C}^{n\times n}$-valued Herglotz functions on $\mathbb{C}^+$ and a large class of $\mathbb{C}^{n\times n}$-positive matrix-valued measures on $\mathbb{R}$. Namely if g is a Herglotz function on the unit disk which obeys the normalization condition assumed at the beginning of this section (vanishing constant imaginary part), then as discussed above it uniquely determined by a regular, positive $\mathbb{C}^{n\times n}$-valued Borel measure σ on the unit circle $\mathbf{T}$ by the formula:

$$g(z) = \int_{\mathbf{T}} \frac{\alpha+z}{\alpha-z}\sigma(d\alpha). \tag{4.2}$$

It follows that the Herglotz function $G := g \circ b$ on $\mathbb{C}_+$ is uniquely determined by the Herglotz measure Σ and the value of $\sigma(\{1\})$ by the formula

$$\begin{aligned} G(z) &= -i\sigma(\{1\})z + \int_{-\infty}^{\infty} \frac{zt+1}{i(t-z)}(\sigma \circ b)(dt) \\ &= -i\sigma(\{1\})z + \frac{1}{i\pi}\int_{-\infty}^{\infty} \frac{zt+1}{(t-z)}\frac{1}{1+t^2}\Sigma(dt). \end{aligned} \tag{4.3}$$

Conversely given any non-negative matrix $P \in \mathbb{C}^{n\times n}$ and positive $\mathbb{C}^{n\times n}$ matrix-valued Borel measure Σ on $\mathbb{R}$ that obeys the condition:

$$\left(\int_{-\infty}^{\infty} \frac{1}{1+t^2} \Sigma(dt)\mathbf{v}, \mathbf{w} \right)_{\mathbb{C}^n} < \infty, \tag{4.4}$$

for any $\mathbf{v}, \mathbf{w} \in \mathbb{C}^n$, there is a unique Herglotz function G on $\mathbb{C}_+$ that obeys equation (4.3), or equivalently obeys:

$$\mathrm{Re}\left(G(z)\right) = P\mathrm{Im}\,(z) + \int_{-\infty}^{\infty} \mathrm{Re}\left(\frac{1}{i\pi}\frac{1}{t-z}\right)\Sigma(dt).$$

It follows that there is a bijective correspondence between Herglotz functions G on $\mathbb{C}_+$ and such pairs (P, Σ), where $P \in \mathbb{C}^{n\times n}$ is positive and Σ is a positive $\mathbb{C}^{n\times n}$ valued measure obeying the condition (4.4). This in turn implies there is a bijective correspondence between contractive analytic functions Θ on $\mathbb{C}_+$ and such pairs (P, Σ). Given Θ we will call the corresponding Σ the Herglotz measure of Θ and we will usually denote this by Σ_Θ. Similarly σ_θ will denote the Herglotz measure of $\theta := \Theta \circ b^{-1}$. Note that since we assume any Herglotz function g_θ obeys our normalization condition (no non-zero imaginary constant part), it follows that σ_θ is unital if and only if $g_\theta(0) = \mathbf{1} = G_\Theta(\mathbf{1})$ which happens if and only if $\theta(0) = 0 = \Theta(i)$.

4.2 Herglotz spaces

Let Θ be a $\mathbb{C}^{n\times n}$–valued contractive analytic function on $\mathbb{C}_+$. The Herglotz space, $\mathcal{L}(\Theta)$ is the abstract reproducing kernel space of analytic $\mathbb{C}^n$-valued functions on $\mathbb{C} \setminus \mathbb{R}$ with reproducing kernel

$$K_w^\Theta(z) := \frac{i}{\pi}\frac{G_\Theta(z) + G_\Theta(w)^*}{z - \overline{w}}.$$

Namely given any $\mathbf{v} \in \mathbb{C}^n$ and $f \in \mathcal{L}(\Theta)$ and $w \in \mathbb{C}\setminus\mathbb{R}$, we have that $K_w\mathbf{v} \in \mathcal{L}(\Theta)$ where $K_w\mathbf{v}(z) := K_w(z)\mathbf{v}$ and,

$$\left(f(z), \mathbf{v}\right)_{\mathbb{C}^n} = \left\langle f, K_z^\Theta \mathbf{v}\right\rangle_\Theta.$$

As shown in [4], if Θ is a Livšic characteristic function so that $\Theta(i) = 0$, and the symmetric linear transformation B with characteristic function Θ is densely defined then one can define a closed simple symmetric linear operator $\mathfrak{Z}_\Theta \in \mathcal{S}_n(\mathcal{L}(\Theta))$ with domain

$$\mathrm{Dom}(\mathfrak{Z}_\Theta) = \{f \in \mathcal{L}(\Theta) |\ zf \in \mathcal{L}(\Theta)\},$$

by

$$(\mathfrak{Z}_\Theta f)(z) := zf(z); \qquad f \in \mathrm{Dom}(\mathfrak{Z}_\Theta),$$

see [4, Theorem 6.3]. Since we do not assume that all of our symmetric linear transformations are densely defined, we will need to extend this slightly:

Lemma 4.3. *Let Θ be a contractive analytic $\mathbb{C}^{n\times n}$-valued function on $\mathbb{C}_+$. The linear transformation $\mathfrak{Z}_\Theta$ defined on the domain*

$$\mathrm{Dom}(\mathfrak{Z}_\Theta) := \{F \in \mathcal{L}(\Theta) |\ zF(z) \in \mathcal{L}(\Theta)\},$$

by

$$(\mathfrak{Z}_\Theta F)(z) = zF(z), \quad F \in \mathrm{Dom}(\mathfrak{Z}_\Theta)$$

belongs to $\mathcal{S}_n(\mathcal{L}(\Theta))$.

The proof of this lemma follows from the vector-valued version of [36, Theorem 5], see also [37]. In particular we use the identity

$$(\overline{w} - w)\left\langle \frac{F - F(w)}{z - w}, \frac{G - G(w)}{z - w}\right\rangle_\Theta = \left\langle F, \frac{G - G(w)}{z - w}\right\rangle_\Theta - \left\langle \frac{F - F(w)}{z - w}, G\right\rangle_\Theta,$$

valid for all $F, G \in \mathcal{L}(\Theta)$ proven in [36, Theorem 5] for the case $n = 1$, and easily verified to also hold for the vector-valued case.

Proof. Let $S_{\pm i} := \{F \in \mathcal{L}(\Theta) | \, F(\pm i) = 0\}$. By de Branges' results on Herglotz spaces, if $F \in S_{-i}$ then

$$(VF)(z) := \frac{z-i}{z+i} F(z) = b(z)F(z) \in \mathcal{L}(\Theta),$$

so that the linear transformation V which acts as multiplication by $b(z)$ obeys $V : S_{-i} \to S_i$. We can show that V is in fact an isometry: if $F \in S_{-i}$ then

$$\begin{aligned} \langle VF, VF \rangle_\Theta &= \left\langle F - \frac{2i}{z+i} F, F - \frac{2i}{z+i} F \right\rangle_\Theta \\ &= \langle F, F \rangle_\Theta - 2i \left(\left\langle \frac{1}{z+i} F, F \right\rangle_\Theta - \left\langle F, \frac{1}{z+i} F \right\rangle_\Theta \right) + \left\langle \frac{2i}{z+i} F, \frac{2i}{z+i} F \right\rangle_\Theta \\ &= \langle F, F \rangle_\Theta , \end{aligned}$$

using the identity stated before the proof.

It is not hard to verify that V is closed, and so $\mathfrak{Z}_\Theta := b^{-1}(V)$ is a well-defined closed symmetric linear transformation. The symmetric linear transformation $\mathfrak{Z}_\Theta$ has indices (n, n) since

$$\mathrm{Ker}(\mathfrak{Z}_\Theta^* + i) = \mathrm{Ker}(V) = \bigvee K_{-i}^\Theta \mathbb{C}^n,$$

and

$$\mathrm{Ker}(\mathfrak{Z}_\Theta^* - i) = \mathrm{Ran}\,(V)^\perp = \bigvee K_i^\Theta \mathbb{C}^n.$$

Similarly,

$$\mathrm{Ker}(\mathfrak{Z}_\Theta^* - z) = \bigvee K_{\overline{z}}^\Theta \mathbb{C}^n,$$

so that

$$\mathcal{L}(\Theta) = \bigvee_{z \in \mathbb{C} \setminus \mathbb{R}} \mathrm{Ker}(\mathfrak{Z}_\Theta^* - z),$$

proving that $\mathfrak{Z}_\Theta$ is simple. It remains to check that the domain of $\mathfrak{Z}_\Theta$ is equal to

$$\mathfrak{D}_\Theta := \{F \in \mathcal{L}(\Theta) | \, zF(z) \in \mathcal{L}(\Theta)\}.$$

Clearly $\mathrm{Dom}(\mathfrak{Z}_\Theta) \subset \mathfrak{D}_\Theta$, and conversely if $F \in \mathfrak{D}_\Theta$ then $G(z) = (z+i)F(z) \in S_{-i} = \mathrm{Ker}(V)^\perp$, and so by definition $(1 - V)G \in \mathrm{Dom}(\mathfrak{Z}_\Theta)$, and

$$(1 - V)G(z) = (z + i)F(z) - (z - i)F(z) = 2iF(z).$$

This proves that $F \in \mathrm{Dom}(\mathfrak{Z}_\Theta)$ so that $\mathfrak{D}_\Theta = \mathrm{Dom}(\mathfrak{Z}_\Theta)$. □

Lemma 4.4. *Let Θ be a contractive analytic function as above. The Livšic characteristic function of $\mathfrak{Z}_\Theta$ is a Frostman shift of Θ:*

$$\Theta_{\mathfrak{Z}_\Theta} = (1 - \Theta(i)^*)(1 - \Theta\Theta(i)^*)^{-1}(\Theta - \Theta(i))(1 - \Theta(i))^{-1}.$$

Note that the above formula reduces to the usual Frostman shift formula in the case where Θ is scalar-valued.

Proof. This is a straightforward calculation using the definition of the characteristic function (equations (2.6), (2.7) and (2.8)) and the reproducing kernel

$$K_w(z) = \frac{i}{\pi} \frac{G_\Theta(z) + G_\Theta(w)^*}{z - \overline{w}},$$

for $\mathcal{L}(\Theta)$. Let $\{e_j\}$ be the standard orthonormal basis of $\mathbb{C}^n$. We can choose

$$u_j = K_{-i}K_{-i}(-i)^{-1/2}e_j, \quad v_j = K_iK_i(i)^{-1/2}e_j \quad \text{and} \quad w_j(z) := K_{\overline{z}}e_j.$$

With this choice of bases, one obtains

$$A(z) = [\left\langle K_{\overline{z}}e_j, K_iK_i(i)^{-1/2}e_k\right\rangle] = K_i(i)^{-1/2}K_{\overline{z}}(i) \quad \text{and} \quad B(z) = K_{-i}(-i)^{-1/2}K_{\overline{z}}(-i).$$

Recall here that

$$\Theta_{\mathfrak{Z}_\Theta}(z) = b(z)B(z)^{-1}A(z).$$

Now observe that

$$K_i(i) = \frac{i}{\pi}\frac{G_\Theta(i) + G_\Theta(i)^*}{2i}.$$

Using that $G_\Theta(\overline{z})^* = -G_\Theta(z)$ for the Herglotz function G_Θ, we also obtain that

$$K_{-i}(-i) = \frac{i}{\pi}\frac{G_\Theta(-i) + G_\Theta(-i)^*}{-2i} = \frac{i}{\pi}\frac{-G_\Theta(i)^* - G_\Theta(i)}{-2i} = K_i(i).$$

It follows that

$$\Theta(z) := \Theta_{\mathfrak{Z}_\Theta}(z) = b(z)B(z)^{-1}A(z) = b(z)K_{\overline{z}}(-i)^{-1}K_{\overline{z}}(i).$$

Substituting in our expression for the reproducing kernel $K_w(z)$ yields

$$\begin{aligned}
\Theta(z) &= b(z)\left(\frac{i}{\pi}\frac{G(-i) + G(\overline{z})^*}{-i-z}\right)^{-1}\left(\frac{i}{\pi}\frac{G(i) + G(\overline{z})^*}{i-z}\right) \\
&= \left(G(-i) + G(\overline{z})^*\right)^{-1}\left(G(i) + G(\overline{z})^*\right) \\
&= \left(-G(i)^* - G(z)\right)^{-1}\left(G(i) - G(z)\right) \\
&= \left(G(i)^* + G(z)\right)^{-1}\left(G(i) - G(z)\right). \qquad \text{(ignore the factor of } -1\text{)}
\end{aligned}$$

We can ignore the factor of -1 since $\Theta(z)$ is defined only up to conjugation by fixed unitaries.

Now straightforward algebra shows that

$$G(z) - G(i) = 2(1 - \Theta(z))^{-1}(\Theta(z) - \Theta(i)(1 - \Theta(i))^{-1},$$

while

$$G(i)^* + G(z) = 2(1 - \Theta(z))^{-1}(1 - \Theta(z)\Theta(i)^*)(1 - \Theta(i)^*)^{-1}.$$

Putting these two formulas together yields the Frostman shift formula. □

In particular if $\Theta(i) = 0$ then Θ is equal to the Livšic characteristic function of $\mathfrak{Z}_\Theta$, and Theorem 2 allows us to conclude:

Corollary 4.5. *If $B \in \mathcal{S}$ has characteristic function Θ then $B \cong \mathfrak{Z}_\Theta$.*

This corollary shows that any $B \in \mathcal{S}_n(\mathcal{H})$ can be represented as multiplication by z, $\mathfrak{Z}_{\Theta_B}$, in a Herglotz space $\mathcal{L}(\Theta_B)$ of analytic $\mathbb{C}^n$-valued functions on $\mathbb{C}\setminus\mathbb{R}$. The following example of symmetric extensions of a symmetric operator B with Θ_B inner will be important:

Example 4.6. Let Θ, Φ be $\mathbb{C}^{n\times n}$-valued inner functions on $\mathbb{C}_+$ such that $\Theta \leq \Phi$. In this case $\Theta^{-1}\Phi$ is also an inner function.

Given any inner function Θ one can define a symmetric linear transformation Z_Θ acting in K^2_Θ by:

$$\mathrm{Dom}(Z_\Theta) := \{f \in K^2_\Theta | \, zf(z) \in K^2_\Theta\},$$

and

$$Z_\Theta f(z) := zf(z), \quad f \in \mathrm{Dom}(Z_\Theta),$$

see for example [3, 4]. It is straightforward to show that the characteristic function of Z_Θ is the Frostman shift of Θ as above so that by Livšic's theorem $Z_\Theta \simeq \mathfrak{Z}_\Theta$.

It follows that since $K^2_\Theta \subset K^2_\Phi$ that $\mathrm{Dom}(Z_\Theta) \subset \mathrm{Dom}(Z_\Phi)$ and that $Z_\Theta \subset Z_\Phi$ so that Z_Θ is unitarily equivalent to a restriction of Z_Φ. In the notation of [5], we write $Z_\Theta \preccurlyeq Z_\Phi$ to denote that Z_Θ is unitarily equivalent to a restriction of Z_Φ, and this defines a pre-order on $\mathcal{S}$. Moreover given any $A \in \mathrm{Ext}(Z_\Phi)$, then the restriction A' of A to its smallest invariant subspace containing K^2_Θ belongs to $\mathrm{Ext}(Z_\Theta)$.

This can be generalized further: Suppose that Φ is an arbitrary contractive analytic function such that $\Phi \geq \Theta$ where Θ is inner. Then by [38, II-6], K^2_Θ is contained isometrically in the deBranges-Rovnyak space K^2_Φ, $K^2_\Theta \subset K^2_\Phi$. Moreover [4, Theorem 7.1] shows that multiplication by $V(z) := \frac{2}{1-\Phi(z)}$ is an isometry from K^2_Φ into $\mathcal{L}(\Phi)$. Hence $V : K^2_\Theta \to \mathcal{L}(\Phi)$, the operator of multiplication by $V(z)$ is an isometry of K^2_Θ into $\mathcal{L}(\Phi)$, and by the definition of $\mathrm{Dom}(Z_\Theta)$, and the definition of $\mathrm{Dom}(\mathfrak{Z}_\Phi)$ in Lemma 4.3, it follows that $V\mathrm{Dom}(Z_\Theta) \subset \mathrm{Dom}(\mathfrak{Z}_\Phi)$ and that $VZ_\Theta V^* \subset \mathfrak{Z}_\Phi$ so that Z_Θ is unitarily equivalent to a restriction of $\mathfrak{Z}_\Phi$. Since $\mathfrak{Z}_\Theta \cong Z_\Theta$, this also shows that $\mathfrak{Z}_\Theta \preccurlyeq \mathfrak{Z}_\Phi$ whenever Θ is inner, Φ is contractive and $\Theta \leq \Phi$. Again the restriction of any $A \in \mathrm{Ext}(\mathfrak{Z}_\Phi)$ to its smallest invariant subspace containing VK^2_Θ belongs to $\mathrm{Ext}_U(Z_\Theta)$. Here recall that given $B \in \mathcal{S}$, $\mathrm{Ext}_U(B)$ is the set of all self-adjoint linear transformations A such that $A \in \mathrm{Ext}(UBU^*)$ for some isometry $U : \mathcal{H} \to \mathcal{K}$.

This example can be generalized even further to the case of arbitrary contractive analytic matrix functions as in [5, Example 9.5] if one extends the definition of $\mathrm{Ext}(B)$ suitably.

Theorem 4.7. *Let $B_1, B_2 \in \mathcal{S}$ with characteristic functions Θ_1, Θ_2. If the characteristic function Θ_1 is inner and $\Theta_1 \leq \Theta_2$ then $B_1 \preccurlyeq B_2$.*

As discussed above, the pre-order $\preccurlyeq$ is defined on $\mathcal{S}$ by $B_1 \preccurlyeq B_2$ if B_1 is unitarily equivalent to a restriction of B_2 [5]. Furthermore if $B_k \in \mathcal{S}(\mathcal{H}_k)$ and $A \in \mathrm{Ext}(B_2)$ then the restriction of A to its smallest invariant subspace containing $\mathcal{H}_2$ belongs to $\mathrm{Ext}_U(B_1)$.

Proof. By Corollary 4.5, $B_j \simeq \mathfrak{Z}_{\Theta_j}$. As discussed in the above example if Θ_1 is inner and $\Theta_1 \leq \Theta_2$ then $\mathfrak{Z}_{\Theta_1} \preccurlyeq \mathfrak{Z}_{\Theta_2}$ so that $B_1 \preccurlyeq B_2$. ☐

Example 4.8. (Sturm-Liouville differential operators) Consider formally symmetric second-order Sturm-Liouville differential operators on intervals $I = [a, b] \subset \mathbf{R}$. Suppose that $p \geqslant 0$, and q are real-valued functions on I such that $1/p$ and q are locally L^1 functions on (a, b), i.e., they belong to L^1 of any compact subset of (a, b). Define the dense domain

$$\mathrm{Dom}(H(p,q,I)^*) := \left\{ f \in L^2(I) \,|\, f, pf' \in L^1_{loc}(I) \text{ and } -(pf')' + qf \in L^2[a,b] \right\},$$

and then define

$$H(p,q,I)^* f = -(pf')' + qf, \quad f \in \mathrm{Dom}(H(p,q,I)^*).$$

The theory of [6, Section 17] shows that

$$H(p,q,I) := (H(p,q,I)^*)^*$$

belongs to $\mathcal{S}_n(L^2[a,b])$ (and is densely defined), where n is either 0, 1, or 2, depending on the properties of p and q. In particular if p, q are sufficiently well-behaved and $I = [a, b]$ is a compact interval then $H(p, q, I)$ will have indices $(2, 2)$, and the characteristic function $\Theta_{H(p,q,I)}$ will be inner (see [4, Example 5.3]). Furthermore, $H(p, q, I)^*$ is its adjoint. Recall here that any closed symmetric linear operator with indices $(0, 0)$ is self-adjoint. It can be shown that

$$\mathrm{Dom}(H(p,q,I)) = \{ f \in \mathrm{Dom}(H(p,q,I)^*) | \, f(a) = 0 = f(b) \text{ and } p(a)f'(a) = 0 = p(b)f'(b) \},$$

[6, Lemma 1, Section 17.3].

The theory of Sturm-Liouville differential operators shows that the canonical self-adjoint extensions of $H(p, q, I)$ can be constructed by extending the domain of $H(p, q, I)$ to include functions in the domain of its adjoint which obey certain boundary conditions (for example Dirichlet or Neumann boundary conditions) [6, Section 17]. Now suppose that $J \subset I$ is a larger subset of $\mathbb{R}$ containing $I = [a, b]$, and let $A \in \mathrm{Ext}(H(p, q, J))$ be a canonical extension of $H(p, q, J)$. Then it is clear that $L^2(I)$ can be viewed as a subspace of $L^2(J)$, that

$\mathrm{Dom}(H(p,q,I)) \subset \mathrm{Dom}(H(p,q,J))$ and that $H(p,q,J)|_{\mathrm{Dom}(H(p,q,I))} = H(p,q,I)$ so that $H(p,q,I) \subset H(p,q,J)$. It follows that A is a self-adjoint extension of $H(p,q,I)$ to the larger Hilbert space L^2_J, and since it can be shown that the projection of L^2_J onto L^2_I is not reducing for $b(A)$, $A \in \mathrm{Ext}(H(p,q,I))$ is a non-canonical extension.

Given any $B \in \mathcal{S}_1(\mathcal{H})$, it is well known that there is a conjugation C_B which commutes with B, *i.e.* $C_B : \mathrm{Dom}(B) \to \mathrm{Dom}(B)$ and $C_B B = BC_B$. Recall here that a conjugation is an anti-linear, idempotent onto isometry [29, Theorem 7.1]. It will be useful for us to extend this construction to the case of arbitrary $B \in \mathcal{S}$. We say that $C : \mathcal{H}_1 \to \mathcal{H}_2$ is a conjugation intertwining $B_1 \in \mathcal{S}_n(\mathcal{H}_1)$ and $B_2 \in \mathcal{S}_n(\mathcal{H}_2)$ provided that $CB_1 = B_2 C$, and C is an anti-linear and onto isometry.

Proposition 4.9. *Let Θ be a contractive $\mathbb{C}^{n\times n}$-valued analytic function in $\mathbb{C}_+$, $n \in \mathbf{N}$. The map $C_\Theta : \mathcal{L}(\Theta) \to \mathcal{L}(\Theta^T)$, defined by $C_\Theta F(z) = F^\dagger(z) := \overline{F(\overline{z})}$ is a conjugation intertwining $\mathfrak{Z}_\Theta$ and $\mathfrak{Z}_{\Theta^T}$, and $C^*_\Theta = C_{\Theta^T}$.*

In the above ^{T} denotes matrix transpose and for a vector $F(z)$, $\overline{F(z)}$ denotes the vector obtained by taking the complex conjugate of each component in the fixed canonical basis of $\mathbb{C}^n$.

Proof. Let $\{e_k\}$ denote the canonical orthonormal basis of $\mathbb{C}^n$. Let $C : \mathbb{C}^n \to \mathbb{C}^n$ denote the conjugation defined by entrywise complex conjugation: if $\mathbf{v} = \sum c_i e_i$ for $c_i \in \mathbb{C}$, then $C\mathbf{v} := \sum \overline{c_i} e_i$. Given any matrix $A \in \mathbb{C}^{n\times n}$, with entries $A = [a_{ij}]$, it is easy to check that $CAC = [\overline{a_{ij}}] = (A^*)^T = (A^T)^*$. By definition, given $F \in \mathcal{L}(\Theta)$, we have that

$$(C_\Theta F)(z) = C(F(\overline{z})).$$

The closed linear span of the evaluation vectors $K^\Theta_w \mathbf{v}$ for $w \in \mathbb{C} \setminus \mathbb{R}$, $\mathbf{v} \in \mathbb{C}^n$ is dense in $\mathcal{L}(\Theta)$. The action of C_Θ on such functions is

$$\begin{aligned}(C_\Theta K^\Theta_w)(z)\mathbf{v} &= CK^\Theta_w(\overline{z})\mathbf{v} = CK^\Theta_w(\overline{z})CC\mathbf{v} \\ &= (K^\Theta_w(\overline{z})^T)^* C\mathbf{v}.\end{aligned}$$

Now

$$\begin{aligned}K^\Theta_w(\overline{z})^T &= \left(\frac{i}{\pi}\frac{G_\Theta(\overline{z}) + G_\Theta(w)^*}{\overline{z} - \overline{w}}\right)^T \\ &= \frac{i}{\pi}\frac{G_{\Theta^T}(\overline{z}) + G_{\Theta^T}(w)^*}{\overline{z} - \overline{w}},\end{aligned}$$

since $G_\Theta = \frac{1+\Theta}{1-\Theta}$ so that $G^T_\Theta = G_{\Theta^T}$. It follows that

$$\begin{aligned}CK^\Theta_w(\overline{z})C &= (K^\Theta_w(\overline{z})^T)^* \\ &= \frac{-i}{\pi}\frac{G_{\Theta^T}(\overline{z})^* + G_{\Theta^T}(w)}{z - w} \\ &= \frac{i}{\pi}\frac{G_{\Theta^T}(z) + G_{\Theta^T}(\overline{w})^*}{z - w} = K^{\Theta^T}_{\overline{w}}(z).\end{aligned}$$

This proves that

$$C_\Theta K^\Theta_w \mathbf{v} = K^{\Theta^T}_{\overline{w}} C\mathbf{v} \in \mathcal{L}(\Theta^T),$$

and it follows from the density of the point evaluation vectors that $C_\Theta : \mathcal{L}(\Theta) \to \mathcal{L}(\Theta^T)$, and that it has dense range. It is clear by definition that C_Θ is anti-linear. To see that it is an (anti-linear) isometry note that

$$\begin{aligned}\left\langle C_\Theta K^\Theta_w \mathbf{v}, C_\Theta K^\Theta_z \mathbf{w}\right\rangle_\Theta &= \left\langle K^{\Theta^T}_{\overline{w}} C\mathbf{v}, K^{\Theta^T}_{\overline{z}} C\mathbf{w}\right\rangle_{\Theta^T} \\ &= \left(K^{\Theta^T}_{\overline{w}}(\overline{z})C\mathbf{v}, C\mathbf{w}\right)_{\mathbb{C}^n} \\ &= \left(CK^\Theta_w(z)CC\mathbf{v}, C\mathbf{w}\right) \\ &= \left(\mathbf{w}, K^\Theta_w(z)\mathbf{v}\right) = \left\langle K^\Theta_z \mathbf{w}, K^\Theta_w \mathbf{v}\right\rangle_\Theta .\end{aligned}$$

Using the fact that linear combinations of such functions are dense in $\mathcal{L}(\Theta)$ and $\mathcal{L}(\Theta^T)$, we conclude that C_Θ is an isometry with dense range, and hence is onto. In other words, C_Θ is anti-unitary, so that $C_\Theta^* C_\Theta = \mathbf{1}$. As is easy to check:

$$C_{\Theta^T} C_\Theta K_w^\Theta \mathbf{v} = C_{\Theta^T} K_{\overline{w}}^{\Theta^T} C\mathbf{v} = K_w^\Theta C^2 \mathbf{v} = K_w^\Theta \mathbf{v},$$

and it follows that $C_\Theta^* = C_{\Theta^T}$.

Finally, since $\mathrm{Dom}(\mathfrak{Z}_\Theta) := \{F \in \mathcal{L}(\Theta) |\ zF \in \mathcal{L}(\Theta)\}$, and similarly for $\mathfrak{Z}_{\Theta^T}$, $C_\Theta \mathrm{Dom}(\mathfrak{Z}_\Theta) = \mathrm{Dom}(\mathfrak{Z}_{\Theta^T})$. Indeed, if $F \in \mathrm{Dom}(\mathfrak{Z}_\Theta)$, then

$$C_\Theta z F(z) = C(\overline{z} F(\overline{z})) = z(C_\Theta F)(z),$$

so that $C_\Theta F \in \mathrm{Dom}(\mathfrak{Z}_{\Theta^T})$, and conversely given any $G \in \mathrm{Dom}(Z_{\Theta^T})$, $C_{\Theta^T} G \in \mathrm{Dom}(\mathfrak{Z}_\Theta)$, and $C_\Theta C_{\Theta^T} G = G$, showing that $C_\Theta \mathrm{Dom}(\mathfrak{Z}_\Theta) = \mathrm{Dom}(\mathfrak{Z}_{\Theta^T})$. The above arguments also show that for any $F \in \mathrm{Dom}(\mathfrak{Z}_\Theta)$,

$$C_\Theta \mathfrak{Z}_\Theta F = \mathfrak{Z}_{\Theta^T} C_\Theta F,$$

completing the proof. □

Corollary 4.10. *Suppose that $B \in \mathcal{S}_n(\mathcal{H})$ has characteristic function Θ_B. Let $B_T \in \mathcal{S}_n(\mathcal{H}_T)$ have characteristic function Θ_B^T. Then there are conjugations $C_B : \mathcal{H} \to \mathcal{H}_T$, and $C_{B^T} = C_B^*$ such that $C_B B = B_T C_B$ and $C_{B^T} B_T = B C_{B^T}$.*

Note that any such conjugation C_B obeys $C_B \mathrm{Ran}\,(B - z) = \mathrm{Ran}\,(B_T - \overline{z})$, $C_B \mathrm{Ker}(B^* - z) = \mathrm{Ker}(B_T^* - \overline{z})$, and $C_B b(B) = b(B_T)^* C_B$.

Proof. We have $B \simeq \mathfrak{Z}_\Theta$ and $B_T \simeq \mathfrak{Z}_{\Theta^T}$. Composing the unitary operators effecting these equivalences with C_Θ yields C_B. □

4.11 Measure spaces

Let Σ be any $\mathbb{C}^{n\times n}$ positive regular matrix-valued measure on $\mathbb{R}$ which obeys the Herglotz condition:

$$\left(\int_{-\infty}^{\infty} \frac{1}{1+t^2} \Sigma(dt)\mathbf{v}, \mathbf{w} \right)_{\mathbb{C}^n} < \infty,$$

for any $\mathbf{v}, \mathbf{w} \in \mathbb{C}^n$. We define the measure space L^2_Σ to be the space of all $\mathbb{C}^n$-valued functions on $\mathbb{R}$ which are square-integrable with respect to Σ, *i.e.* $f \in L^2_\Sigma$ provided that

$$\int_{-\infty}^{\infty} \big(\Sigma(dt) f(t), f(t)\big)_{\mathbb{C}^n} < \infty.$$

for any $z \in \mathbb{C} \setminus \mathbb{R}$, define the $\mathbb{C}^{n\times n}$ matrix function

$$\delta_z(t) := \frac{i}{\pi} \frac{1}{t - \overline{z}} \mathbf{1}_{n\times n}.$$

Suppose that Θ is a contractive analytic function such that

$$\mathrm{Re}\,\big(G_\Theta(z)\big) = P\mathrm{Im}\,(z) + \int_{-\infty}^{\infty} \mathrm{Re}\left(\frac{i}{\pi} \frac{1}{t - z} \right) \Sigma(dt).$$

The deBranges isometry

$$W_\Theta : L^2_\Sigma \to \mathcal{L}(\Theta),$$

defined by

$$\big((W_\Theta h)(z), \mathbf{v}\big)_{\mathbb{C}^n} := \left(\frac{1}{i\pi} \int_{-\infty}^{\infty} \overline{\frac{1}{\pi(t - \overline{z})}} \Sigma(dt) h(t), \mathbf{v} \right) = \langle h, \delta_z \mathbf{v} \rangle_\Sigma\,,$$

where $\langle\cdot,\cdot\rangle_\Sigma$ denotes the inner product in L^2_Σ is an isometry of $L^2_\Theta := L^2_\Sigma$ into $\mathcal{L}(\Theta)$. The range of W_Θ is $\mathcal{L}(\Psi) \subset \mathcal{L}(\Theta)$ where

$$G_\Psi(z) = G_\Theta(z) + izP,$$

and the orthogonal complement of the range of W_Θ is the closed linear span of the constant functions $\bigvee P\mathbb{C}^n$. One can then check that the reproducing kernel for $\mathcal{L}(\Theta)$ is given by the formula

$$\left(K^\Theta_w(z)\mathbf{v},\mathbf{w}\right)_{\mathbb{C}^n} = \left((\pi W\delta_w(z) + \frac{P}{\pi})\mathbf{v},\mathbf{w}\right) = \langle\delta_w\mathbf{v},\delta_z\mathbf{w}\rangle_\Sigma + \left(\frac{P}{\pi}\mathbf{v},\mathbf{w}\right)_{\mathbb{C}^n},$$

that is,

$$K^\Theta_w(z) = \frac{P}{\pi} + \frac{1}{\pi^2}\int_{-\infty}^{\infty}\frac{1}{t-\overline{w}}\frac{1}{t-z}\Sigma(dt). \tag{4.5}$$

Also notice that if $P = 0$ and Θ is a characteristic function so that $\Theta(i) = 0$, that this implies that $G_\Theta(i) = \mathbf{1}$ so that

$$\mathbf{1} = \int_{-\infty}^{\infty}\mathrm{Re}\left(\frac{1}{i\pi}\frac{1}{t-i}\right)\Sigma(dt) = \int_{-\infty}^{\infty}\frac{1}{1+t^2}\Sigma(dt),$$

and this implies that the vectors $\delta_i e_k$, $1 \le k \le n$ are an orthonormal set.

5 Non-canonical representations of symmetric operators

We are now sufficiently prepared to begin pursuing the main theory and results of this paper. For any $A \in \mathrm{Ext}(B)$ we can construct a representation of B as multiplication on a space of analytic functions on $\mathbb{C}\setminus\mathbb{R}$ as follows:

If $\mathrm{Dom}(A) \subset \mathcal{K} \supset \mathcal{H}$, let

$$\mathcal{K}_z := \mathcal{K} \ominus \mathrm{Ran}\,(B-\overline{z}) = (\mathcal{K}\ominus\mathcal{H}) \oplus \mathrm{Ker}(B^*-z).$$

Here B is viewed as a linear transformation acting in $\mathcal{H}$ so that $\mathrm{Ker}(B^*-z) := \mathcal{H}\ominus\mathrm{Ran}\,(B-\overline{z})$.

For any $w,z \in \mathbb{C}\setminus\mathbb{R}$, if A is densely defined (so that $A = b^{-1}(U)$ and U does not have 1 as an eigenvalue) let

$$U_{w,z} := (A-w)(A-z)^{-1}. \tag{5.1}$$

If however $A = b^{-1}(U)P_U(\mathbf{T}\setminus\{1\})$ and U is a unitary extension of $V = b(B)$ which has 1 as an eigenvalue let

$$U_{w,z} := \left((i-w) + U(i+w)\right)\left((i-z) + U(i+z)\right)^{-1}. \tag{5.2}$$

These two formulas coincide when U does not have 1 as an eigenvalue.

It is not difficult to verify as in [29, Section 1.2] that (regardless of whether A is densely defined or not) for any $w,z \in \mathbb{C}\setminus\mathbb{R}$, $U_{w,z}$ has the following properties:

1. $U_{w,z}$ is invertible.
2. $U_{w,z} : \mathcal{K}_w \to \mathcal{K}_z$ is a bijection.

Note that

$$P_\mathcal{H} U_{w,z}\mathrm{Ker}(B^*-w) \subset P_\mathcal{H}\left(\mathrm{Ker}(B^*-z)\oplus(\mathcal{K}\ominus\mathcal{H})\right) \subset \mathrm{Ker}(B^*-z).$$

Given any fixed $w \in \mathbb{C}\setminus\mathbb{R}$, let $J_w : \mathbb{C}^n \to \mathrm{Ker}(B^*-w)$ be a bounded isomorphism (a bounded linear map with bounded inverse). We can then define the map

$$\Gamma^w_A : \mathbb{C}\setminus\mathbb{R} \to \mathcal{B}(\mathbb{C}^n,\mathcal{H}),$$

by

$$\Gamma_A^w(z) := P_{\mathcal{H}} U_{w,\bar{z}} P_w J_w = P_{\mathcal{H}}(A-w)(A-\bar{z})^{-1} J_w, \tag{5.3}$$

(the last equality holds for the case where A is densely defined) where P_w projects onto $\mathrm{Ker}(B^* - w)$ and it follows that if $A \in \mathrm{Ext}(B)$ is actually a canonical element of $\mathrm{Ext}(B)$ that Γ_A is a *model* for B as defined in [4]. Namely, recall:

Definition 5.1. Given $B \in \mathcal{S}_n(\mathcal{H})$, let $\mathcal{J}$ be a Hilbert space with $\dim(\mathcal{J}) = n$. A map $\Gamma : \mathbb{C} \setminus \mathbb{R} \to \mathcal{B}(\mathcal{J}, \mathcal{H})$, the space of bounded linear maps from $\mathcal{J}$ to $\mathcal{H}$, is a *model* for B if it satisfies the following conditions:

$$\Gamma : \mathbb{C} \setminus \mathbb{R} \to \mathcal{B}(\mathcal{J}, \mathcal{H}) \quad \text{is co-analytic;} \tag{5.4}$$

$$\Gamma(\lambda) : \mathcal{J} \to \mathrm{Ran}\,(B - \lambda I)^{\perp} \quad \text{is invertible for each } \lambda \in \mathbb{C} \setminus \mathbb{R}; \tag{5.5}$$

$$\Gamma(z)^* \Gamma(\lambda) : \mathcal{J} \to \mathcal{J} \quad \text{is invertible when } \lambda, z \in \mathbb{C}_+ \text{ and when } \lambda, z \in \mathbb{C}_-; \tag{5.6}$$

$$\bigvee_{\mathrm{Im}(\lambda)=0} \mathrm{Ran}\,(\Gamma(\lambda)) = \mathcal{H}, \tag{5.7}$$

where $\bigvee$ denotes the closed linear span.

Recall that as shown in [4], any model Γ for $B \in \mathcal{S}_n(\mathcal{H})$ can be used to construct a reproducing kernel Hilbert space of analytic functions $\mathcal{H}_\Gamma$ on $\mathbb{C} \setminus \mathbb{R}$ and a unitary $U_\Gamma : \mathcal{H} \to \mathcal{H}_\Gamma$ such that the image of B under this unitary transformation acts as multiplication by z.

Now if $A \in \mathrm{Ext}(B)$ is non-canonical then Γ_A^w as defined in equation (5.3) does not necessarily satisfy the conditions of a model as defined in Definition 5.1. Despite this Γ_A^w has similar properties to a model and can still be used to construct a reproducing kernel Hilbert space of analytic functions $\mathcal{H}_A$ on $\mathbb{C} \setminus \mathbb{R}$, and (at least in the case under consideration where Θ_B is inner) an isometry $U_A : \mathcal{H} \to \mathcal{H}_A$ such that $U_A B U_A^*$ again acts as multiplication by z in $\mathcal{H}_A$.

This motivates the definition of a non-canonical model which includes these generalized models Γ_A arising from non-canonical $A \in \mathrm{Ext}(B)$:

Definition 5.2. Let $\mathcal{J}$ be any n–dimensional Hilbert space and suppose that $B \in \mathcal{S}_n(\mathcal{H})$. If $\mathcal{B}(\mathcal{J}, \mathcal{H})$ is the space of bounded linear maps from $\mathcal{J}$ to $\mathcal{H}$, we say that $\Gamma : \mathbb{C} \setminus \mathbb{R} \to \mathcal{B}(\mathcal{J}, \mathcal{H})$ is a *quasi-model* for $B \in \mathcal{S}_n(\mathcal{H})$ if Γ satisfies the following two conditions:

$$\Gamma : \mathbb{C} \setminus \mathbb{R} \to \mathcal{B}(\mathcal{J}, \mathcal{H}) \quad \text{is co-analytic;} \tag{5.8}$$

$$\Gamma(z) : \mathcal{J} \to \mathrm{Ker}(B^* - \bar{z}). \tag{5.9}$$

Given a quasi-model Γ, we define

$$m_\pm := \max_{z \in \mathbb{C}_\pm} \dim\left(\mathrm{Ker}(\Gamma(z))^{\perp}\right), \tag{5.10}$$

Γ is then said to have *rank* (m_-, m_+), $0 \le m_\pm \le n$. The quasi-model Γ is said to have full rank, or simply to be full, if $m_+ = n = m_-$.

5.3 Basic properties of quasi-models

Definition 5.4. Let Γ be a quasi-model of rank (m_+, m_-). Let Π_Γ^+ be the set of all points in $\mathbb{C}_+$ for which $\dim\left(\mathrm{Ker}(\Gamma(z)^{\perp})\right) = m_+$, and define Π_Γ^- similarly. Let $\Sigma_\Gamma^\pm := \mathbb{C}_\pm \setminus \Pi_\Gamma^\pm$. We will also use the notation $\Pi_\Gamma = \Pi_\Gamma^+ \cup \Pi_\Gamma^-$ and $\Sigma_\Gamma = \Sigma_\Gamma^+ \cup \Sigma_\Gamma^-$. In other words, Π_Γ^+ is the set of all points $z \in \mathbb{C}_+$ such that $\dim\left(\mathrm{Ran}\,(\Gamma(z))\right) = \dim\left(\mathrm{Ker}(\Gamma(z))^{\perp}\right)$ achieves its maximum value $m_+ \le n$.

We will now show that any quasi-model Γ of rank (n,n) has a property similar to the property (5.6) for a model.

Proposition 5.5. *If $B \in \mathcal{S}_n(\mathcal{H})$ and Γ is a quasi-model for B then $\Gamma(z)^*\Gamma(w)$ is a quasi-affinity on $\mathfrak{J}$ whenever $m_+ = n$ and $z, w \in \Pi_\Gamma^+$ or whenever $m_- = n$ and $z, w \in \Pi_\Gamma^-$.*

Remark 5.6. Note that in the case where $n < \infty$, which is the case we are primarily studying, when $\Gamma(z)^*\Gamma(w)$ is a quasi-affinity, it is acting between finite dimensional spaces and hence is in fact bounded and invertible. Also the reason this proposition is important is that we will shortly construct a reproducing kernel Hilbert space $\mathcal{H}_\Gamma$ whose reproducing kernel is $K_w(z) = \Gamma^*(z)\Gamma(w)$, and it will be useful to know when this is invertible.

This proposition will be the consequence of the following:

Proposition 5.7. *For each $z \in \mathbb{C} \setminus \mathbb{R}$, let $\{\delta_k(z)\}_{k=1}^n$ be a basis for* $\mathrm{Ker}(B^* - z)$*. Then the linear operator Y on $l^2(\mathbf{N})$ with entries*

$$Y(w,z) := \left[\langle \delta_j(w), \delta_k(z)\rangle\right]_{1\le j,k\le n},$$

is a quasi-affinity for any $z, w \in \mathbb{C}_+$ or $z, w \in \mathbb{C}_-$, i.e. *it is injective and has dense range (and hence an inverse which is potentially unbounded).*

The proof of this proposition needs a little set up. Given a closed linear transformation T with domain $\mathrm{Dom}(T) \subset \mathcal{H}$, a point $z \in \mathbb{C}$ is called a *regular* point of T if $T - z$ is bounded below on $\mathrm{Dom}(T)$, *i.e.*, $\|(T-z)f)\| \ge c_z\|f\|$ for all $f \in \mathrm{Dom}(T)$. Let Ω_T denote the set of regular points of T. If $B \in \mathcal{S}_n(\mathcal{H})$, then since B is symmetric we have that $\mathbb{C} \setminus \mathbb{R} \subset \Omega_B \subset \mathbb{C}$. The symmetric linear transformation B is called regular if $\Omega_B = \mathbb{C}$. For any $z \in \Omega_B$, let $\mathfrak{G}_z$ be the closure of the linear relation: $\mathfrak{G}(B) \dotplus \{(h_z, zh_z)|\ h_z \in \mathrm{Ker}(B^* - z)\}$, and $\dotplus$ denotes the non-orthogonal direct sum of linearly independent subspaces.

Lemma 5.8. *If $z \in \mathbb{C} \setminus \mathbb{R}$ then there is a closed linear operator B_z extending B such that $\mathfrak{G}(B_z) = \mathfrak{G}_z$.*

Proof. It suffices to prove that $\mathfrak{G}_z$ is the graph of a densely defined closed linear operator.

Clearly $\mathfrak{G}(B_z) \subset B^*$. To prove that $\mathfrak{G}(B_z)$ is the graph of a linear transformation, we need to prove that the intersection of the multi-valued part of B^* with $\mathfrak{G}_z$ is the zero element:

$$\{(0,g)|\ g \in B^*(0)\} \cap \mathfrak{G}_z = \{(0,0)\},$$

where recall that $B^*(0) = \mathrm{Dom}(B)^\perp$.

Suppose not, then we can find a sequence $(f_n) \subset \mathrm{Dom}(B)$ and a sequence $h_n \in \mathrm{Ker}(B^* - z)$ such that $(f_n + h_n, Bf_n + zh_n) \to (0, g)$ where $g \perp \mathrm{Dom}(B)$. It follows that

$$(B-z)f_n = Bf_n + zh_n - z(f_n + h_n) \to g - 0 = g.$$

Since $\mathrm{Ran}\,(B-z)$ is closed it follows that there is an $f \in \mathrm{Dom}(B)$ such that

$$(B-z)f = g \perp \mathrm{Dom}(B).$$

However this would then imply that

$$0 = \langle g, f\rangle = \left\langle (B-z)f, f\right\rangle = \langle Bf, f\rangle - z\langle f, f\rangle,$$

which is impossible as B is symmetric and $z \in \mathbb{C}\setminus\mathbb{R}$. This proves that $\mathfrak{G}_z$ is the graph of a linear transformation B_z, it remains to prove that B_z is densely defined.

To prove that B_z is a linear operator, *i.e.* densely defined, suppose that $\phi \in \mathcal{H}$ is orthogonal to $\mathrm{Dom}(B_z)$. Then $\phi \perp \mathrm{Dom}(B)$ and $\phi \perp \mathrm{Ker}(B^* - z)$. Hence $\phi \in \mathrm{Ran}\,(B - \overline{z})$ and so $\phi = (B-\overline{z})f$ for some $f \in \mathrm{Dom}(B)$. But ϕ is orthogonal to $\mathrm{Dom}(B)$ as well so that

$$0 = \langle f, \phi\rangle = \left\langle f, (B-\overline{z})f\right\rangle,$$

showing that

$$\langle Bf, f\rangle = z\langle f, f\rangle,$$

which as before is impossible as B is symmetric. □

Lemma 5.9. *Suppose that $z \in \mathbb{C}\setminus\mathbb{R}$. The spectrum of the operator B_z is contained in $\overline{\mathbb{C}_+}$ or $\overline{\mathbb{C}_-}$ when $z \in \mathbb{C}_+$ or $\mathbb{C}_-$, respectively.*

Since B_z is a closed linear operator, the proof is identical to that of [4, Lemma 2.6], and we omit it.

Proof. (of Proposition 5.7) Given a unit vector $\mathbf{c} \in \mathbb{C}^n$ (we take $\mathbb{C}^\infty := \ell^2(\mathbf{N})$), let

$$\Delta_{\mathbf{c}}(z) := \sum_k \overline{c_k}\delta_k(z).$$

Now observe that

$$Y(w,z)\mathbf{c} = \left(\left\langle \delta_j(w), \Delta_{\mathbf{c}}(z)\right\rangle\right)_{1\le j\le n}.$$

Now if $Y(w,z)$ was not injective then there would be a $\mathbf{c} \in \mathbb{C}^n$ for which $Y\mathbf{c} = 0$, and hence $0 = \left\langle \delta_j(w), \Delta_{\mathbf{c}}(z)\right\rangle$ so that $\psi_z := \Delta_{\mathbf{c}}(z) \perp \mathrm{Ker}(B^* - w)$ and hence $\psi_z \in \mathrm{Ran}\,(B - \overline{w})$, $\psi_z = (B-\overline{w})f$ for some $f \in \mathrm{Dom}(B)$. But then, since $\overline{w}$ does not belong to the spectrum of B_z,

$$(z-\overline{w})^{-1}\psi_z = (B_z - \overline{w})^{-1}\psi_z = f,$$

which shows that $\psi_z \in \mathrm{Dom}(B)$, contradicting the fact that B is symmetric.

Hence $Y(w,z)$ is injective whenever $w, z \in \mathbb{C}_+$ or in $\mathbb{C}_-$. But then $Y^*(w,z) = Y(z,w)$ is also injective, proving that $Y(w,z)$ also always has dense range. This proves that $Y(z,w)$ is always a quasi-affinity of $\mathcal{B}(\ell^2(\mathbf{N}))$ whenever z, w are both in $\mathbb{C}_+$ or are both in $\mathbb{C}_-$. □

Proof. (of Proposition 5.5)

If $z, w \in \Pi_\Gamma^+$ this follows from the observation that given any orthonormal basis $\{j_k\}$ of $\mathcal{J}$, and $z \in \Pi_\Gamma^+$, $\delta_k(\overline{z}) := \Gamma(z)j_i$ forms a basis for $\mathrm{Ker}(B^* - \overline{z})$, and that

$$\Gamma(z) = \sum \langle\cdot, j_i\rangle\, \delta_i(\overline{z}),$$

so that

$$\Gamma^*(z)\Gamma(w) = \left[\left\langle \delta_j(\overline{z}), \delta_k(\overline{w})\right\rangle\right]_{1\le j,k\le n}.$$

The proof of the other half of the proposition is analogous. □

For the remainder of this section we will assume that $n < \infty$, although many of our arguments generalize to the case $n = \infty$ without too much difficulty. Recall that Π_Γ^+ is the set of all points $z \in \mathbb{C}_+$ such that $\dim\left(\mathrm{Ran}\left(\Gamma(z)\right)\right) = \dim\left(\mathrm{Ker}(\Gamma(z))^\perp\right)$ achieves its maximum value $m_+ \le n$, and that Π_Γ^- is defined similarly.

Lemma 5.10. *The sets $\Sigma_\Gamma^\pm = \mathbb{C}_\pm \setminus \Pi_\Gamma^\pm$ are contained in the zero-sets of non-zero analytic functions in $\mathbb{C}_\pm$ (and hence are purely discrete with accumulation points lying only on $\mathbb{R}\cup\{\infty\}$).*

This lemma shows that $\Gamma(z)$ achieves its maximum rank on a set of points which is the complement of the zero set of a non-zero analytic function on $\mathbb{C}\setminus\mathbb{R}$. In particular this set of points, $\Pi_\Gamma = \Pi_\Gamma^+ \cup \Pi_\Gamma^-$, is dense in $\mathbb{C}\setminus\mathbb{R}$.

Proof. Choose any $w \in \Pi_\Gamma^+$. Let $\{j_k\}$ be an orthonormal basis of $\mathcal{J}$ such that $\{j_k\}_{k=1}^{m_+}$ is an orthonormal basis of $\mathrm{Ker}(\Gamma(w))^\perp$. Let $\{v_k\}_{k=1}^{m_+}$ be the basis of $\mathrm{Ran}\left(\Gamma(w)\right)$ defined by $v_k = \Gamma(w)j_k$ and set

$$D_w(z) := \left[\left\langle \Gamma(w)j_k, \Gamma(z)j_l\right\rangle\right]_{1\le k,l\le m_+},$$

and let $\delta_w(z) := \det D_w(z)$. Then δ_w is analytic (as a function of z) in $\mathbb{C}_+$ and δ_w is not identically zero since $\delta_w(w) = \det D_w(w)$, and it is clear that by construction $D_w(w)$ is invertible. Now if $z \in \mathbb{C}_+$ is any point such that $\delta_w(z) \neq 0$ then $D_w(z)$ is invertible and hence $\Gamma(z)|_{\mathrm{Ker}(\Gamma(w))^\perp}$ is invertible as a map onto its range. Let $\widetilde{j}_k := P_z j_k$ where P_z projects onto $\mathrm{Ker}(\Gamma(z))^\perp$. The $\widetilde{j}_k$ form a linearly independent set since otherwise the set of all

$$\Gamma(z)j_k = \Gamma(z)\widetilde{j}_k,$$

would not be linearly independent, contradicting the fact that $\Gamma(z)|_{\mathrm{Ker}(\Gamma(w))^\perp}$ is invertible. It follows that

$$\dim\left(\mathrm{Ker}(\Gamma(z))^\perp\right) \geq m_+ = \max_{z \in \mathbb{C}_+} \dim\left(\mathrm{Ker}(\Gamma(z)^\perp)\right),$$

for any $z \in \mathbb{C}_+$ such that $\delta_w(z) \neq 0$, proving the claim. □

Corollary 5.11. *Given any $w \in \Pi^\pm_\Gamma$ we have that the set*

$$\mathbb{C}_\pm \setminus \{z \in \mathbb{C}_\pm |\ \Gamma(z)^* \Gamma(w)|_{\mathrm{Ker}(\Gamma(w)^\perp)} \text{ is invertible }\},$$

is contained in the zero set of an analytic function which is not identically zero.

Lemma 5.12. *Suppose that $n < \infty$. If $m_+ = n$ then $\bigvee_{z \in \mathbb{C}_+} \Gamma(z)\mathcal{J} = \bigvee_{z \in \mathbb{C}_+} \mathrm{Ker}(B^* - \overline{z})$. Similarly if $m_- = n$ then $\bigvee_{z \in \mathbb{C}_-} \Gamma(z)\mathcal{J} = \bigvee_{z \in \mathbb{C}_-} \mathrm{Ker}(B^* - \overline{z})$. Consequently if $m_+ = n = m_-$ then the simplicity of B implies that $\bigvee_{z \in \mathbb{C}\setminus\mathbb{R}} \Gamma(z)\mathcal{J} = \mathcal{H}$.*

Proof. This is intuitively clear. Since B is simple, $\bigvee_{z \in \mathbb{C}\setminus\mathbb{R}} \mathrm{Ker}(B^* - z)$ is dense in $\mathcal{H}$. By definition if $z \in \mathbb{C}_+$ and $z \notin \Sigma^+_\Gamma$ and $m_+ = n$ then $\mathrm{Ker}(B^* - \overline{z}) = \Gamma(z)\mathcal{J}$. By Lemma 5.10 the set Π^+_Γ of all $z \in \mathbb{C}_+$ for which $\mathrm{Ran}\left(\Gamma(z)\right) = \mathrm{Ker}(B^* - \overline{z})$ is dense in $\mathbb{C}_+$.

If $f \in \mathcal{H}$ and $f \perp \bigvee_{z \in \mathbb{C}_+} \Gamma(z)\mathcal{J}$ then $f \perp \mathrm{Ker}(B^* - \overline{z})$ for all $z \in \Pi^+_\Gamma$. Let $\widetilde{\Gamma}$ be a canonical model for B, and let $\widetilde{f}(z) := \widetilde{\Gamma}(z)^* f$. Since $f \perp \mathrm{Ker}(B^* - \overline{z}) = \mathrm{Ran}\left(\widetilde{\Gamma}(z)\right)$ for all $z \in \Pi^+_\Gamma$, the $\mathcal{J}$-valued analytic function $\widetilde{f}(z)$ vanishes everywhere on Π^+_Γ. Since this set is dense in $\mathbb{C}_+$, $\widetilde{f} = 0$ identically on $\mathbb{C}_+$. This shows that $f \perp \bigvee_{z \in \mathbb{C}_+} \mathrm{Ker}(B^* - \overline{z})$. The same argument in $\mathbb{C}_-$ completes the proof. □

Definition 5.13. We say that a quasi-model Γ is a *generalized* or *non-canonical model* for B if

$$\bigvee_{z \in \mathbb{C}\setminus\mathbb{R}} \mathrm{Ran}\left(\Gamma(z)\right) = \mathcal{H}.$$

By Lemma 5.12, any full rank quasi-model (a rank (n, n) quasi-model, i.e. $n = m_\pm = \max_z \in \mathbb{C}_\pm \dim\left(\mathrm{Ker}(\Gamma(z))^\perp\right)$) is a generalized model for B. The next proposition verifies that the linear maps Γ^w_A defined for $A \in \mathrm{Ext}(B)$ and $w \in \mathbb{C} \setminus \mathbb{R}$ in equation (5.3) satisfy our definition of a quasi-model.

Remark 5.14. Suppose that the characteristic function Θ of B is inner. If this is the case then we will show that for any $A \in \mathrm{Ext}(B)$, that $\bigvee_{z \in \mathbb{C}_-} \mathrm{Ran}\left(\Gamma^w_A(\overline{z})\right) = \mathcal{H}$ for any $w \in \mathbb{C}_+$ and $\bigvee_{z \in \mathbb{C}_+} \mathrm{Ran}\left(\Gamma^w_A(\overline{z})\right) = \mathcal{H}$ whenever $w \in \mathbb{C}_-$. Recall here that Γ^w_A is defined in Equation (5.3).

To see this note that in this case that B is unitarily equivalent to Z_Θ, which acts as multiplication by z in some model space K^2_Θ. Suppose that $U : \mathcal{H} \to K^2_\Theta$ is this unitary transformation such that $U^* Z_\Theta U = B$. Let $C_\Theta = \dagger \circ \Theta^*$ be the canonical anti-linear isometry from K^2_Θ onto $K^2_{\Theta^T}$, where T denotes transpose, as defined in [39, Claim 3]. The existence of C_Θ also follows from our Corollary 4.10.

Suppose that $w \in \mathbb{C}_+$. Then by Lemma 5.12, since $m_- = n$ for any Γ_A^w (because $\Gamma_A^w(\overline{w})$ is invertible),

$$\begin{aligned}\bigvee_{z\in\mathbb{C}_-} \operatorname{Ran}\left(\Gamma_A^w(z)\right) &= \bigvee_{z\in\mathbb{C}_+} \operatorname{Ker}(B^* - z)\\ &= U^* \bigvee_{z\in\mathbb{C}_+} \operatorname{Ker}(Z_\Theta^* - z)\\ &= U^* \bigvee \{C_\Theta k_z^{\Theta^T}\}\\ &= U^* K_\Theta^2 = \mathcal{H}.\end{aligned}$$

Similarly if $w \in \mathbb{C}_-$ then

$$\begin{aligned}\bigvee_{z\in\mathbb{C}_+} \operatorname{Ran}\left(\Gamma_A^w(z)\right) &= U^* \bigvee_{z\in\mathbb{C}_-} \operatorname{Ker}(Z_\Theta^* - z)\\ &= U^* \bigvee \{k_z^\Theta\}\\ &= U^* K_\Theta^2 = \mathcal{H}.\end{aligned}$$

This proves that if Θ_B is inner, then every quasi-model Γ_A^w for $A \in \operatorname{Ext}(B)$ and $w \in \mathbb{C} \setminus \mathbb{R}$ is a generalized model:

Proposition 5.15. *If $B \in \mathcal{S}_n(\mathcal{H})$ with Θ_B inner and $A \in \operatorname{Ext}(B)$, then for any $w \in \mathbb{C} \setminus \mathbb{R}$ one can construct a generalized model Γ_A^w for B by defining $\mathcal{J} := \mathbb{C}^n$, $J_w : \mathcal{J} \to \operatorname{Ker}(B^* - w)$ a bounded isomorphism and setting*

$$\Gamma_A^w(z) := P_\mathcal{H} U_{w,\overline{z}} J_w.$$

The quasi-model Γ_A^w has rank (n, m_+) if $w \in \mathbb{C}_+$ and rank (m_-, n) if $w \in \mathbb{C}_-$ where $0 \le m_\pm \le n$.

We will usually assume that J_w is chosen to be an onto isometry. Recall that if A is such that $A = b^{-1}(U)$ and $1 \notin \sigma_p(U)$, then $U_{wz} = P_\mathcal{H}(A - w)(A - \overline{z})^{-1}$, as in equation (5.1). In the exceptional case where $1 \in \sigma_p(U)$, U_{wz} is given by equation (5.2).

Proof. First, clearly Γ_A^w is anti-analytic on $\mathbb{C} \setminus \mathbb{R}$. Also as discussed previously, $\Gamma_A^w(\overline{z}) \in \operatorname{Ker}(B^* - z)$ since $U_{w,z}$ maps $\operatorname{Ker}(B^* - w)$ into $(\mathcal{K} \ominus \mathcal{H}) \oplus \operatorname{Ker}(B_A^* - z)$ (as discussed at the beginning of this section). Finally, by the above Remark 5.14, $\bigvee_{z\in\mathbb{C}\setminus\mathbb{R}} \Gamma_A^w(z)\mathbb{C}^n = \mathcal{H}$ so that Γ_A^w is a generalized model. □

Note that by construction $\Gamma_A^w(\overline{w}) = J_w$, which is invertible by assumption.

Given any $A \in \operatorname{Ext}(B)$, we are free to choose $w \in \mathbb{C} \setminus \mathbb{R}$ in the construction of a quasi-model Γ_A^w associated with A. For the remainder of this paper we will choose $w = -i$ unless otherwise specified and define

$$\Gamma_A(z) := \Gamma_A^{-i}(z),$$

which (excluding the exceptional case where $b(A)$ has 1 as an eigenvalue) is equal to

$$\Gamma_A(z) = P_\mathcal{H}(A + i)(A - \overline{z})^{-1} J_{-i},$$

and $\Gamma_A(i) = J_{-i}$. We will also simply write J for J_{-i} where $J = P_{-i}J : \mathbb{C}^n \to \operatorname{Ker}(B^* + i)$, and it will often be convenient to choose J to be an isometry.

6 Construction of the model reproducing kernel Hilbert space

Given any quasi-model Γ for $B \in \mathcal{S}_n(\mathcal{H})$, we can construct a reproducing kernel Hilbert space $\mathcal{H}_\Gamma$ as follows:

Definition 6.1. For $f \in \mathcal{H}$ define

$$\hat{f}(z) := \Gamma^*(z) f,$$

an analytic function on $\mathbb{C} \setminus \mathbb{R}$, and let $\mathcal{H}_\Gamma$:= the vector space of all the functions $\hat{f}$.

Let $\mathcal{H}_\Gamma^{-1} = \bigvee_{z \in \mathbb{C}\setminus\mathbb{R}} \operatorname{Ran}\left(\Gamma(z)\right)$, $\mathcal{H}_\Gamma^{-1} \subset \mathcal{H}$. Then clearly $\mathcal{H}_\Gamma$ is the set of all functions $\hat{f}$ for $f \in \mathcal{H}_\Gamma^{-1}$, and if $f \perp \mathcal{H}_\Gamma^{-1}$ then $\hat{f} = 0$. We define an inner product on $\mathcal{H}_\Gamma$ by

$$\left\langle \hat{f}, \hat{g} \right\rangle_\Gamma := \langle f, g \rangle ,$$

whenever $f, g \in \mathcal{H}_\Gamma^{-1}$.

According to Definition 5.13, we call Γ a generalized model if $\mathcal{H}_\Gamma^{-1} = \mathcal{H}$.

We say that the reproducing kernel Hilbert space $\mathcal{H}_\Gamma$ has the division property in $\mathbb{C}_\pm$ if whenever $\hat{f} \in \mathcal{H}_\Gamma$ and $\hat{f}(w) = 0$ for $w \in \Pi_\Gamma^\pm$ we have that

$$\frac{\hat{f}(z)}{z - w} \in \mathcal{H}_\Gamma .$$

Recall here that Π_Γ^+ is the set of all points $z \in \mathbb{C}_+$ such that $\dim\left(\operatorname{Ran}\left(\Gamma(z)\right)\right) = \dim\left(\operatorname{Ker}(\Gamma(z))^\perp\right)$ achieves its maximum value $m_+ \leq n$, and Π_Γ^- is defined similarly.

Proposition 6.2. *With the above inner product $\mathcal{H}_\Gamma$ is a reproducing kernel Hilbert space of analytic functions on $\mathbb{C} \setminus \mathbb{R}$ with reproducing kernel*

$$k_w^\Gamma(z) = \Gamma(z)^* \Gamma(w),$$

and point evaluation vectors

$$k_w^\Gamma j = U_\Gamma \Gamma(w) j,$$

for $j \in \mathcal{J}$. If the rank of Γ is (m_+, m_-) then $\mathcal{H}_\Gamma$ has the division property in $\mathbb{C}_\pm$ whenever $m_\pm = n$.

The map $U_\Gamma : \mathcal{H} \to \mathcal{H}_\Gamma$ defined by $U_\Gamma f = \hat{f} = \Gamma^*(\cdot) f$ is a co-isometry with initial space $\mathcal{H}_\Gamma^{-1}$, and is unitary if and only if Γ is a generalized model for B. If Γ is a generalized model then $Z_\Gamma := U_\Gamma B U_\Gamma^{-1}$ acts as multiplication by z on the domain $U_\Gamma \operatorname{Dom}(B)$, and if either m_+ or m_- is equal to n then

$$\operatorname{Dom}(Z_\Gamma) = \{\hat{f} |\ z\hat{f}(z) \in \mathcal{H}_\Gamma\}.$$

Recall that if Θ_B is inner then given any $A \in \operatorname{Ext}(B)$, and $w \in \mathbb{C} \setminus \mathbb{R}$, Proposition 5.15 shows that any quasi-model Γ_A^w is a generalized model with indices (n, m_+) or (m_-, n).

Proof. This is all fairly straightforward to check. First of all one should verify that $\|\hat{f}\|_\Gamma = 0$ implies that $f \perp \mathcal{H}_\Gamma^{-1}$, *i.e.* that $\hat{f}(z) = \Gamma(z)^* f = 0$ for all $z \in \mathbb{C} \setminus \mathbb{R}$. Indeed $\Gamma(z)^* f = 0$ for $z \in \mathbb{C} \setminus \mathbb{R}$ if and only if $\left\langle f, \Gamma(z) j \right\rangle = 0$ for all $z \in \mathbb{C} \setminus \mathbb{R}$, and $j \in \mathcal{J}$ which happens if and only if $f \perp \operatorname{Ran}\left(\Gamma(z)\right)$ for all $z \in \mathbb{C} \setminus \mathbb{R}$, in other words $f \perp \mathcal{H}_\Gamma^{-1}$.

Now given any $j \in \mathcal{J}$ and $f \in \mathcal{H}_\Gamma^{-1}$,

$$\left\langle \hat{f}(w), j \right\rangle_{\mathcal{J}} = \langle f, \Gamma(w) j \rangle_{\mathcal{H}} = \left\langle \hat{f}, U_\Gamma \Gamma(w) j \right\rangle_\Gamma , \tag{6.1}$$

and it follows from this that for any $j \in J$, $k_w j := U_\Gamma \Gamma(w) j$ are reproducing kernel vectors in $\mathcal{H}_\Gamma$ and the reproducing kernel is given by

$$\begin{aligned} \left\langle k_w(z) j_1, j_2 \right\rangle_{\mathcal{J}} &= \langle k_w j_1, k_z j_2 \rangle_\Gamma = \left\langle \Gamma(w) j_1, \Gamma(z) j_2 \right\rangle_{\mathcal{H}} \\ &= \left\langle \Gamma(z)^* \Gamma(w) j_1, j_2 \right\rangle_{\mathcal{J}} . \end{aligned}$$

Now suppose U_Γ is unitary and define $Z_\Gamma := U_\Gamma B U_\Gamma^{-1}$ on $U_\Gamma \operatorname{Dom}(B)$. Let us first show that Z_Γ acts as multiplication by z on its domain. If $f \in \operatorname{Dom}(B)$ then

$$Z_\Gamma \hat{f} = U_\Gamma B f$$

so that for any $j \in \mathcal{J}$,

$$\begin{aligned} \left\langle (U_\Gamma Bf)(z), j \right\rangle_{\mathcal{J}} &= \left\langle Bf, \Gamma(z)j \right\rangle_{\mathcal{H}} = \left\langle f, B^\star \Gamma(z)j \right\rangle && (6.2) \\ &= z \left\langle f, \Gamma(z)j \right\rangle = \left\langle z\hat{f}(z), j \right\rangle_{\mathcal{J}}, && (6.3) \end{aligned}$$

showing that $Z_\Gamma \hat{f}(z) = z\hat{f}(z)$.

Now suppose that $m_+ = n$, and let's prove that $\mathcal{H}_\Gamma$ has the division property in $\mathbb{C}_+$. In this case if $\hat{f} \in \mathcal{H}_\Gamma$ and $\hat{f}(w) = 0$ then

$$0 = \left\langle \hat{f}(w), j \right\rangle = \left\langle f, \Gamma(w)j \right\rangle,$$

for any $j \in J$. If $w \in \Pi_\Gamma^+$, then (by definition of Π_Γ^+) $\Gamma(w) : \mathcal{J} \to \mathrm{Ker}(B^\star - \overline{w})$ is onto which implies that $f \in \mathrm{Ran}\,(B - w)$. Then $f = (B - w)g$, and $\hat{f} = (Z_\Gamma - w)\hat{g}$, or

$$\hat{g}(z) = \frac{\hat{f}(z)}{z - w}.$$

It remains to prove that if $m_+ = n$ and $\hat{f} \in \mathcal{H}_\Gamma$ is such that $z\hat{f}(z) \in \mathcal{H}_\Gamma$ then $\hat{f} \in \mathrm{Dom}(Z_\Gamma)$. If $\hat{f}$ and $z\hat{f} \in \mathcal{H}_\Gamma$ then so is $(z - w)\hat{f} =: \hat{g}$ for any fixed $w \in \Pi_\Gamma^+$, and some $g \in \mathcal{H}$. Since $\hat{g}$ vanishes at w, it follows that $\Gamma^\star(w)g = 0$, so that $g \perp \mathrm{Ran}\left(\Gamma(w)\right) = \mathrm{Ker}(B^\star - \overline{w})$ since $w \in \Pi_\Gamma$. It follows that $g = (B - w)h$ for some $h \in \mathcal{H}$ so that $\hat{g}(z) = (z - w)\hat{h}(z)$ for any $z \in \mathbb{C} \setminus \mathbb{R}$. But since $\hat{g}(z) = (z - w)\hat{f}(z)$ it follows that $\hat{f} = \hat{h}$ so that $f = h \in \mathrm{Dom}(B)$. An analogous argument in the lower half-plane $\mathbb{C}_+$ completes the proof. □

If $\Gamma = \Gamma_A$ for $A \in \mathrm{Ext}(B)$, we will usually write $\mathcal{H}_A$ for $\mathcal{H}_\Gamma$ and Z_A for Z_Γ.

Example 6.3. (An example of Z_A with indices (n, n) where $m_+ = m < n$.)

Suppose that $B \in \mathcal{S}_n(\mathcal{H})$ and Θ_B is inner so that by Proposition 5.15, Γ_A^w is a generalalized model for B, for any $A \in \mathrm{Ext}(B)$ and $w \in \mathbb{C} \setminus \mathbb{R}$.

Let V := the partial isometric extension of $b(B)$ to $\mathcal{H}$. Given any contraction $C \in \mathbb{C}^{n\times n}$ define

$$\hat{C} := J_- C J_+^\star$$

where $J_\pm : \mathbb{C}^n \to \mathrm{Ker}(B^\star \mp i)$ are fixed isometries. Let

$$V(C) := V + \hat{C},$$

a contractive extension of V and let $(U_C, \mathcal{K})$ be the minimal unitary dilation of $V(C)$. Now choose C to be a projection in $\mathbb{C}^{n\times n}$. Let us assume that $V(C)$ does not have 1 as an eigenvalue. This is the case, for example, if B is densely defined (see *e.g* [2, Lemma 6.1.3]). Then it follows from [31, Proposition 6.1, Chapter 2], that 1 is not an eigenvalue of U so that $b^{-1}(U_C) =: A_C \in \mathrm{Ext}(B)$ and $U_C = b(A_C)$. Define

$$\Gamma_C(z) := \Gamma_{A_C}^i(z) = P_\mathcal{H}(A_C - i)(A_C - \overline{z})^{-1} J_+.$$

Now

$$\Gamma_C(i) = P_\mathcal{H}(A_C - i)(A_C + i)^{-1} J_+ = P_\mathcal{H} b(A_C) P_\mathcal{H} J_+ = V(C)J_+ = \hat{C}J_+,$$

since $b(A_C) = U_C$ is an extension of $V(C)$. It follows that

$$\Gamma_C(i)(I - C) = J_- C(I - C) = 0,$$

where $I \in \mathbb{C}^{n\times n}$ is the identity matrix. Now given any $z \in \mathbb{C}_+$,

$$\begin{aligned} \Gamma_C(z) &= P_\mathcal{H}(A_C - i)(A_C - \overline{z})^{-1} J_+ \\ &= P_\mathcal{H}(A_C + i)(A_C - \overline{z})^{-1}(A_C - i)(A_C - \overline{i})^{-1} P_\mathcal{H} J_+. && (6.4) \end{aligned}$$

Since both $z, i \in \mathbb{C}_+$, by dilation theory this is simply equal to

$$\Gamma_C(z) = P_\mathcal{H}(A_C + i)(A_C - \overline{z})^{-1} P_\mathcal{H} b(A_C) P_\mathcal{H} J_+ = P_\mathcal{H}(A_C + i)(A_C - \overline{z})^{-1} P_\mathcal{H} \Gamma_C(i),$$

so that $\Gamma_C(z)(I-C) = 0$ as before. To see this note that since $U_C = b(A_C)$ is a dilation of $V(C)$, that for any $n \in \mathbf{N} \cup \{0\}$,

$$P_{\mathcal{H}} b(A_C)^n P_{\mathcal{H}} = (P_{\mathcal{H}} b(A_C) P_{\mathcal{H}})^n$$

It follows that

$$P_{\mathcal{H}}(A_C + i)^{-n} P_{\mathcal{H}} = (P_{\mathcal{H}}(A_C+i)^{-1} P_{\mathcal{H}})^n.$$

Given any $z \in \mathbb{C}_-$ that lies in the open ball of radius 1 about $z = -i$ we have that $(A_C - z)^{-1}$ can be expressed as a power series in $(A_C + i)^{-1}$, and it follows from this that the resolvent formula:

$$\begin{aligned}(z-w)P_{\mathcal{H}}(A_C - z)^{-1}(A_C - w)^{-1}P_{\mathcal{H}} &= P_{\mathcal{H}}(A_C - w)^{-1}P_{\mathcal{H}} - P_{\mathcal{H}}(A-z)^{-1}P_{\mathcal{H}} \\ &= (z-w)P_{\mathcal{H}}(A-z)^{-1}P_{\mathcal{H}}(A-w)^{-1}P_{\mathcal{H}},\end{aligned}$$

holds for all $z, w \in \mathbb{C}_-$.

Hence $\Gamma(z)(I-C)$ is identically zero in $\mathbb{C}_+$ so that

$$m_+ = \max_{z \in \mathbb{C}_+} \mathrm{Ker}(\Gamma(z))^{\perp} = \dim(\mathrm{Ran}(C)).$$

Similarly using $\Gamma = \Gamma^{-i}_{A_C}$ instead, one can construct an example of Z_A with indices (n, n) where $n > m_-$.

6.4 Alternate formulas for the Livšic characteristic function

In this subsection we pause to compute an alternate formula for the Livšic characteristic function. This will be useful, in particular, for computing formulas for the reproducing kernel of $\mathcal{H}_\Gamma$ in the next subsection.

Suppose that $B \in \mathcal{S}_n(\mathcal{H})$ where $n < \infty$. As mentioned in the introduction the Livšic characteristic function of B is defined using isomorphisms $J_z : \mathbb{C}^n \to \mathrm{Ker}(B^* - z)$ such that $J_{\pm i}$ are onto isometries. If $A \in \mathrm{Ext}(B)$ is canonical we can define

$$J_z := \Gamma^i_A(\overline{z}) = (A-i)(A-z)^{-1}J_i,$$

where $J_i : \mathbb{C}^n \to \mathrm{Ker}(B^* - i)$ is a fixed onto isometry. As discussed in the introduction, one can define

$$A(z) := J^*_{-i}J_z \qquad B(z) := J^*_i J_z,$$

and then

$$\Theta_B(z) = b(z)B(z)^{-1}A(z).$$

Note however that

$$\begin{aligned}A(z) = J^*_{-i}J_z &= J^*_i(A+i)(A-i)^{-1}(A-i)(A-\overline{z})^{-1}J_i \\ &= J^*_i(A+i)(A-\overline{z})^{-1}J_i \\ &= \left((A-i)(A-z)^{-1}J_i\right)^* J_i = J^*_{\overline{z}}J_i = B(\overline{z})^*,\end{aligned} \tag{6.5}$$

so that $A(z) = B(\overline{z})^*$, $A(z) = J^*_{\overline{z}}J_i$ and $B(z) = J^*_{\overline{z}}J_{-i}$ for $z \in \mathbb{C} \setminus \mathbb{R}$.

6.5 Reproducing kernel formulas for $\mathcal{H}_\Gamma$

Let Γ be a generalized model for B of rank (m_+, m_-) where at least one of $m_\pm$ is equal to n. Then by Proposition 6.2 we have an onto isometry $U_\Gamma : \mathcal{H} \to \mathcal{H}_\Gamma$ such that

$$U_\Gamma B = Z_\Gamma U_\Gamma,$$

so that Z_Γ is unitarily equivalent to B.

For any $w \in \mathbb{C} \setminus \mathbb{R}$ let P_w be the projection onto $\mathrm{Ran}\,(B - w) = \mathrm{Ker}(B^* - \overline{w})^\perp$, and let $Q_w := U_\Gamma P_w U_\Gamma^*$, the projection onto $\mathrm{Ran}\,(Z_\Gamma - w)$. Now define

$$L_w := U_\Gamma b_{\overline{w}}(B) P_w U_\Gamma^* = b_{\overline{w}}(Z_\Gamma) Q_w,$$

the partial isometric extension of $b_{\overline{w}}(Z_\Gamma)$ to all of $\mathcal{H}_\Gamma$. Here we define

$$b_w(z) = \frac{z - w}{z - \overline{w}}.$$

It is clear that

$$L_w = Q_{\overline{w}} b_{\overline{w}}(Z_\Gamma) Q_w,$$

and that $L_w^* = L_{\overline{w}}$.

We can now calculate formulas for the reproducing kernel of $\mathcal{H}_\Gamma$, using the same procedure as in [4, Section 4]. Let $k_w(z) = k_w^\Gamma(z)$ denote the reproducing kernel of $\mathcal{H}_\Gamma$. Now given any $u, v \in \mathcal{J}$ and $\alpha \in \mathbb{C} \setminus \mathbb{R}$,

$$\begin{aligned}
\left\langle (L_\alpha^* k_w)(z)u, v \right\rangle &= \left\langle L_\alpha^* k_w u, k_z v \right\rangle \\
&= \langle k_w u, L_\alpha k_z v \rangle = \overline{\left\langle b_{\overline{\alpha}}(Z_\Gamma) Q_\alpha k_z v, k_w u \right\rangle} \\
&= \overline{b_{\overline{\alpha}}(w)} \left\langle k_w u, Q_\alpha k_z v \right\rangle \\
&= \frac{1}{\overline{b_\alpha(w)}} \left(\left\langle k_w(z)u, v \right\rangle - \left\langle \left((1 - Q_\alpha)k_w\right)(z)u, v \right\rangle \right). \qquad (6.6)
\end{aligned}$$

But also,

$$\begin{aligned}
\left\langle (L_\alpha^* k_w)(z)u, v \right\rangle &= \left\langle (L_{\overline{\alpha}} k_w)(z)u, v \right\rangle = b_\alpha(z) \left\langle Q_{\overline{\alpha}} k_w u, k_z v \right\rangle \\
&= b_\alpha(z) \left(\left\langle k_w(z)u, v \right\rangle - \left\langle \left((1 - Q_{\overline{\alpha}})k_w\right)(z)u, v \right\rangle \right). \qquad (6.7)
\end{aligned}$$

Solving for $\left\langle k_w(z)u, v \right\rangle$ and using that $u, v \in \mathcal{J}$ were arbitrary yields:

$$k_w^\Gamma(z) = \frac{\left((1 - Q_\alpha)k_w\right)(z) - b_\alpha(z)\overline{b_\alpha(w)} \left((1 - Q_{\overline{\alpha}})k_w\right)(z)}{1 - b_\alpha(z)\overline{b_\alpha(w)}}, \qquad (6.8)$$

for any $\alpha \in \mathbb{C} \setminus \mathbb{R}$.

Now suppose Γ is a rank (m_-, n) quasi-model for B and that Z_Γ is unitarily equivalent to B. This happens for example if $\Gamma = \Gamma_A$ for some $A \in \mathrm{Ext}(B)$ and Θ_B is inner. Also choose $\mathcal{J} := \mathbb{C}^n$, and $J : \mathbb{C}^n \to \mathrm{Ker}(B^* + i)$ to be an isometry, and $\alpha = i$ in equation (6.8).

Define

$$J_z := \Gamma_A(\overline{z}) : \mathbb{C}^n \to \mathrm{Ker}(B^* - z); \quad z \in \mathbb{C}_-.$$

Then $J_{-i} = J$ is an isometry and also choose $J_i : \mathbb{C}^n \to \mathrm{Ker}(B^* - i)$ to be a fixed isometry. Recall that $k_w = U_A \Gamma(w)$, and notice that $(1 - Q_{-i}) = U_A J_i J_i^* U_A^*$. It follows that

$$\left((1 - Q_{-i})k_w\right)(z) = J_{\overline{z}}^* J_i J_i^* J_{\overline{w}},$$

and similarly that

$$\left((1 - Q_i)k_w\right)(z) = J_{\overline{z}}^* J_{-i} J_{-i}^* J_{\overline{w}}.$$

It follows that our formula for the reproducing kernel in $\mathcal{H}_\Gamma$ can be written:

$$k_w^\Gamma(z) = \frac{J_{\overline{z}}^* J_{-i} J_{-i}^* J_{\overline{w}} - b(z)\overline{b(w)} J_{\overline{z}}^* J_i J_i^* J_{\overline{w}}}{1 - b(z)\overline{b(w)}}. \qquad (6.9)$$

Now in the case where both $z, w \in \Pi_\Gamma$ (in particular for Γ_A we have that Π_A^+ is dense in $\mathbb{C}_+$) we have that $J_{\overline{w}}$ and $J_{\overline{z}}$ are isomorphisms and it follows from Subsection 6.4 that $J_{\overline{z}}^* J_{-i} = B(z)$ and $J_{\overline{z}}^* J_i = A(z)$, where

$$\Theta_B(z) = b(z) B(z)^{-1} A(z).$$

Hence for any $z, w \in \Pi_\Gamma$,

$$k_w^\Gamma(z) = \frac{B(z)B(w)^* - b(z)A(z)A(w)^*\overline{b(w)}}{1 - b(z)\overline{b(w)}} \tag{6.10}$$

$$= B(z)\left(\frac{\mathbf{1} - \Theta_B(z)\Theta_B(w)^*}{1 - b(z)\overline{b(w)}}\right)B(w)^*. \tag{6.11}$$

Recall here that $\Pi_A^+ := \Pi_{\Gamma_A}^+$ is the set of all points $z \in \mathbb{C}_+$ such that $\dim\left(\mathrm{Ran}\left(\Gamma_A(z)\right)\right) = \dim\left(\mathrm{Ker}(\Gamma_A(z))^\perp\right)$ achieves its maximum value $m_+ = n$, and that by Lemma 5.10, Π_A^+ is dense in $\mathbb{C}_+$.

7 Cyclicity

The goal of this section is to show that the characteristic function Θ_B of B is inner implies that $\mathrm{Ker}(B^* - w)$ is cyclic for any $A \in \mathrm{Ext}(B)$ and $w \in \mathbb{C}\setminus\mathbb{R}$. This will enable us, in the subsequent section, to extend the isometry $U_A : \mathcal{H} \to \mathcal{H}_A$ to an isometry $V_A : \mathcal{K} \to \mathcal{K}_A$ where A is self-adjoint in $\mathcal{K}$, $\mathcal{K}_A \supset \mathcal{H}_A$ is a larger reproducing kernel Hilbert space on $\mathbb{C}\setminus\mathbb{R}$ containing $\mathcal{H}_A$, and $V_A|_{\mathcal{H}_A} = U_A$. This larger space $\mathcal{K}_A$ contains information about the extension $A \in \mathrm{Ext}(B)$ that will be key for our characterization of $\mathrm{Ext}(B)$.

Here we say that a subspace $S \subset \mathcal{K}$ is cyclic for $A \in \mathrm{Ext}(B)$ if A is self-adjoint with $\mathrm{Dom}(A) \subset \mathcal{K}$ and

$$\bigvee \mathrm{vN}(A)S = \mathcal{K},$$

where $\mathrm{vN}(A)$ is the von Neumann algebra generated by the unitary operator $b(A)$.

It will be convenient to apply some of the dilation theory for contractions as developed in [31]. We briefly review these tools below:

Given a contraction $T \in B(\mathcal{H})$, recall that the defect indices of T are defined to be the pair of positive integers $(\mathfrak{d}_T, \mathfrak{d}_{T^*})$ where

$$\mathfrak{d}_T := \dim\left(\overline{\mathrm{Ran}\left(\sqrt{1 - T^*T}\right)}\right).$$

Namely $\mathfrak{d}_T := \dim(\mathfrak{D}_T)$ where

$$\mathfrak{D}_T := \mathrm{Ran}\left(D_T = \sqrt{1 - T^*T}\right).$$

Given $B \in \mathcal{S}_1(\mathcal{H})$, we will be studying the partial isometry

$$V := b_w(B)Q_w$$

where Q_w is the projection onto $\mathrm{Ran}(B - \overline{w}) = \mathrm{Ker}(B^* - w)^\perp$ for some fixed $w \in \mathbb{C}\setminus\mathbb{R}$ and $b_w(B)$ is the w–Cayley transform of B,

$$b_w(z) = \frac{z - w}{z - \overline{w}}.$$

This is a partial isometry, and it is clear that the defect indices of V are equal to the deficiency indices of $b_w(B)$, namely (n, n). A contraction is called c.n.u. (completely non-unitary) if it has no non-trivial unitary restriction. It is clear that since B is simple, this implies that V is c.n.u. The model theory of Nagy-Foias [31] associates a contractive operator-valued function Θ_T called the Nagy-Foias characteristic function of T, to any c.n.u. contraction T. This function is defined by

$$\Theta_T(z) := (-T + zD_{T^*}(1 - zT^*)^{-1}D_T)|_{\mathfrak{D}_T}; \quad z \in \mathbf{D}.$$

In our case where $T = V$ is a partial isometry, this expression simplifies to:

$$\Theta_V(z) = zP_-(1 - zV^*)^{-1}P_+,$$

where P_+, P_- are the projectors onto $\mathfrak{D}_V = \mathrm{Ker}(B^* - w)$ and $\mathfrak{D}_{V^*} = \mathrm{Ker}(B^* - \overline{w})$ respectively, $P_+ = I - Q_w$, $P_- = I - Q_{\overline{w}}$. Since V is a partial isometry, in the case where $w = i$, the Nagy-Foias characteristic function Θ_V of $V = b_i(B)Q_w$ coincides with the Livšic characteristic function,

$$\theta_{b_i(B)} := \Theta_B \circ b_i^{-1},$$

of the isometric linear transformation $b_i(B)$, as shown for example in [2, Section 6]. Here recall that two operator-valued analytic functions Θ_1, Θ_2 on $\mathbf{D}$ are said to coincide if $\Theta_1(z) = U\Theta_2(z)V$ for fixed unitaries U, V, and for all $z \in \mathbf{D}$.

Now recall that any contraction T acting on $\mathcal{H}$ has a minimal unitary dilation U acting on some larger Hilbert space $\mathcal{K} \supset \mathcal{H}$. Recall that a unitary U on $\mathcal{K} \supset \mathcal{H}$ is called a unitary dilation of T if for any $n \in \mathbf{N} \cup \{0\}$ we have that

$$T^n = P_{\mathcal{H}} U^n|_{\mathcal{H}}.$$

Such a dilation is called minimal if $\mathcal{K}$ is the smallest reducing subspace for U containing $\mathcal{H}$, and the minimal unitary dilation of T is unique up to a unitary transformation that fixes the Hilbert space $\mathcal{H}$ [40, Theorem 4.3]. Since our contraction $V = b_w(B)Q_w$ is c.n.u. (because B is simple), it follows from [31, II.6.4], that the spectral measure of the minimal unitary dilation U of V is equivalent to Lebesgue measure. This just means that any of the positive Borel measures defined by $\sigma(\Omega) = \langle \chi_\Omega(U)f, f\rangle$, where $\Omega \subset \mathbf{T}$ is a Borel set and $f \in \mathcal{H}$ is fixed are equivalent (have the same sets of measure zero) to Lebesgue measure. Here χ_Ω denotes the characteristic function of the Borel set Ω, and $\chi_\Omega(U)$ is a projection by the functional calculus for normal operators. It follows that U has no eigenvalues so that $b_w^{-1}(U)$ is a densely defined non-canonical self-adjoint extension of B. Moreover the fact that U is minimal implies that $\mathcal{K} \ominus \mathcal{H}$ contains no non-trivial reducing subspace S for U (since otherwise $U|_{\mathcal{K}\ominus S}$ would be the minimal unitary dilation of V). Hence

$$b_w^{-1}(U) \in \mathrm{Ext}(B).$$

Now as in [31, II.2] set

$$\mathcal{L} := \overline{(U - V)\mathcal{H}} = \bigvee U\mathrm{Ker}(B^* - w),$$

and let

$$\mathcal{R}_\star := \mathcal{K} \ominus \left(\overline{\bigoplus_{n\in\mathbf{Z}} U^n \mathcal{L}} \right) = \mathcal{K} \ominus \left(\overline{\bigoplus_{n\in\mathbf{Z}} U^n \mathrm{Ker}(B^* - w)} \right).$$

Now by [31, Proposition 2.1 VI.2], the Nagy-Foias characteristic function Θ_V is inner (has unitary boundary values on $\mathbf{T}$ almost everywhere with respect to Lebesgue measure) if and only if both $V^k \to 0$ and $(V^*)^k \to 0$ in the strong operator topology. Note that if $n < \infty$ then since V has equal defect indices, if Θ_V has isometric boundary values almost everywhere then it is inner. Since Θ_V coincides with the Livšic characteristic function of $b_w(B)$ (this is a consequence of the fact that V is a partial isometry, as discussed above), we conclude that Θ_B is inner if and only if both $V^k \to 0$ strongly and $(V^*)^k \to 0$ strongly. That is, $V = b_w(B)Q_w$ is such that its Nagy-Foias characteristic function Θ_V is inner if and only if the Livsic characteristic function $\theta_{b_w(B)} = \Theta_B \circ b_w^{-1}$ is inner if and only if Θ_B, the Livšic characteristic function of B, is inner. In the terminology of [31], if Θ_B is inner so that $V^k \to 0$ and $(V^*)^k \to 0$ strongly, and V has defect indices (n, n), V is called a contraction of class $C_0(n)$.

By [31, II.3.1] the projection $P_\star$ onto $\mathcal{R}_\star$ can be calculated by the formula:

$$P_\star h = \lim_{n\to\infty} U^{-n} V^n h. \tag{7.1}$$

Note that $\mathrm{Ker}(B^* - w)$ is cyclic for $b_w^{-1}(U) \in \mathrm{Ext}(B)$ if and only if $P_\star = 0$.

Theorem 7.1. *Suppose $B \in \mathcal{S}_n(H)$, Q_w is the projection onto* $\mathrm{Ran}\,(B - \overline{w})$*, and $P_w = 1 - Q_w$ projects onto* $\mathrm{Ker}(B^* - w)$*. Let $V = b_w(B)Q_w$, U the minimal unitary dilation of V, and $A = b_w^{-1}(U) \in$* $\mathrm{Ext}(B)$*. Then for any $h \in \mathcal{H}$,*

$$(1 - P_\star)h = \sum_{j=0}^{\infty} U^{-j} P_w U^j h = \sum_{j=0}^{\infty} U^{-j} P_w V^j h. \tag{7.2}$$

Lemma 7.2. *Let $B \in \mathcal{S}_n(\mathcal{H})$, $A \in$* $\mathrm{Ext}(B)$*. For any $h \in \mathcal{H}$ and $k \in \mathbf{N}$, the following formula holds.*

$$h = \sum_{j=0}^{k} b_w^\dagger(A)^j P_w (b_w(B)Q_w)^j h + b_w^\dagger(A)^{k+1} (b_w(B)Q_w)^{k+1} h. \tag{7.3}$$

In the above recall that $b_w(z) := \frac{z-w}{z-\overline{w}}$ and $b_w^\dagger(z) = \overline{b_w(\overline{z})} = \frac{z-\overline{w}}{z-w} = b_{\overline{w}}(z)$.

Proof. This clearly holds if $h \in \mathrm{Ran}\,(B-\overline{w})^\perp$. If $h \perp \mathrm{Ker}(B^* - w)$ then

$$h = Q_w h = b_w^\dagger(B) h_1,$$

for some $h_1 \in \mathrm{Ran}\,(B-w) = \mathrm{Dom}(b_w^\dagger(B))$. Now

$$h_1 = Q_w h_1 + P_w h_1,$$

and if we define $h_2 := Q_w h_1$ then $h_2 = b_w^\dagger(B) h_3$ for some $h_3 \in \mathrm{Ran}\,(B-w)$. Now

$$h_3 = b_w(B) h_2 = b_w(B) Q_w h_1 = b_w(B) Q_w b_w(B) Q_w h = (b_w(B) Q_w)^2 h,$$

and

$$\begin{aligned} h &= b_w^\dagger(B) h_1 = b_w^\dagger(B)(P_w h_1 + h_2) && (7.4)\\ &= b_w^\dagger(B)(P_w h_1 + b_w^\dagger(B) h_3) && (7.5)\\ &= b_w^\dagger(A)(P_w h_1 + b_w^\dagger(A) h_3) && (7.6)\\ &= b_w^\dagger(A) P_w b_w(B) Q_w h + b_w^\dagger(A)^2 (b_w(B) Q_w)^2 h. && (7.7) \end{aligned}$$

Repeating this process again yields $h_4 := Q_w h_3 =: b_w^\dagger(B) h_5$ and

$$\begin{aligned} h &= b_w^\dagger(B)(P_w h_1 + h_2)\\ &= b_w^\dagger(A)\left(P_w(b_w(B)Q_w)h + b_w^\dagger(A)(h_4 + P_w h_3)\right)\\ &= b_w^\dagger(A) P_w (b_w(B)Q_w) h + b_w^\dagger(A)^2 P_w (b_w(B)Q_w)^2 h + b_w^\dagger(A)^3 (b_w(B)Q_w)^3 h. \end{aligned}$$

The pattern is now apparent. Repeating this process k times yields $h_{2k+1} = (b_w(B)Q_w)^{k+1}$ and one obtains the formula stated above, namely,

$$h = \sum_{j=0}^{k} b_w^\dagger(A)^j P_w (b_w(B)Q_w)^j h + b_w^\dagger(A)^{k+1} (b_w(B)Q_w)^{k+1} h.$$

□

Proof. (Theorem 7.1) In the case where $A = b_w^{-1}(U)$ where U is the minimal unitary dilation of $V = b_w(B)Q_w$, the formula (7.3) becomes:

$$\begin{aligned} h &= \sum_{j=0}^{k} U^{-j} P_w V^j h + U^{-(k+1)} V^{k+1} h\\ &= \sum_{j=0}^{k} U^{-j} P_w U^j h + U^{-(k+1)} V^{k+1} h && (7.8) \end{aligned}$$

Now we use the formula (7.1) of Nagy-Foias to conclude that if $A = b_w^{-1}(U)$ where U is the minimal unitary dilation of V, that $U^{-(k+1)} V^{k+1} h \to P_\star h$, proving the formula (7.2) and the theorem. □

Corollary 7.3. *Suppose that $B \in \mathcal{S}_n(\mathcal{H})$. Then* $\mathrm{Ker}(B^* - w)$ *and* $\mathrm{Ker}(B^* - \overline{w})$ *are cyclic for every $A \in \mathrm{Ext}(B)$ if and only if Θ_B is inner. If Θ_B is inner then the formulas*

$$h = \sum_{j=0}^{\infty} b_w^\dagger(A)^j P_w (b_w(B)Q_w)^j h, \qquad (7.9)$$

hold for any $A \in \mathrm{Ext}(B)$ and $h \in \mathcal{H}$.

Remark 7.4. Let $\{w_j\}$ be some fixed orthonormal basis of $\mathrm{Ker}(B^* - w)$, and let $J_w : \mathbb{C}^n \to \mathrm{Ker}(B^* - w)$ be defined by $J_w e_k = w_k$, where $\{e_k\}$ is an orthonormal basis of $\mathbb{C}^n$. Consider L^2_Σ where Σ is the $\mathbb{C}^{n\times n}$ matrix-valued positive Borel measure defined by $\Sigma(\Omega) = J_w^* P_w P_A(\Omega) P_w J_w$, $P_A(\Omega) := \chi_\Omega(A)$, where χ_Ω is the characteristic function of the Borel set Ω. The above corollary shows in particular that for any fixed $h \in \mathcal{H}$ there is a vector function $\mathbf{f} = (f_1, ..., f_n) \in L^2_\Sigma$ such that

$$h = f_1(A)w_1 + f_2(A)w_2 + ... + f_n(A)w_n,$$

and that, remarkably, this equation holds independently of the choice of $A \in \mathrm{Ext}(B)$, *i.e.* the same $\mathbf{f}$ works for all $A \in \mathrm{Ext}(B)$ when h is held fixed. Although we will not pursue this in this paper, this fact can be used to provide a new proof, and a generalization of the Alexandrov isometric measure theorem, [41, Theorem 2].

Proof. By Lemma 7.2, given any $A \in \mathrm{Ext}(B)$ and $h \in \mathcal{H}$,

$$h = \sum_{j=0}^{k} b_w^\dagger(A)^j P_w (b_w(B)Q_w)^j h + b_w^\dagger(A)^{k+1}(b_w(B)Q_w)^{k+1} h.$$

Hence to prove the formula (7.9), it suffices to show that $\|(b_w(B)Q_w)^k h\| = \|b_w^\dagger(A)^k (b_w(B)Q_w)^k) h\| \to 0$.

If Θ_B is inner then $V^n \to 0$ strongly (where recall $V = b_w(B)Q_w$) so that

$$0 = \lim_{n\to\infty} \|V^n h\|,$$

and so the formula (7.9) holds. If $A = b_w^{-1}(U)$, then the fact that $\mathrm{Ker}(B^* - w)$ is cyclic for A follows from the fact that $\mathcal{R}_\star = \{0\}$. For arbitrary $A \in \mathrm{Ext}(B)$, the formula (7.9) shows that the cyclic subspace S_w for any fixed $A \in \mathrm{Ext}(B)$ generated by $\mathrm{Ker}(B^* - w)$ contains $\mathcal{H}$. Hence if A is self-adjoint in $\mathcal{K}$, then $S_w = \mathcal{K}$, as otherwise $\mathcal{K} \ominus S_w$ would be a non-trivial subspace of $\mathcal{K} \ominus \mathcal{H}$ which is reducing for A (this contradicts one of our assumptions on $\mathrm{Ext}(B)$). This proves that $\mathrm{Ker}(B^* - w)$ is cyclic for any $A \in \mathrm{Ext}(B)$.

Conversely if $\mathrm{Ker}(B^* - w)$ is cyclic for any $A \in \mathrm{Ext}(B)$, then it is cyclic for $b_w^{-1}(U)$ where U is the minimal unitary dilation of $V = b_w(B)Q_w$, and it follows from the definition of $R_\star$ that $P_\star = 0$, and hence $T^n \to 0$ strongly. If $n < \infty$ this implies T is a contraction of class $C_0(n)$, implying that the characteristic function Θ_B of B is inner as discussed previously. If $n = \infty$ our assumption that $\mathrm{Ker}(B^* - \overline{w})$ is cyclic also implies that $(T^*)^k \to 0$ strongly. This, together with the fact that T^k converges strongly to 0 implies that Θ_B is inner. □

Note that the above proof also shows:

Corollary 7.5. *If* $B \in \mathcal{S}_n(\mathcal{H})$, $n < \infty$, *and there is a* $w \in \mathbb{C}\backslash\mathbb{R}$ *such that* $\mathrm{Ker}(B^* - w)$ *is cyclic for every* $A \in \mathrm{Ext}(B)$, *then* Θ_B *is inner.*

8 A larger reproducing kernel Hilbert space $\mathcal{K}_A \supset \mathcal{H}_A$

Definition 8.1. Given any $A \in \mathrm{Ext}(B)$ and $z \in \mathbb{C} \setminus R$, let

$$\Omega_A(z) := U_{-i,z} J, \tag{8.1}$$

where recall that provided $A = b^{-1}(U)$ and U does not have 1 as an eigenvalue then

$$U_{-i,z} J = (A + i)(A - \overline{z})^{-1} J,$$

where recall that $J = J_{-i} = P_{-i} J_{-i}$ and $J : \mathbb{C}^n \to \mathrm{Ker}(B^* + i)$. In the exceptional case where $A \in \mathrm{Ext}(B)$ is defined using a unitary extension U of $b(B)$ and $1 \in \sigma_p(U)$, recall that $U_{w,z}$ is given by formula (5.2). We will assume in this section that J is an isometry. Note that

$$\Gamma_A(z) = P_{\mathcal{H}} \Omega_A(z). \tag{8.2}$$

We define a new reproducing kernel Hilbert space K_A as the abstract $\mathbb{C}^n$-valued reproducing kernel Hilbert space on $\mathbb{C} \setminus \mathbb{R}$ with reproducing kernel

$$K_w(z) := \Omega(z)^* \Omega(w).$$

In the above and in what follows we will often simply write Ω for Ω_A, Γ for Γ_A and $k_w(z)$, $K_w(z)$ for the reproducing kernels of $\mathcal{H}_A$ and $\mathcal{K}_A$, respectively. The existence of $\mathcal{K}_A$ follows from the fact that $K_w(z)$ is a positive kernel function, and the abstract theory of reproducing kernel Hilbert spaces [42, Theorem 10.11].

Observe that the difference

$$K_w(z) - k_w(z) = \Omega(z)^* (\mathbf{1} - P_{\mathcal{H}}) \Omega(w),$$

is a positive kernel function. The theory of reproducing kernel Hilbert spaces then implies that $\mathcal{H}_A$ is contractively contained in $\mathcal{K}_A$ [42, Theorem 10.20]. In other words the embedding $E_A : \mathcal{H}_A \to \mathcal{K}_A$ defined by $Eh = h$ for all $h \in \mathcal{H}_A$ is a contraction, $\|h\|_{\mathcal{K}_A} \leq \|h\|_{\mathcal{H}_A}$.

Definition 8.2. Suppose that Θ_B is inner. Given $A \in \text{Ext}(B)$ self-adjoint in $\mathcal{K} \supset \mathcal{H}$, recall that we define $U_A : \mathcal{H} \to \mathcal{H}_A$ by

$$U_A(f)(z) = \hat{f}(z) = \Gamma(z)^* f.$$

Now define a linear map $V_A : \mathcal{K} \to \mathcal{K}_A$ by

$$(V_A f)(z) = \Omega_A(z)^* f,$$

for $f \in \mathcal{K}$.

Note that if $g \in \mathcal{H}$ that

$$(V_A g)(z) = J^* (A - z)^{-1} (A - i) g = \Gamma^*(z) g = (U_A g)(z),$$

so that for any $g \in \mathcal{H}$,

$$U_A g(z) = V_A g(z).$$

Hence if $E_A : \mathcal{H}_A \to \mathcal{K}_A$ is the contractive embedding then

$$V_A P_{\mathcal{H}} = E_A U_A. \tag{8.3}$$

For $\mathbf{v} \in \mathbb{C}^n$ the function $K_w \mathbf{v}$ defined by

$$K_w \mathbf{v}(z) := K_w(z) \mathbf{v},$$

is a point evaluation vector in $\mathcal{K}_A$, *i.e.*

$$\langle h, K_w \mathbf{v} \rangle_{\mathcal{K}_A} = \big(h(w), \mathbf{v} \big)_{\mathbb{C}^n},$$

for any $h \in \mathcal{K}_A$. Also observe that if $\mathbf{u} \in \mathbb{C}^n$, then

$$K_w \mathbf{u} = V_A \Omega(w) \mathbf{u},$$

is the $\mathbf{u}$ point-evaluation vector in $\mathcal{K}_A$ at w.

Proposition 8.3. *The linear map $V_A : \mathcal{K} \to \mathcal{K}_A$ is an isometry of $\mathcal{K}$ onto $\mathcal{K}_A$. Hence if $h \in \mathcal{H}$, then*

$$\|V_A h\|_{\mathcal{K}_A} = \|h\| = \|U_A h\|_{\mathcal{H}_A},$$

so that $\mathcal{H}_A \subset \mathcal{K}_A$ isometrically and $U_A = V_A|_{\mathcal{H}}$.

Proof. Recall that since we assume that B is such that Θ_B is inner, Corollary 7.3 implies that $\text{Ker}(B^* + i)$ is cyclic for A.

Since $\mathrm{Ker}(B^* + i)$ is cyclic, $\mathcal{K}$ is spanned by linear combinations of vectors of the form $\Omega(w)J\mathbf{v}$ for $w \in \mathbb{C}\setminus\mathbb{R}$ and $\mathbf{v} \in \mathbb{C}^n$. In particular for any $\mathbf{v} \in \mathbb{C}^n$, the vector $V_A\Omega(w)\mathbf{v} \in \mathcal{K}_A$ since

$$(V_A\Omega(w)\mathbf{v})(z) := (\Omega(z)^*\Omega(w))\mathbf{v} = K_w(z)\mathbf{v},$$

and $K_w\mathbf{v} \in \mathcal{K}_A$. The set of all point evaluation vectors $K_w\mathbf{v}$, $K_w\mathbf{v}(z) := K_w(z)\mathbf{v}$ for $w \in \mathbb{C} \setminus \mathbb{R}$ are by definition dense in $\mathcal{K}_A$ so that this also proves V_A is onto $\mathcal{K}_A$.

To see that V_A is an isometry use that vectors of the form $f = \sum_j c_j\Omega(w_j)\mathbf{v}_j$, for $\mathbf{v}_j \in \mathbb{C}^n$ and $w_j \in \mathbb{C}$ are dense in $\mathcal{K}$, so that

$$\begin{aligned} \langle f, f\rangle &= \sum_{ij} c_i\overline{c_j}\left\langle \Omega(w_i)\mathbf{v}_i, \Omega(w_j)\mathbf{v}_j\right\rangle_{\mathcal{K}} && (8.4)\\ &= \sum_{ij} c_i\overline{c_j}\left(K_{w_i}(w_j)\mathbf{v}_i, \mathbf{v}_j\right)_{\mathbb{C}^n} && (8.5)\\ &= \sum_{ij} c_i\overline{c_j}\left\langle K_{w_i}\mathbf{v}_i, K_{w_j}\mathbf{v}_j\right\rangle_{\mathcal{K}_A} && (8.6)\\ &= \langle V_Af, V_Af\rangle_{\mathcal{K}_A}. && (8.7)\end{aligned}$$

Now if $h \in \mathcal{H}$, then

$$\|E_AU_Ah\|_{\mathcal{K}_A} = \|V_Ah\|_{\mathcal{K}_A} = \|h\|_{\mathcal{H}} = \|U_Ah\|_{\mathcal{H}_A}.$$

Hence the contractive embedding $E_A : \mathcal{H}_A \to \mathcal{K}_A$ is actually an isometric inclusion, and $\mathcal{H}_A \subset \mathcal{K}_A$ as a Hilbert subspace.

□

8.4 Cauchy transforms and characteristic functions for $A \in \mathrm{Ext}(B)$

For any $A \in \mathrm{Ext}(B)$, let $U := b(A)$ be the corresponding unitary extension of $V := b(B)$, and define σ_U as the $\mathbb{C}^{n\times n}$ matrix-valued measure on the unit circle $\mathbf{T}$ given by

$$\sigma_U(\Omega) = \pi J^* P_U(\Omega)J,$$

where $P_U(\Omega) := \chi_\Omega(U)$ is the projection-valued measure of U defined using the functional calculus and recall that $J : \mathbb{C}^n \to \mathrm{Ker}(B^* + i) = \mathrm{Ker}(V)$ is a fixed isometry. We also define the $\mathbb{C}^{n\times n}$ positive matrix-valued measure on $\mathbb{R}$, Σ_A by

$$\Sigma_A(\Omega) := \int_\Omega \pi(1+t^2)J^*P_A(dt)J,$$

and note that if $\sigma_A(\Omega) := J^*P_A(\Omega)J$, then $\sigma_A = \sigma_U \circ b$, where $b(z) = \frac{z-i}{z+i}$ as before.

Definition 8.5. If $A \in \mathrm{Ext}(B)$ with $A = b^{-1}(U)$, let $\Phi[A; B]$ be the contractive analytic function on $\mathbb{C}_+$ corresponding to the pair $(\sigma_U(\{1\}), \Sigma_A)$ as described in Section 4. When there is no chance of confusion we will suppress dependence on B and use the simplified notation Φ_A for $\Phi[A; B]$. We call $\Phi[A; B]$ the characteristic function of the self-adjoint extension A relative to the symmetric linear transformation B, or simply the characteristic function of A when it is clear which B is used in the definition of $\Phi[A; B]$. If $V \in \mathcal{V}_n(\mathcal{H})$ and $U \in \mathrm{Ext}(V)$, the characteristic function $\phi[U; V]$ of the unitary extension U relative to the partial isometry V is defined analogously.

In more detail, if $\phi := \phi[U; V]$, then

$$\mathrm{Re}\left(g_\phi(z)\right) = \int_{\mathbf{T}} \mathrm{Re}\left(\frac{\alpha+z}{\alpha-z}\right)\sigma_U(d\alpha),$$

where

$$\phi = \frac{g_\phi - \mathbf{1}}{g_\phi + \mathbf{1}}$$

Equivalently if we impose the normalization condition discussed in Section 4 $(\mathrm{Im}\left(g_\phi(0)\right) = 0)$,

$$g_\phi(z) = \int_{\mathbf{T}} \frac{\alpha + z}{\alpha - z} \sigma_U(d\alpha).$$

By the relationship between Herglotz functions on the disk and upper half-plane, as discussed in Section 4, we have that

$$\mathrm{Re}\left(G_{\Phi_A}(z)\right) = \sigma_U(\{1\})\mathrm{Im}\,(z) + \int_{-\infty}^{\infty} \mathrm{Re}\left(\frac{1}{i\pi}\frac{1}{t-z}\right) \Sigma_A(dt),$$

or equivalently

$$\begin{aligned} G_{\Phi_A}(z) &= -iz\sigma_U(\{1\}) + \frac{i}{\pi}\int_{-\infty}^{\infty} \frac{tz+1}{t-z}\frac{1}{1+t^2}\Sigma_A(dt) \\ &= -iz\sigma_U(\{1\}) + \int_{-\infty}^{\infty} \frac{tz+1}{i(t-z)}(\sigma_U \circ b)(dt) \\ &= -iz\sigma_U(\{1\}) + \int_{-\infty}^{\infty} \frac{tz+1}{i(t-z)} J^* P_A(dt) J, \\ &= -iJ^*\left(zP_{b(A)}(\{1\}) + (Az+1)(A-z)^{-1}\right)J. \end{aligned} \tag{8.8}$$

In particular if U does not have 1 as an eigenvalue, then Φ_A is uniquely determined by Σ_A. Note that since U is unitary, the projection-valued measure P_U is unital which implies that σ_U is a unital probability measure so that $g_\phi(0) = \mathbf{1}$, and this in turn implies that $\phi(0) = 0$, and that

$$\Phi[A; B](i) = 0,$$

for any $A \in \mathrm{Ext}(B)$.

Theorem 8.6. *If $\widetilde{\Phi}_A$ is the contractive analytic function with Herglotz function πG_{Φ_A}, then $\mathcal{K}_A = \mathcal{L}(\widetilde{\Phi}_A)$.*

In particular if $U = b(A)$ does not have 1 as an eigenvalue then $\mathcal{K}_A$ is the space of Cauchy transforms of the positive operator-valued measure $\pi\Sigma_A$.

Proof. Let $\widetilde{\Phi} := \widetilde{\Phi}_A$. It suffices to show that $K_w(z) = K_w^{\widetilde{\Phi}}(z)$ where $K_w(z) = \Omega(z)^*\Omega(w)$ is the reproducing kernel for $\mathcal{K}_A$. First

$$K_w(z) = \Omega(z)^*\Omega(w) = J^* U_{-i,z}^* U_{-i,w} J,$$

where $U_{-i,z}$ is given by equation (5.2) so that

$$\begin{aligned} K_w(z) &= 4J^*\left((i+z)U + (i-z)\right)^{-1}\left((\overline{w}-i)U^* - (\overline{w}+i)\right)^{-1} J \\ &= \frac{4\sigma_U(\{1\})}{\left((i+z)+(i-z)\right)\left((\overline{w}-i)-(\overline{w}+i)\right)} + \frac{4}{\pi}\int_{\mathbf{T}\setminus\{1\}} \frac{1}{(i+z)\alpha + (i-z)}\frac{1}{(\overline{w}-i)\overline{\alpha} - (\overline{w}+i)}\sigma_U(d\alpha) \\ &= \sigma_U(\{1\}) + \frac{1}{\pi^2}\int_{-\infty}^{\infty} \frac{1}{(t-z)(t-\overline{w})}\pi\Sigma_A(dt) \\ &= K_w^{\widetilde{\Phi}}(z), \end{aligned}$$

where the last equality follows from equation (4.5) and the definition of $\widetilde{\Phi}_A$. ◻

Now let us compute the Livšic characteristic function of the operator $\mathfrak{Z} := \mathfrak{Z}_{\widetilde{\Phi}_A} \in \mathcal{S}_n(\mathcal{L}(\widetilde{\Phi}_A))$ which acts as multiplication by the independent variable in $\mathcal{L}(\widetilde{\Phi}_A) = \mathcal{K}_A$.

Recall that $A \in \mathrm{Ext}(B)$ is self-adjoint in $\mathcal{K} \supset \mathcal{H}$ where $B \in \mathcal{S}_n(\mathcal{H})$. Note that $K_i(i) = I = K_{-i}(-i)$ so that if we define $j_z : \mathbb{C}^n \to \mathcal{K}_A = \mathcal{L}(\widetilde{\Phi}_A)$ by

$$j_z\mathbf{c} = V_A\Omega_A(\overline{z})\mathbf{c} = K_z\mathbf{c},$$

then $j_{\pm i}$ are isometries and if

$$C(z) := j_{-i}^\star j_z; \qquad D(z) = j_i^\star j_z$$

then

$$\widetilde{\Phi}_A(z) = b(z)D(z)^{-1}C(z),$$

is the Livšic characteristic function of $\mathfrak{Z} = \mathfrak{Z}_{\widetilde{\Phi}_A}$.

Note that if $M^A := M^{\pi\Sigma_A}$ is the self-adjoint operator of multiplication by the independent variable in $L^2_{\pi\Sigma_A}(\mathbb{R})$, and $W : L^2_{\pi\Sigma_A} \to \mathcal{K}_A = \mathcal{L}(\widetilde{\Phi}_A)$ is the deBranges Cauchy transform isometry as described in Subsection 4.11, then $\mathfrak{Z}^A := WM^AW^\star$ is a canonical self-adjoint extension of the symmetric linear transformation $\mathfrak{Z} = \mathfrak{Z}_{\widetilde{\Phi}_A}$. It follows that $j_z = \Gamma(\overline{z})$ where $\Gamma = \Gamma^i_{\mathfrak{Z}^A}$ is a canonical model for $\mathfrak{Z}$.

Also note that by Section 6.4 we have that if

$$\widetilde{C}(z) = j_{\overline{z}}^\star j_i = K_{-i}(z), \qquad \widetilde{D}(z) = j_{\overline{z}}^\star j_{-i} = K_i(z),$$

then $\widetilde{C}(z) = C(z)$ and $\widetilde{D}(z) = D(z)$.

It follows that if we define

$$\widetilde{\Lambda}_A(z) = b(z)K_i(z)^{-1}K_{-i}(z) \qquad \text{and} \qquad \Lambda_A(z) = b(z)K_{\overline{z}}(-i)^{-1}K_{\overline{z}}(i), \tag{8.9}$$

then $\widetilde{\Lambda}_A = \Lambda_A$. This is verified directly in the lemma below.

Lemma 8.7. *The contractive analytic functions Λ_A and $\widetilde{\Lambda}_A$ are both equal to $\Phi_A = \Phi[B; A]$.*

Proof. Since Λ_A is the characteristic function of $\mathfrak{Z}_{\widetilde{\Phi}_A}$, and since $K_w^{\widetilde{\Phi}_A}(z) = \pi K_w^{\Phi_A}(z)$, it follows that

$$\Lambda_A(z) = b(z)K_{\overline{z}}^{\Phi_A}(-i)^{-1}K_{\overline{z}}^{\Phi_A}(i).$$

This shows that Λ_A is the Livšic characteristic function of $\mathfrak{Z}_{\Phi_A}$, and Lemma 4.4 of Section 4 implies that Λ_A is the Frostman shift of Φ_A which vanishes at i. However since $\Phi_A(i) = 0$, this Frostman shift is just equal to Φ_A and $\Phi_A = \Lambda_A$.

Now, $\widetilde{\Lambda}_A(z) = b(z)K_i(z)^{-1}K_{-i}(z)$. Using that $G_A(\overline{z})^\star = -G_A(z)$, one can calculate that

$$\begin{aligned} b(z)K_i(z)^{-1}K_{-i}(z) &= (G_A(z) + G_A(i)^\star)^{-1}(G_A(z) - G_A(i)) \\ &= b(z)K_{\overline{z}}(-i)^{-1}K_{\overline{z}}(i) = \Lambda_A(z). \end{aligned}$$

This shows that $\widetilde{\Lambda}_A(z) = \Lambda_A(z)$. □

Theorem 8.8. *Given any $A \in \mathrm{Ext}(B)$, we have that $\Phi_A \geq \Theta_B$, i.e. $\Theta_B(z)^{-1}\Phi_A(z)$ is a contractive analytic function in $\mathbb{C}_+$.*

Proof. Consider again the symmetric linear transformation $\mathfrak{Z}$ which acts as multiplication by z in $\mathcal{L}(\widetilde{\Phi}_A) = \mathcal{K}_A$, where $\widetilde{\Phi}$ is the contractive analytic function corresponding to the measure $\pi\Sigma_A$. We can construct a canonical model for $\mathfrak{Z}$ by choosing $\mathcal{J} := \mathbb{C}^n$ with orthonormal basis $\{e_j\}$ and defining

$$\Gamma(z)\mathbf{c} := K_z\mathbf{c},$$

for $\mathbf{c} \in \mathbb{C}^n$ where $K_z(w)$ is the reproducing kernel for $\mathcal{K}_A$. If we do this we find that the abstract model space $(\mathcal{K}_A)_\Gamma$ is simply equal to $\mathcal{K}_A$ and that U_Γ is just the identity on $\mathcal{K}_A$. Hence it follows from Section 6.5, and in fact from [4], that we can express the reproducing kernel for $\mathcal{K}_A$ as

$$K_z(z) = \frac{K_i(z)K_i(i)^{-1}K_i(z)^\star - |b(z)|^2 K_{-i}(z)K_{-i}(-i)^{-1}K_{-i}(z)^\star}{1 - |b(z)|^2}.$$

We can write this as

$$(1 - |b(z)|^2)K_z(z) = \widetilde{D}(z)\widetilde{D}(z)^* - |b(z)|^2\widetilde{C}(z)\widetilde{C}(z)^*,$$

where $\Phi_A(z) = \Lambda_A(z) = \widetilde{\Lambda}_A(z) = b(z)\widetilde{D}(z)^{-1}\widetilde{C}(z)$, and $\widetilde{D}(z) = K_i(z)$, $\widetilde{C}(z) = K_{-i}(z)$ as before.

Also note that if $k_w(z)$ is the reproducing kernel for $\mathcal{H}_A$, then for any $z \in \Pi_A^+$ (which is dense in $\mathbb{C}_+$) we can write

$$(1 - |b(z)|^2)k_z(z) = B(z)B(z)^* - |b(z)|^2A(z)A(z)^*,$$

where $\Theta_B(z) = b(z)B(z)^{-1}A(z)$ and $B(z) = k_i(z) = \Gamma_A(z)^*\Gamma_A(i) = \Gamma_A(z)^*J = \Omega_A(z)^*\Omega_A(i) = K_i(z)$. Hence $B(z) = \widetilde{D}(z)$.

Now since $A \in \mathrm{Ext}(B)$, $\mathcal{H}_A$ is isometrically contained in $\mathcal{K}_A$ so that $K_z(z) - k_z(z) \geq 0$. Hence we have that

$$\widetilde{D}(z)\widetilde{D}(z)^* - |b(z)|^2\widetilde{C}(z)\widetilde{C}(z)^* \geq \widetilde{D}(z)\widetilde{D}(z)^* - |b(z)|^2A(z)A(z)^*. \tag{8.10}$$

so that

$$A(z)A(z)^* \geq \widetilde{C}(z)\widetilde{C}(z)^*,$$

and hence (using that $B(z) = \widetilde{D}(z)$)

$$B^{-1}(z)A(z)A(z)^*B^{-1}(z)^* \geq \widetilde{D}(z)^{-1}\widetilde{C}(z)\widetilde{C}(z)^*(\widetilde{D}(z)^*)^{-1}.$$

Since $\widetilde{\Lambda}_A(z) = \Lambda_A(z) = \Phi_A(z)$, this shows that

$$\Theta_B(z)\Theta_B(z)^* \geq \Phi_A(z)\Phi_A(z)^*, \tag{8.11}$$

proving the theorem.

□

Example 8.9. Consider the finite dimensional partial isometry V:

$$V := \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

Clearly $V \in \mathcal{V}_1(\mathbb{C}^2)$.

Now let

$$U := \begin{pmatrix} 0 & 3/5 & 4/5 \\ 1 & 0 & 0 \\ 0 & 4/5 & -3/5 \end{pmatrix}.$$

This is a unitary matrix acting on $\mathbb{C}^3$, and $U|_{\mathrm{Ker}(V)^\perp} = V|_{\mathrm{Ker}(V)^\perp}$ so that $V \subseteq U$ and so if $B := b^{-1}(B) \in \mathcal{S}_1(\mathbb{C}^2)$ then we have that $A := b^{-1}(U) \in \mathrm{Ext}(B)$. (It is easy to check that the smallest reducing subspace for U containing $\mathcal{H} = E\mathbb{C}^2$ is all of $\mathbb{C}^3$. Here E denotes the canonical isometry from $\mathbb{C}^2$ into $\mathbb{C}^3$).

Our goal is to calculate Φ_A and to verify that $\Phi_A \geq \Theta_B$.

First we calculate Θ_B, the characteristic function of $B = b^{-1}(V) = i(1 + V)(1 - V)^{-1}$. We will denote the standard bases of $\mathbb{C}^n$ by $\{e_k\}$. Now

$$\mathrm{Ker}(B^* - i) = \mathrm{Ker}(V) = \bigvee\{e_2\} \quad \text{and} \quad \mathrm{Ker}(B^* + i) = \mathrm{Ran}\,(V)^\perp = \bigvee\{e_1\}.$$

To calculate the Livšic characteristic function we also need to determine $\mathrm{Ker}(B^* - z)$. First we calculate $\mathrm{Ran}\,(B - z)$:

$$\mathrm{Ran}\,(B - z) = i(1 + V)\mathrm{Ker}(V)^\perp - z(1 - V)\mathrm{Ker}(V)^\perp = \big((i - z) + (i + z)V\big)\,\mathrm{Ker}(V)^\perp.$$

Since $\mathrm{Ker}(V)^\perp$ is spanned by e_1 and $Ve_1 = e_2$, we get that $\mathrm{Ran}\,(B - z)$ is spanned by

$$\big((i - z), (i + z)\big)^T,$$

(T denotes transpose). It follows that if $(c, d)^T \in \mathrm{Ker}(B^* - \overline{z})$, that

$$(\overline{c}, \overline{d}) \cdot (i - z, i + z) = 0,$$

and this shows that $\mathrm{Ker}(B^* - z)$ is spanned by

$$w(z) := (z - i, z + i)^T.$$

Finally

$$\Theta_B(z) = b(z)\frac{(w(z), e_1)}{(w(z), e_2)} = \left(\frac{z-i}{z+i}\right)^2.$$

To calculate Φ_A, we first need to calculate the projection-valued measure of U. We begin by calculating the eigenvalues and eigenvectors of U: We have

$$\det(\lambda - U) = \lambda^3 + 3/5\lambda^2 - 3/5\lambda - 1 = (\lambda - \lambda_1)(\lambda - \lambda_2)(\lambda - \lambda_3),$$

where $\lambda_1 = 1$, $\lambda_2 := -4/5 + i3/5 =: \beta$ and $\lambda_3 = \overline{\lambda_2} = \overline{\beta}$. A normalized eigenvector for $\lambda_1 = 1$ is:

$$\hat{b}_1 := (2/3, 2/3, 1/3)^T,$$

and (non-normalized) eigenvectors for $\beta, \overline{\beta}$ are:

$$\mathbf{b}_2 = (1, \beta, 5/4(\beta^2 - 3/5)\beta)^T,$$

and

$$\mathbf{b}_3 = (1, \overline{\beta}, 5/4(\overline{\beta}^2 - 3/5)\overline{\beta})^T.$$

It follows that the projection-valued measure of U is given by

$$P_U = \sum_{i=1}^{3} \left(\cdot, \hat{b}_i\right) \hat{b}_i \delta_{\lambda_i},$$

where the δ_{λ_i} are Dirac point measures of weight one at the points λ_i, and the $\hat{b}_i$ are normalized eigenvectors to the eigenvalues λ_i. Now the scalar measure σ_U which determines ϕ_U, where $\Phi_A = \phi_U \circ b$, is given by

$$\sigma_U(\Omega) = \left\langle v, P_U(\Omega)v \right\rangle,$$

where $v = e_1$ is a unit vector spanning $\mathrm{Ran}\,(V)^\perp = \mathrm{Ker}(B^* + i)$. Hence

$$\sigma_U(\Omega) = \sum_{k=1}^{3} |\left(e_1, \hat{b}_k\right)|^2 \delta_{\lambda_k}.$$

Now $\left(e_1, \hat{b}_1\right) = 2/3$, and since $\mathbf{b}_2 = C\mathbf{b_3}$ is the component-wise complex conjugate of $\mathbf{b}_3$, it follows that $|\left(e_1, \hat{b}_2\right)|^2 = |\left(e_1, \hat{b}_3\right)|^2 =: a$. Finally since P_U is unital, σ_U must be a probability measure:

$$1 = \sum_{k=1}^{3} |\left(e_1, \hat{b}_k\right)|^2 = 4/9 + 2a,$$

proving that $a = 5/18$. In conclusion,

$$\sigma_U = \frac{4}{9}\delta_1 + \frac{5}{18}\delta_\beta + \frac{5}{18}\delta_{\overline{\beta}},$$

where $\beta = -4/5 + i3/5$. It follows that

$$g_{\phi_U}(w) = \int_{\mathbf{T}} \frac{\alpha + w}{\alpha - w}\sigma_U(d\alpha),$$

$$G_{\Phi_A}(z) = -i\sigma_U(\{1\})z + \int_{-\infty}^{\infty} \left(\frac{zt+1}{i(t-z)}\right)\widetilde{\sigma}_U(dt),$$

where $\widetilde{\sigma}_U := \sigma_U \circ b$. An easy calculation shows that $b^{-1}(\beta) = 1/3$ and $b^{-1}(\overline{\beta}) = -1/3$, and so it follows that

$$G_{\Phi_A}(z) = -i\frac{4}{9}z - i\frac{5}{18}\frac{z/3+1}{1/3-z} - i\frac{5}{18}\frac{z/3-1}{1/3+z}.$$

Notice that $G_{\Phi_A}(i) = 1$ as expected since we must have $\Phi_A(i) = 0$. Hence

$$\begin{aligned}\Phi_A(z) &= \frac{\left(\frac{4}{9} + \frac{5}{18}\frac{z+3}{1-3z} + \frac{5}{18}\frac{z-3}{1+3z}\right) - i}{\left(\frac{4}{9} + \frac{5}{18}\frac{z+3}{1-3z} + \frac{5}{18}\frac{z-3}{1+3z}\right) + i}.\\ &= \frac{z(1-3z)(1+3z) + \frac{5}{8}\left((z+3)(1+3z) + (z-3)(1-3z)\right) - i\frac{9}{4}(1-3z)(1+3z)}{z(1-3z)(1+3z) + \frac{5}{8}\left((z+3)(1+3z) + (z-3)(1-3z)\right) + i\frac{9}{4}(1-3z)(1+3z)}.\end{aligned}$$

The numerator simplifies to

$$n(z) = -9z^3 + i\frac{81}{4}z^2 + \frac{27}{2}z - i\frac{9}{4}.$$

Let $p(z) = \frac{n(z)}{-9} = z^3 - i\frac{9}{4}z^2 - \frac{3}{2}z + \frac{i}{4}$. It follows that $\Phi_A(z)$ is the product of three Blaschke factors, one for each of the roots of $p(z)$. It is easy to calculate that $p(z)$ factors as $p(z) = (z-i)^2(z-\frac{i}{4})$, and so (up to a unimodular constant),

$$\Phi_A(z) = \frac{(z-i)^2(z-i/4)}{(z+i)^2(z+i/4)},$$

which is indeed greater or equal to

$$\Theta_B(z) = \left(\frac{z-i}{z+i}\right)^2.$$

Definition 8.10. We say that $A_1 \sim A_2$ if $\Phi_{A_1} = \Phi_{A_2}$. This is clearly an equivalence relation. Let $\mathrm{ext}(B) := \mathrm{Ext}(B)/\sim$. That is $\mathrm{ext}(B)$ is the set of all $\sim$ equivalence classes of $\mathrm{Ext}(B)$.

Suppose that $A_1, A_2 \in \mathrm{Ext}(B)$ are such that $A_k = b^{-1}(U_k)$ for $U_k \in \mathrm{Ext}(b(B))$ which do not have 1 as an eigenvalue. Then:

Theorem 8.11. *$A_1 \sim A_2$ if and only if A_1 is unitarily equivalent to A_2 via a unitary U whose restriction to $\mathcal{H}$ is the identity.*

The above result is easily extended to include the exceptional case where one (or both) A_1, A_2 are defined using $U_1, U_2 \in \mathrm{Ext}(b(B))$ where 1 is an eigenvalue of either or both of U_1 or U_2. Namely the statement of the theorem becomes: Suppose $A_1, A_2 \in \mathrm{Ext}(B)$ are defined using $U_1, U_2 \in \mathrm{Ext}(b(B))$. Then $A_1 \sim A_2$ if and only if $U_1 \simeq U_2$ via a unitary U which fixes $\mathcal{H}$.

Proof. If such a unitary U exists then

$$\Sigma_1(\Omega) := \Sigma_{A_1}(\Omega) = \int_{\Omega} \pi(1+t^2)J^*P_1(dt)J,$$

and

$$\begin{aligned}J^*P_1(dt)J &= J^*U^*UP_1(dt)J\\ &= J^*U^*P_2(dt)UJ\\ &= J^*P_2(dt)J,\end{aligned} \tag{8.12}$$

since $UJ = J$ as $U|_{\mathcal{H}} = \mathbf{1}_{\mathcal{H}}$. It follows that $\Sigma_1 = \Sigma_2$ which implies $\Phi_1 = \Phi_2$.

Conversely suppose that $\Phi_1 = \Phi_{A_1} = \Phi_{A_2} = \Phi_2$. It follows then that $\Sigma_1 = \Sigma_2$ so that

$$J^*P_1(\Omega)J = J^*P_2(\Omega)J.$$

It follows that for any bounded Borel function g on $\mathbb{R}$,

$$J^* g(A_1)J = J^* g(A_2)J.$$

Since $\mathrm{Ker}(B^* + i) = J\mathbb{C}^n$ is cyclic for A_j (by Theorem 7.3 since Θ_B is inner), for $j = 1, 2$, it follows that we can define a unitary $U : \mathcal{K}_1 \to \mathcal{K}_2$ as follows. Let $\{v_k = Je_k\}$ be an orthonormal basis of $P_{-i}\mathcal{H}$. Any $f \in \mathcal{K}_1$ can be written

$$f = f_1(A_1)v_1 + \ldots + f_n(A_1)v_n,$$

and define

$$Uf = f_1(A_2)v_1 + \ldots + f_n(A_2)v_n.$$

Since Θ_B is inner, Corollary 7.3 and Remark 7.4 imply that if $f \in \mathcal{H} \subset \mathcal{K}_j$, $j = 1, 2$, then $f_1, \ldots, f_n$ can be fixed so that $Uf = f$ and U is the identity on $\mathcal{H}$. The linear map U is isometric because

$$\begin{aligned} \left\langle f_k(A_1)v_k, f_j(A_1)v_j \right\rangle &= \left\langle J^*\overline{f_j}(A_1)f_k(A_1)Je_k, e_j \right\rangle \\ &= \left\langle J^*\overline{f_j}(A_2)f_k(A_2)Je_k, e_j \right\rangle \\ &= \left\langle Uf_k(A_1)v_k, Uf_j(A_1)v_j \right\rangle. \end{aligned} \tag{8.13}$$

The map U is also onto because $\mathrm{Ker}(B^* + i)$ is cyclic for A_1 and A_2 by Theorem 7.3 again. □

Remark 8.12. Suppose that $A \in \mathrm{Ext}_U(B)$, which is to say that there is an isometry $U : \mathcal{H} \to \mathcal{K}$ such that $A \in \mathrm{Ext}(UBU^*)$. In this case we define $\Phi_A := \Phi[A; UBU^*]$.

Note that if $A \in \mathrm{Ext}_U(B)$ has characteristic function Φ_A, then there is a corresponding $A' \in \mathrm{Ext}(B)$ such that $\Phi_{A'} = \Phi_A$. This follows from Naimark's dilation theorem [40, Theorem 4.6].

Indeed if $A \in \mathrm{Ext}_U(B)$ so that $A \in \mathrm{Ext}(UBU^*)$ for some isometry $U : \mathcal{H} \to \mathcal{K}$ then

$$Q(\Omega) := P_{\mathcal{H}} U^* P_A(\Omega) U P_{\mathcal{H}},$$

is a positive operator-valued measure acting on $\mathcal{H}$. Assume for now that A is defined using a $W \in \mathrm{Ext}(Ub(B)U^*)$ which does not have 1 as an eigenvalue so that $A = b^{-1}(W)$.

Since $A = b^{-1}(W)$ and $1 \notin \sigma_p(W)$, A is a densely defined self-adjoint operator and $P_A(\mathbb{R}) := \chi_{\mathbb{R}}(A) = \mathbf{1}_{\mathcal{K}}$, as otherwise $P_A(\mathbb{R})\mathcal{K}$ is a non-trivial reducing subspace for A which contains $U\mathcal{H}$. This would contradict our assumption that $A \in \mathrm{Ext}_U(B)$. In other words the projection-valued measure of A is unital.

By Naimark's dilation theorem there is a larger Hilbert space $\mathcal{K}' \supset \mathcal{H}$ and a unital projection-valued measure $P(\Omega)$ acting on $\mathcal{K}'$ such that the compression

$$P_{\mathcal{H}} P(\Omega) P_{\mathcal{H}} = Q(\Omega),$$

for any Borel set Ω. This projection-valued measure P is called a dilation of Q, and it can be chosen to be minimal in the sense that $\mathcal{K}' = \bigvee P(\Omega)\mathcal{H}$. If A' is the self-adjoint operator corresponding to this projection valued measure,

$$A' := \int_{-\infty}^{\infty} t P(dt),$$

then it follows that $A' \in \mathrm{Ext}(B)$. It is also clear that by definition, $\Phi_A = \Phi_{A'}$.

If A is defined using $W \in \mathrm{Ext}(Ub(B)U^*)$ with $1 \in \sigma_p(U)$, define $Q(\Omega) = P_{\mathcal{H}} P_U(\Omega) P_{\mathcal{H}}$, a unital positive operator-valued measure (POVM) on the unit circle. Again apply Naimark's dilation theorem to obtain a unitary operator U' on $\mathcal{K}' \supset \mathcal{H}$. As before it follows that if $A' \in \mathrm{Ext}(B)$ is defined using $U' \in \mathrm{Ext}(b(B))$, that $\Phi_{A'} = \Phi_A$.

Theorem 8.13. *The map $A \in \mathrm{ext}(B) \mapsto \Phi_A$ is a bijection onto the set of all contractive analytic functions Φ_A which are greater or equal to Θ_B.*

Recall that $\Phi_A \geq \Theta_B$ means that $\Theta_B^{-1}\Phi_A$ is a contractive analytic function. This needs some setup: Given $B \in \mathcal{S}_n(\mathcal{H})$ with characteristic function Θ_B let $V := b(B)(1 - P_i)$, the partial isometric extension of $b(B)$ where as before P_i projects onto $\mathrm{Ker}(B^* - i)$. Fix a choice of isometries $J_{\pm i} : \mathbb{C}^n \to \mathrm{Ker}(B^* \pm i)$. Recall as described in the introduction that all unitary extensions of V are indexed by $U \in \mathcal{U}(n)$: Given any $U \in \mathcal{U}(n)$,

$$V(U) := b(B)(1 - P_i) + J_{-i}UJ_i^*,$$

is a unitary extension of V, and $B(U) := b^{-1}(V(U))$ is a self-adjoint extension of B (provided $V(U)$ does not have 1 as an eigenvalue). All self-adjoint extensions of B are constructed in this way.

Define $\theta_V := \Theta_B \circ b^{-1}$, a contractive analytic function on the unit disc, $\mathbf{D}$. Recall that the Alexandrov-Clark measures for θ_V are defined as the $n \times n$ matrix-valued measures δ_U for any $U \in \mathcal{U}(n)$ (the group of $n \times n$ unitary matrices) associated with the Herglotz functions

$$g_U := \frac{1 + \theta_V U^*}{1 - \theta_V U^*},$$

via the Herglotz representation theorem for the unit disk *i.e.*

$$\mathrm{Re}\left(g_U(z)\right) = \int_{\mathbf{T}} \mathrm{Re}\left(\frac{\alpha + z}{\alpha - z}\right) \delta_U(d\alpha).$$

Let $G_U := g_U \circ b$ be the corresponding Herglotz function on $\mathbb{C}_+$. We define the Alexandrov-Clark measures of Θ_B to be the measures Δ_U on $\mathbb{R}$ such that

$$\mathrm{Re}\left(G_U(z)\right) = \delta_U(\{1\})\mathrm{Im}\,(z) + \int_{-\infty}^{\infty} \mathrm{Re}\left(\frac{1}{i\pi}\frac{1}{t - z}\right) \Delta_U(dt).$$

Recall that as discussed in Section 4 (see equation (4.1)) we have that

$$\Delta_U(\Omega) := \int_{\Omega} \pi(1 + t^2)(\delta_U \circ b)(dt),$$

where $(\delta_U \circ b)(\Omega) = \delta_U(b(\Omega))$ and $b(z) = \frac{z-i}{z+i}$, $b : \mathbb{R} \to \mathbf{T} \setminus \{1\}$.

Now let Z denote the unitary operator of multiplication by z in $L^2_\theta(\mathbf{T})$ (the L^2 space of vector-valued functions on $\mathbf{T}$ which are square integrable with respect to the measure $\delta_\mathbf{1}$).

Let $\{b_j^-(z) = e_j\}$ be a basis for the constant functions in L^2_θ. Since $\Theta(i) = 0 = \theta(0)$, it follows that this is an orthonormal basis. Similarly define $b_j^+(z) := \frac{1}{z}e_j$. For any $C \in \mathbb{C}^{n\times n}$ let

$$Z(C) := Z + P_+(\hat{C} - 1)P_- Z,$$

where $P_\pm$ projects onto the closed span of the $b_j^\pm$, and $\hat{C} = J_+ C J_-^*$ where $J_\pm$ are the isometries defined by $J_\pm e_k = b_k^\pm$. Then as shown in [32] $Z(0)$ has Livšic characteristic function θ_V, and so it follows that there is a unitary transformation $W : \mathcal{H} \to L^2_\theta$ that implements the equivalences $Z(0) \simeq V = b(B)(1 - P_i)$, and $Z(U) \simeq V(U)$ for any $U \in \mathcal{U}(n)$, and such that $W : \mathrm{Ker}(B^* - i) = \mathrm{Ker}(V) \to \mathrm{Ker}(Z(0)) = \bigvee b_j^-$ sends $u_j \mapsto b_j^-$ [2, 32], where $\{u_j\}$ is an orthonormal basis of $\mathrm{Ker}(B^* - i)$.

Moreover the results of [2] show that

$$\delta_U(\Omega) = \left[\langle \chi_\Omega(Z(U))b_i^-, b_j^-\rangle\right].$$

Using the fact that $G_U = g_U \circ b$, and the relationship between Herglotz functions and measures on the upper half-plane and the disk as described in Section 4, it follows that

$$\mathrm{Re}\left(G_U(w)\right) = \delta_U(\{1\})\mathrm{Im}\,(w) + \int_{-\infty}^{\infty} \mathrm{Re}\left(\frac{1}{i\pi}\frac{1}{t - z}\right) \pi(1 + t^2)\widetilde{\Delta}_U(dt),$$

where $\widetilde{\Delta}_U := \delta_U \circ b$ so that

$$\begin{aligned} \widetilde{\Delta}_U(\Omega) &= \left[\left\langle \chi_{b(\Omega)}(Z_U) b_i^+, b_j^+ \right\rangle\right] \\ &= \left[\left\langle \chi_{b(\Omega)}(b(B(U))) u_i, u_j \right\rangle\right] \\ &= \left[\left\langle \chi_{\Omega}(B(U)) u_i, u_j \right\rangle\right], \end{aligned} \tag{8.14}$$

and

$$\delta_U(\{1\}) = \left[\left\langle \chi_{\{1\}}(Z(U)) b_i^+, b_j^+ \right\rangle\right] = \left[\left\langle \chi_{\{1\}}(b(B(U))) u_i, u_j \right\rangle\right].$$

Theorem 8.14. *For any $U \in \mathcal{U}(n)$, $\Phi_{B(U)} = U^* \Theta_B$.*

More precisely, recall that the Livšic characteristic function Θ_B is only defined up to conjugation by fixed unitary matrices. The above theorem is saying that if one fixes a choice of Θ_B, then there is a canonical self-adjoint extension $B(\mathbf{1})$ of B such that $\Phi_{B(\mathbf{1})} = \Theta_B$, where $b(B(\mathbf{1})) = b(B)(1 - P_i) + J_{-i}J_i^*$ for some fixed choice of isometries $J_{\pm i} : \mathbb{C}^n \to \mathrm{Ker}(B^* \pm i)$. After this choice of Θ_B and $J_{\pm i}$ is fixed we have that $\Phi_{B(U)} = U^* \Theta_B$, where recall that $b(B(U)) = b(B)(1 - P_i) + J_{-i}UJ_i^*$.

Proof. Let $B_T \in \mathcal{S}_n(\mathcal{H}_T)$ be a symmetric linear transformation with characteristic function Θ_B^T, and let $\{\widetilde{u}_j\}$, $\{\widetilde{v}_j\}$ be orthonormal bases of $\mathrm{Ker}(B_T^* - i)$ and $\mathrm{Ker}(B_T^* + i)$, respectively. Here recall that ^{T} denotes matrix transpose and if $B \in \mathcal{S}$ has characteristic function Θ, B_T is that element of $\mathcal{S}$ with characteristic function Θ^T.

By Corollary 4.10, there is a conjugation $C_T := C_{B_T} : \mathcal{H}_T \to \mathcal{H}$ which intertwines B_T and B. Let $\{u_k\}$, $\{v_k\}$ be the orthonormal bases of $\mathrm{Ker}(B^* - i)$ and $\mathrm{Ker}(B^* + i)$ respectively given by $C_T\widetilde{u}_j = v_j$ and $C_T\widetilde{v}_j = u_j$. Further recall that $C_T^* = C_B$ is a conjugation intertwining B and B_T so that $C_B v_j = \widetilde{u}_j$ and $C_B u_j = \widetilde{v}_j$. Also define $J : \mathbb{C}^n \to \mathrm{Ker}(B^* - i)$ by $Je_k = v_k$, for some orthonormal basis $\{e_k\}$ of $\mathbb{C}^n$.

Let V and V_T be the partial isometric extensions of the Cayley transforms of B, and B_T. Given any $U \in \mathcal{U}(n)$, let

$$V(U) := V + \hat{U} := V + \sum_{i,j} U_{ij} \langle \cdot, u_i \rangle v_j.$$

The set of all $V(U)$, for $U \in \mathcal{U}(n)$ is is the set of all canonical unitary extensions of V, and the set of all $B(U) := b^{-1}(V(U))$ is the set of all canonical self-adjoint extensions of B. Similarly define

$$V_T(U) := V_T + \widetilde{U} := V_T + \sum_{i,j} U_{ij} \langle \cdot, \widetilde{u}_i \rangle \widetilde{v}_j.$$

Consider the self-adjoint extension $B_T(U) = b^{-1}(V_T(U))$, where V_T is the partial isometric extension of $b(B_T)$. Then

$$\mathrm{Dom}(B_T(U)) = \mathrm{Ran}\left(1 - V_T(U)\right) = \mathrm{Dom}(B_T) + \left(1 - \widetilde{U}\right)\widetilde{S}_{-i},$$

where $\widetilde{S}_{\pm i} = \widetilde{P}_{\pm i}\mathcal{H}$, and $\widetilde{P}_{\pm i}$ are the projections onto $\mathrm{Ker}(B_T^* \pm i)$. Similarly define $S_{\pm i}$ and $P_{\pm i}$. As above, $\widetilde{U}$ is defined by

$$\widetilde{U} = \sum_{ij} U_{ij} \langle \cdot, \widetilde{u}_i \rangle \widetilde{v}_j : \widetilde{S}_i \to \widetilde{S}_{-i}.$$

Given any $g \in \mathrm{Dom}(B_T(U))$, it follows that there is some $\widetilde{f} = \sum \left\langle \widetilde{f}, \widetilde{u}_i \right\rangle \widetilde{u}_i \in \widetilde{S}_i$ and $g_T \in \mathrm{Dom}(B_T)$ such that

$$\begin{aligned} g &= g_T + \sum \left\langle \widetilde{f}, \widetilde{u}_i \right\rangle \widetilde{u}_i - \sum U_{ij} \left\langle \widetilde{f}, \widetilde{u}_i \right\rangle \widetilde{v}_j \\ &= g_T + \widetilde{f} - \widetilde{U}\widetilde{f}, \end{aligned}$$

so that

$$B_T(U)g = B_T g_T + i\widetilde{f} + i\widetilde{U}\widetilde{f}.$$

Now $C_T g_T = g_B \in \mathrm{Dom}(B)$, and

$$\begin{aligned} C_T g &= g_B + \sum \overline{\left\langle \widetilde{f}, \widetilde{u}_i \right\rangle} v_i - \sum \overline{U_{ij}} \overline{\left\langle \widetilde{f}, \widetilde{u}_i \right\rangle} u_j \\ &= g_B + f - \hat{W} f, \end{aligned} \tag{8.15}$$

where $C_T \widetilde{f} = f := \sum \overline{\left\langle \widetilde{f}, \widetilde{u}_i \right\rangle} v_i \in S_{-i}$ and

$$\hat{W} = \sum_{ij} \overline{U_{ij}} \langle \cdot, v_i \rangle u_j.$$

Comparing this to

$$\hat{U}^* = \sum_{ij} \overline{U_{ji}} \langle \cdot, v_i \rangle u_j,$$

we see that $\hat{W} = \widehat{U^T}^*$

Now if $R \in \mathfrak{U}(n)$ then $b(B(R))^* = V^* + \hat{R}^*$ and if $b^\dagger(z) = \frac{z+i}{z-i}$ then its inverse with respect to composition is $b^{-1}(z)^\dagger = -i\frac{1+z}{1-z}$, so that we also have that $\mathrm{Dom}(B(R)) = \mathrm{Ran}\left(1 - V(R)^*\right)$. It follows that

$$C_T g = g_B + f - \widehat{U^T}^* f \in \mathrm{Dom}(B(U^T)),$$

and

$$B(U^T) C_T g = B g_B - if - i\widehat{U^T}^* f,$$

while

$$C_T B_T(U) g = C_T B_T g_T + C_T(i\widetilde{f} + i\widetilde{U f}) = B(U^T) C_T g,$$

and this proves that

$$C_T B_T(U) = B(U^T) C_T. \tag{8.16}$$

It further follows that

$$C_T V_T(U) = V(U^T)^* C_T.$$

Now let δ_U be the Alexandrov-Clark measure associated with the Herglotz functions

$$g_U(z) := \frac{1 + \theta^T U^*}{1 - \theta_T U^*},$$

where $\theta^T := \Theta^T \circ b$, and as before let let $\widetilde{\Delta}_U := \delta_U \circ b^{-1}$. As discussed before this proof, the results of [2] show that

$$\widetilde{\Delta}_U(\Omega) = \left[\langle \chi_\Omega(B_T(U)) \widetilde{u}_i, \widetilde{u}_j \rangle\right],$$

so that

$$\begin{aligned} \widetilde{\Delta}_U(\Omega) &= \left[\langle C_T \widetilde{u}_j, C_T \chi_\Omega(B_T(U)) \widetilde{u}_i \rangle\right] \\ &= \left[\left\langle u_j, \chi_\Omega(B(U^T)) u_i \right\rangle\right] \\ &= (J^* P_{B(U^T)}(\Omega) J)^T. \end{aligned}$$

Similarly,

$$\begin{aligned} \delta_U(\{1\}) &= \left[\langle C_B C_T \chi_{\{1\}}(V_T(U)) \widetilde{u}_i, \widetilde{u}_j \rangle\right] \\ &= \left[\left\langle v_j, \chi_{\{1\}}(V(U^T)^*) v_i \right\rangle\right] \\ &= \left[\left\langle v_j, \chi_{\{1\}}(V(U^T)) v_i \right\rangle\right] \\ &= (J^* P_{V(U^T)}(\{1\}) J)^T. \end{aligned} \tag{8.17}$$

In conclusion we have that if $\Phi := \Phi_{B(U^T)}$, that $G_\Phi^T = G_U$, so that

$$G_\Phi = G_U^T = \frac{1 + (U^*)^T \Theta_B}{1 - (U^*)^T \Theta_B}.$$

This proves that $\Phi_{B(U^T)} = (U^T)^* \Theta_B$, or equivalently that $\Phi_{B(U)} = U^* \Theta_B$. □

Proof. (of Theorem 8.13)

This map is automatically injective by the definition of ext(B). To show that it is surjective, let Φ be a contractive analytic function such that $\Phi \geq \Theta_B$, *i.e.* $\Theta_B^{-1}\Phi$ is a contractive analytic function and $\Phi(i) = 0$. Let $\Theta := \Theta_B$.

Now we have $B \simeq \mathfrak{Z}_\Theta$ acting in $\mathcal{L}(\Theta)$, and by Corollary 4.5, $\mathfrak{Z}_\Theta \preccurlyeq \mathfrak{Z}_\Phi$. Furthermore by Theorem 8.14 we have that there is a canonical self-adjoint extension A of $\mathfrak{Z}_\Phi$ whose characteristic function $\Phi_A = \Phi[A; \mathfrak{Z}_\Phi]$ relative to $\mathfrak{Z}_\Phi$ is Φ. Moreover one can see from Example 4.6 that the isometry $V : \mathcal{L}(\Theta) \to \mathcal{L}(\Phi)$ which obeys $V\mathfrak{Z}_\Theta \subset \mathfrak{Z}_\Phi V$ also satisfies $VP_{-i} = Q_{-i}V$ and $V^* VP_{-i} = P_{-i}$ where P_{-i} projects onto $\mathrm{Ker}(\mathfrak{Z}_\Theta^* + i)$ while Q_{-i} projects onto $\mathrm{Ker}(\mathfrak{Z}_\Phi^* + i)$. To see this note that since $\Theta(i) = 0 = \Phi(i)$ that the reproducing kernel functions for $\mathcal{L}(\Theta)$ and $\mathcal{L}(\Phi)$ obey

$$K_i^\Theta(z) = \frac{2}{1-\Theta(z)}\frac{i}{\pi}\frac{1}{z+i} \quad \text{and} \quad K_i^\Phi(z) = \frac{2}{1-\Phi(z)}\frac{i}{\pi}\frac{1}{z+i}.$$

Observe that as in Example 4.6,

$$V_1(z) = \frac{1-\Theta(z)}{2},$$

is an isometry of $\mathcal{L}(\Theta)$ onto K_Θ^2, that K_Θ^2 is isometrically contained in K_Φ^2 (since Θ is inner), and that multiplication by

$$V_2(z) := \frac{2}{1-\Phi(z)},$$

is an isometry of K_Φ^2 into $\mathcal{L}(\Phi)$. Since V acts as multiplication by $V(z) = V_2(z)V_1(z)$, it is an isometry that obeys $VK_i^\Theta \mathbf{v} = K_i^\Phi \mathbf{v}$ for any $\mathbf{v} \in \mathbb{C}^n$.

It follows that the isometry $V : \mathcal{L}(\Theta) \to \mathcal{L}(\Phi)$ obeys $V\mathrm{Ker}(\mathfrak{Z}_\Theta^* + i) = \mathrm{Ker}(\mathfrak{Z}_\Phi^* + i)$. This shows that the characteristic function $\Phi_A = \Phi_A[A; \mathfrak{Z}_\Phi] = \Phi$ of A with respect to $\mathfrak{Z}_\Phi$ is the same as the characteristic function of $A \in \mathrm{Ext}_U(B)$ with respect to B. By Remark 8.12, there is an $A' \in \mathrm{Ext}(B)$ with $\Phi[A'; B] = \Phi_A = \Phi$. □

9 Outlook

There are several directions in which the results of this paper can be extended.

We have assumed throughout that $B \in \mathcal{S}$ has an inner Livšic characteristic function. A good portion of the theory we have developed here does not depend on this (or on the assumption that $n < \infty$), and it would be good to generalize the results contained here to the case where the Livšic function is an arbitrary contractive analytic operator-valued function (vanishing at $z = i$). We have done some work on this already, in particular Example 4.6 can be generalized to show that if $\Theta \leq \Phi$ are arbitrary contractive analytic functions that there is a bounded multiplier $V : \mathcal{L}(\Theta) \to \mathcal{L}(\Phi)$ which intertwines $\mathfrak{Z}_\Theta$ and $\mathfrak{Z}_\Phi$ (see [5, Example 8.5]). Also if $A \in \mathrm{Ext}(B)$ where Θ_B is not inner, then one can show that in general $\mathcal{H}_A$ is only boundedly contained in $\mathcal{K}_A$. Our results here also have direct applications to the study of the natural pre-orders defined on partial isometries in [5]. In particular given any $V \in \mathcal{V}_n$ with inner characteristic function θ_V, we can completely characterize the set of all partial isometries $W \in \mathcal{V}$ such that $V \preccurlyeq W$ in terms of the characteristic functions of V and W. Recall here that $\mathcal{V}$ denotes the set of all c.n.u. partial isometries defined on separable Hilbert spaces which have equal deficiency indices. We are currently working on generalizing these results to the case of arbitrary $V \in \mathcal{V}$ (and perhaps to more general contractions) and will include these results in a future paper.

There should be several interesting consequences of the results already obtained in this paper. For example as discussed in Remark 7.4, we can use the theory developed here to provide an alternate proof and generalization of the Alexandrov isometric measure theorem, [41, Theorem 2]. In fact the result we obtain is a generalization of the operator theoretic result of Krein [29, Chapter 1, Corollary 2.1] which uses the theory of entire symmetric operators and hence holds for the case where Θ_B is a meromorphic scalar-valued inner function. We point out that this result of Krein can be used to prove the Alexandrov isometric measure theorem (for the case where the inner function Θ is meromorphic), and that de Branges has also proven this result in the case where Θ is meromorphic in his book [36, Theorem 32]. Our generalization holds for arbitrary inner matrix functions. Our theory should also allow us to extend the main result of [45] to the case of arbitrary inner functions and vector-valued nearly invariant subspaces.

Finally, there is a natural bijection between the sets $\mathrm{Ext}(B)$ and $\mathrm{POVM}(B)$, the set of all unital positive operator valued measures which diagonalize B. That is $Q \in \mathrm{POVM}(B)$ if and only if

$$A := \int_{-\infty}^{\infty} tQ(dt) \in \mathrm{Ext}(B).$$

A straightforward application of Naimark's dilation theorem shows that $\mathrm{POVM}(B)$ is a convex set, and we think it could be interesting to study the properties of this convex set. For example, we would like to determine its extreme points, and to study its Choquet theory. It is known that $\mathrm{POVM}(B)$ is a face in the set of all unital positive-operator valued measures on $\mathbb{R}$ [46, Theorem 13.6.3], and consequently that every projection valued measure corresponding to a canonical $A \in \mathrm{Ext}(B)$ is an extreme point of this set (although this can be proven directly). Naimark has proven that if $B \in \mathcal{S}_n(\mathcal{H})$ and $A \in \mathrm{Ext}(B)$ is self-adjoint in $\mathcal{K}$ where $\mathcal{K} \ominus \mathcal{H}$ is finite dimensional, then the positive operator-valued measure corresponding to A is an extreme point of $\mathrm{POVM}(B)$ [47]. Moreover it has been shown that if $B \in \mathcal{S}_n(\mathcal{H})$, then the set of all $Q \in \mathrm{POVM}(B)$ which correspond to $A \in \mathrm{Ext}(B)$ defined on $\mathcal{K}$ with $\mathcal{K} \ominus \mathcal{H}$ finite dimensional is dense in a natural topology on $\mathrm{POVM}(B)$ [48]. It should be interesting to see whether the extreme points of $\mathrm{POVM}(B)$ can be given a function theoretic characterization in terms of the characteristic functions $\Phi[A; B]$ of the corresponding extensions $A \in \mathrm{Ext}(B)$ of B.

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