1. Von Neumann theory of defect indices

1.1. **Cayley transform of a symmetric operator.**

The *Cayley transform* is the map $\kappa : z \mapsto \frac{z-\mathrm{i}}{z+\mathrm{i}}$, mapping $\mathbb{R}\cup\{\infty\}$ to the unit circle $\mathbb{S}^1$, with inverse $\kappa^{-1}(z) = \mathrm{i}\frac{1+z}{1-z}$.

It can be naturally extended to symmetric operators. In fact if T is symmetric, then

$$\|(T-z)u\|^2 = \|(T-\mathrm{Re}z)u\|^2 + |\mathrm{Im}z|^2\|u\|^2,\ u \in \mathrm{Dom}\,T,$$

which implies that $(T-z)$ is injective for $z \in \mathbb{C}\setminus\mathbb{R}$ with

$$\|u\| \leq |\mathrm{Im}z|^{-1}(T-z)u\|,\ u \in \mathrm{Dom}\,T.$$

We can hence consider the bounded operator

$$(T+\mathrm{i})^{-1} : (T+\mathrm{i})\,\mathrm{Dom}\,T \to \mathrm{Dom}\,T,$$

and the *Cayley transform* $\kappa(T)$ defined as

$$\kappa(T) = (T-\mathrm{i})(T+\mathrm{i})^{-1},\ \mathrm{Dom}\,\kappa(T) = (T+\mathrm{i})\,\mathrm{Dom}\,T.$$

We see that $\|\kappa(T)u\| = \|u\|$, ie $\kappa(T)$ is an isometry.

1.1.1. *Isometries.* If U is an isometry with a closed domain $\mathrm{Dom}\,U$, then U is often called a *partial isometry*, for example in the polar decomposition of bounded operators. If U is an isometry, U is closed iff $\mathrm{Dom}\,U$ is closed iff $\Gamma(U)$ is closed.

If U is a closed isometry, we denote by U^{ext} the extension of U to $\mathcal{H}$ defined by setting $U^{\mathrm{ext}}_{|\,\mathrm{Dom}\,U^\perp} = \{0\}$.

To study the Cayley transform we need to relate the graphs of T and of $\kappa(T)$. This can be easily done if we use the framework of *linear relations.*

1.2. **Linear relations.**

A *linear relation* $\mathcal{R}$ on a Hilbert space $\mathcal{H}$ is a linear subspace $\mathcal{R} \subset \mathcal{H}\oplus\mathcal{H}$, and we write $u_1\,\mathcal{R}\,u_2$ if $(u_1,u_2) \in \mathcal{R}$. Let $\pi_i : \mathcal{H}\oplus\mathcal{H} \to \mathcal{H}$ for $i = 1,2$ the projection on the first or second component. $\mathcal{R} = \Gamma(T)$ for some linear operator T iff $\pi_1 : \mathcal{R} \to \mathcal{H}$ is injective. We have then $\mathrm{Dom}\,T = \pi_1(\mathcal{R})$, $\mathrm{Ran}T = \pi_2(\mathcal{R})$.

Definition 1.1. (1) $\mathcal{R}$ *is* symmetric *if* $\mathcal{R} \subset (q\mathcal{R})^\perp$ *for* $q = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}$*;*

(2) $\mathcal{R}$ *is* selfadjoint *if* $\mathcal{R} = (q\mathcal{R})^\perp$*;*

(3) $\mathcal{R}$ *is* isometric *if* $\mathcal{R} \subset (\hat{q}\mathcal{R})^\perp$ *for* $\hat{q} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$*;*

(4) $\mathcal{R}$ *is* unitary *if* $\mathcal{R} = (\hat{q}\mathcal{R})^\perp$*.*

Clearly $\mathcal{R}$ symmetric, selfadjoint, isometric, unitary iff $\mathcal{R}^{\mathrm{cl}}$ is so.

One checks that T symmetric, selfadjoint, isometric iff $\Gamma(T)$ is symmetric, selfadjoint, isometric. However to define T^* uniquely one needs to require that $\mathrm{Dom}\,T$ is dense in $\mathcal{H}$, which corresponds for relations to $\pi_1(\mathcal{R})$ dense in $\mathcal{H}$.

$\mathcal{R}$ is isometric iff $\|u_1\| = \|u_2\|$, $\forall(u_1,u_2) \in \mathcal{R}$, hence $\mathcal{R}$ isometric iff $\mathcal{R} = \Gamma(U)$ for some isometry U.

If $\mathcal{R}$ is isometric with $\pi_1\mathcal{R}$ dense, then $\pi_1\mathcal{R}^{\mathrm{cl}} = \mathcal{H}$ so $\mathcal{R} = \Gamma(U)$, $\mathcal{R}^{\mathrm{cl}} = \Gamma(U^{\mathrm{cl}})$, U^{cl} is an isometry with domain $\mathcal{H}$. If $\mathcal{R}$ is also unitary, then $(U^{\mathrm{cl}}\mathcal{H})^\perp \subset U^{\mathrm{cl}}\mathcal{H}$ hence $(U^{\mathrm{cl}}\mathcal{H})^\perp = \{0\}$ hence $\mathrm{Ran}U^{\mathrm{cl}} = \mathcal{H}$ and U^{cl} is unitary in the usual sense, ie $U^{\mathrm{cl}}(U^{\mathrm{cl}})^* = (U^{\mathrm{cl}})^*U^{\mathrm{cl}} = \mathbb{1}$.

1.2.1. *Cayley transform.* We set $\kappa = \begin{pmatrix} \mathrm{i} & 1 \\ -\mathrm{i} & 1 \end{pmatrix}$, acting on $\mathcal{H}\oplus\mathcal{H}$, so that $\kappa^{-1} = \frac{1}{2}\begin{pmatrix} -\mathrm{i} & \mathrm{i} \\ 1 & 1 \end{pmatrix}$.

Lemma 1.2. *$\mathcal{R}$ is symmetric, resp. selfadjoint iff $\kappa(\mathcal{R})$ is isometric, resp. unitary.*

Proof. follows from $2q = \kappa^* \hat{q} \kappa$.□

If $\kappa(T) = (T - \mathrm{i})(T + \mathrm{i})^{-1}$ for T symmetric, is the Cayley transform for operators, then $\kappa(\Gamma(T)) = \Gamma(\kappa(T))$.

The condition $\pi_1(\mathcal{R})$ dense is equivalent to $(\pi_1 - \pi_2)(\kappa(\mathcal{R}))$ dense, using the expression for κ^{-1}.

Proposition 1.3. (1) *$\mathcal{R}_1 \subset \mathcal{R}_2 \;\Leftrightarrow \kappa(\mathcal{R}_1) \subset \kappa(\mathcal{R}_2)$;*
(2) *$\mathcal{R}$ closed iff $\kappa(\mathcal{R})$ closed;*
(3) *If $\mathcal{R}$ is symmetric, then $\mathcal{R}$ is closed iff $\pi_i(\kappa(\mathcal{R}))$ closed.*

Proof. : (1) is stupid, (2) is also stupid since κ is continuous, bijective. (3) follows from the fact that $\kappa(\mathcal{R})$ is isometric. □

Translating the above proposition to the case of linear operators, we obtain the following result:

Theorem 1.4. (1) *The Cayley transform $\kappa : T \mapsto \kappa(T)$ is an order preserving bijection between the class of symmetric operators on $\mathcal{H}$ and the class of isometries on $\mathcal{H}$ such that $\mathrm{Im}(\mathbb{1} - U)$ is dense.*
(2) *If one of the four objects $T, \mathrm{Im}(T + \mathrm{i}), \mathrm{Im}(T - \mathrm{i}), \kappa(T)$ is closed, so are the others.*

1.3. **Selfadjoint extensions of symmetric operators.** Let us first note that if T is symmetric, then T is closeable with $T^{\mathrm{cl}} = T^{**}$ and T^{cl} is symmetric. Therefore any closed symmetric extension of T (hence in particular any selfadjoint extension of T, if it exists), is also a closed symmetric extension of T^{cl}. It follows that to discuss the selfadjoint extensions of T we can assume that T is closed.

From Thm. 1.4 we see that it suffices to discuss isometric (or unitary) extensions of a (closed) isometry.

Definition 1.5. *Let T be a symmetric operator. We set*

$$K^{\pm} = \mathrm{Im}(T \pm \mathrm{i})^{\perp} = \mathrm{Ker}(T^* \mp \mathrm{i}) = \mathrm{Im}(T^{\mathrm{cl}} \pm \mathrm{i})^{\perp} = \mathrm{Ker}((T^{\mathrm{cl}})^* \mp \mathrm{i}),$$

and $n^{\pm} = \mathrm{dim} K^{\pm}$.

The spaces $K^{\pm}$, resp. cardinal numbers $n^{\pm}$ are called the *defect spaces*, resp. *defect indices* of T. In the sequel we assume that T is closed, so that $U = \kappa(T)$ is closed. We note that if $U = \kappa(T)$, then

$$K^{+} = \mathrm{Dom}\, U^{\perp},\ K^{-} = \mathrm{Ran} U^{\perp}.$$

1.3.1. *Isometric extensions of isometries.* Let U be a closed isometry. We have $\mathcal{H} = \mathrm{Dom}\, U \oplus^{\perp} K^{+} = \mathrm{Ran} U \oplus^{\perp} K^{-}$ and we can write the extension U^{ext} (see 1.1.1) in corresponding matrix form as

$$U^{\mathrm{ext}} = \begin{pmatrix} U & 0 \\ 0 & 0 \end{pmatrix}.$$

If U_1 is a closed isometric extension of U, then we have by an easy computation:

$$U_1^{\mathrm{ext}} = \begin{pmatrix} U & 0 \\ 0 & V_1 \end{pmatrix},$$

where $V_1 : K^{+} \to K^{-}$ is a closed isometry. In particular U_1 is unitary iff $V_1 : K^{+} \to K^{-}$ is unitary.

Going back to symmetric operators using the Cayley transform, we obtain the following result.

Proposition 1.6. *Let T be a symmetric operator. Then the closed symmetric extensions of T are in bijection with the closed isometries from K^+ to K^-.*

Let V such a closed isometry. Then the associated extension T_V of T is given by:

$$\begin{aligned} &\operatorname{Dom} T_V = \{u + (\mathbb{1} - V)r : u \in \operatorname{Dom} T, r \in \operatorname{Dom} V\}, \\ &T_V(u + (\mathbb{1} - V)r) = Tu + \mathrm{i}(\mathbb{1} + V)r. \end{aligned} \tag{1.1}$$

As a corollary we obtain the following theorem about selfadjoint extensions of symmetric operators.

Theorem 1.7. *Let T be symmetric with defect indices $n^\pm$ and defect spaces $K^\pm$. Then the following holds:*

(1) *T has selfadjoint extensions iff $n^+ = n^-$. The selfadjoint extensions of T are in bijection with the unitary operators from K^+ to K^-. If V is such a unitary operator the associated selfadjoint extension T_V is given by* (1.1)*.*

(2) *T^{cl} is selfadjoint iff $n^+ = n^- = 0$. In this case T has a unique selfadjoint extension and is said* essentially selfadjoint*.*

If $n^+ \neq n^-$ and $n^+ = 0$ or $n^- = 0$, T is said *maximal symmetric*.