9. Self-adjoint extensions of symmetric operators

* In this section we assume that S is a densely defined, symmetric operator

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9.1. Assumption: S is an operator on $\mathcal{H}$ for which
a) $\overline{D(S)} = \mathcal{H}$
b) $\forall \phi, \psi \in D(S)$: $(\phi, S\psi) = (S\phi, \psi)$

* If S satisfies a) and b), then by Thrm 5.10.c)
$\Rightarrow$ S is closable, and $\bar{S}$ satisfies Assumption 9.1.
* If $V \in C^\infty(\mathbb{R}^d, \mathbb{R})$, then $S = (H_0 + V)|_D$ is symmetric with the domain $D := C_c^\infty(\mathbb{R}^d)$.

(Proof: $\psi, \phi \in D \Rightarrow (\phi, S\psi) = \underbrace{(\phi, -\tfrac{1}{2}\Delta\psi)}_{\overset{\text{part. int.}}{=} (-\frac{1}{2}\Delta\phi, \psi)} + \underbrace{(\phi, V\psi)}_{\overset{V \text{ is real}}{=} (V\phi, \psi)} = (S\phi, \psi)$ $\square$)

* The goal of this section is to find out if such operators S have self-adjoint extensions, and what these might be. This can be done via the following tool:

9.2. Proposition: Let T be a symmetric operator: $\forall \phi, \psi \in D(T)$, $(\phi, T\psi) = (T\phi, \psi)$.

Then there exists a unique mapping $\mathcal{C}_T : R(T+i) \to R(T-i)$ for which
$$\mathcal{C}_T(T\psi + i\psi) = T\psi - i\psi \quad \forall \psi \in D(T).$$
In addition, $\mathcal{C}_T$ is an operator, bijective, and an isometry.

Proof: Let $R_\pm := R(T \pm i) := \{T\psi \pm i\psi \mid \psi \in D(T)\}$.
Clearly, R_+ and R_- are subspaces of $\mathcal{H}$.
Also, for any $\psi \in D(T)$,

$$\|T\psi \pm i\psi\|^2 = (T\psi, T\psi) + (T\psi, \pm i\psi) + (\pm i\psi, T\psi) + (\pm i\psi, \pm i\psi)$$
$$= \|T\psi\|^2 + \|\psi\|^2 \pm i \underbrace{(T\psi, \psi)}_{= (\psi, T\psi)} \mp i(\psi, T\psi)$$

Therefore, as T is symmetric,

(*) $$\|T\psi \pm i\psi\|^2 = \|T\psi\|^2 + \|\psi\|^2 \quad \forall \psi \in D(T).$$

Thus, if $(T+i)\psi = 0 \Rightarrow 0 = \|T\psi\|^2 + \|\psi\|^2$ $\Rightarrow \psi = 0$. Therefore, $T+i$ is one-to-one, and there is a mapping $(T+i)^{-1}: R(T+i) \to D(T+i)$. Since $D(T+i) = D(T) = D(T-i)$, we can then define $\mathcal{C}_T := (T-i)(T+i)^{-1}$ for which $D(\mathcal{C}_T) = R(T+i)$ and $R(\mathcal{C}_T) = R(T-i)$. But as also $T-i$ is one-to-one by (*), $\mathcal{C}_T$ is invertible, and $\mathcal{C}_T^{-1} = (T+i)(T-i)^{-1}$.

Clearly, then $\forall \psi \in D(T): \mathcal{C}_T(T\psi + i\psi)$
$$\underset{D(T+i)=D(T)}{=} \mathcal{C}_T(T+i)\psi = (T-i)\psi = T\psi - i\psi.$$

If $\mathcal{C}_T'$ is another mapping $R(T+i) \to R(T-i)$ with this property, then $\forall \phi \in R(T+i)$
$$\mathcal{C}_T'\phi = \mathcal{C}_T'(T+i)\underbrace{(T+i)^{-1}\phi}_{=:\psi} = \mathcal{C}_T'(T\psi + i\psi)$$
$$= T\psi - i\psi = (T-i)(T+i)^{-1}\phi = \mathcal{C}_T\phi$$
$\Rightarrow \mathcal{C}_T' = \mathcal{C}_T$. This proves the stated uniqueness.

$\mathcal{C}_T$ is bijective, and it is linear, since the inverse of an operator is always linear.

(A operator, one-to-one $\Rightarrow \exists A^{-1}: R(A) \to D(A)$, and $\forall \psi_1, \psi_2 \in R(A)$, $\alpha_1, \alpha_2 \in \mathbb{C}$, let $\phi_1 = A^{-1}\psi_1$, $\phi_2 = A^{-1}\psi_2$ when $\alpha_1\psi_1 + \alpha_2\psi_2 \in R(A)$ and $\alpha_1\psi_1 + \alpha_2\psi_2 = \alpha_1 A\phi_1 + \alpha_2 A\phi_2$
$= A(\alpha_1\phi_1 + \alpha_2\phi_2)$
$\Rightarrow A^{-1}(\alpha_1\psi_1 + \alpha_2\psi_2) = \alpha_1\phi_1 + \alpha_2\phi_2 = \alpha_1 A^{-1}\psi_1 + \alpha_2 A^{-1}\psi_2$.)

Thus $\mathcal{C}_T$ is an operator. Now, if $\psi \in R(T+i)$ $\Rightarrow \exists\, \phi = (T+i)^{-1}\psi \in D(T)$, and

$$\|\mathcal{C}_T\psi\|^2 = \|(T-i)\phi\|^2 \overset{(*)}{=} \|T\phi\|^2 + \|\phi\|^2$$
$$\underset{(*)}{=} \|(T+i)\phi\|^2 = \|\psi\|^2.$$

$\Rightarrow \|\mathcal{C}_T\psi\| = \|\psi\| \quad \forall \psi \in D(\mathcal{C}_T)$, and $\mathcal{C}_T$ is an isometry. $\square$

9.3. Definition For a symmetric operator T on $\mathcal{H}$, the linear isometry $\mathcal{C}_T$ defined in Prop. 9.2. is called the <u>Cayley-transform</u> of T.

9.4. Theorem Let T and T' be <u>symmetric</u> operators. Then

o) $R(1-\mathcal{C}_T) = D(T)$ and $1-\mathcal{C}_T$ is 1-1.

a) $\mathcal{C}_{T'} = \mathcal{C}_T \Rightarrow T' = T$

b) $T \subset T' \Leftrightarrow \mathcal{C}_T \subset \mathcal{C}_{T'}$

c) T is closed $\Leftrightarrow \mathcal{C}_T$ is closed

d) If T is densely defined, T is closable and
$$\mathcal{C}_{\bar{T}} = \overline{\mathcal{C}_T}.$$

Conversely, if V is an operator on $\mathcal{H}$ for which $\|V\psi\| = \|\psi\| \ \forall \psi \in D(V)$ ($\Leftrightarrow$ V is an isometry) <u>and</u> $1-V$ is one-to-one, then the mapping

$$T = i(1+V)(1-V)^{-1} : R(1-V) \to R(1+V)$$

is a symmetric operator, and $\mathcal{C}_T = V$.

<u>Proof</u>: Let us first prove "o)" and then the "converse". Suppose $\psi \in R(1-\mathcal{C}_T)$
$\Rightarrow \exists \phi \in D(\mathcal{C}_T) = R(T+i)$ s.t. $\psi = \phi - \mathcal{C}_T\phi$.
But then $\exists \phi_0 \in D(T)$ s.t. $\phi = T\phi_0 + i\phi_0$
$\Rightarrow \mathcal{C}_T\phi = \mathcal{C}_T(T\phi_0 + i\phi_0) = T\phi_0 - i\phi_0$
$\Rightarrow \psi = T\phi_0 + i\phi_0 - T\phi_0 + i\phi_0 = 2i\phi_0 \in D(T)$.

Conversely, if $\psi_0 \in D(T)$, then $\phi := T\psi_0 + i\psi_0 \in D(\mathcal{C}_T)$ and

$$\mathcal{C}_T \phi = \mathcal{C}_T(T\psi_0 + i\psi_0) = T\psi_0 - i\psi_0.$$

$\Rightarrow$

$$\phi - \mathcal{C}_T\phi = T\psi_0 + i\psi_0 - T\psi_0 + i\psi_0 = 2i\psi_0$$

$\Rightarrow$

$$\psi_0 = \frac{1}{2i}(\phi - \mathcal{C}_T\phi) = (1-\mathcal{C}_T)\left(\frac{1}{2i}\phi\right) \in R(1-\mathcal{C}_T).$$

This proves $R(1-\mathcal{C}_T) = D(T)$.

Also, if $(1-\mathcal{C}_T)\phi = 0$ for some $\phi \in D(\mathcal{C}_T)$,

$\Rightarrow$ $0 = \psi = 2i\phi_0$ in the above.

$\Rightarrow$ $\phi_0 = 0$ $\Rightarrow$ $\phi = T\phi_0 + i\phi_0 = 0$.

Thus $1-\mathcal{C}_T$ is 1-1, and we have proven "a)".

To prove the "converse", let us assume V is an operator and an isometry, for which $1-V$ is 1-1. Then

$$(1-V)^{-1} : R(1-V) \to D(1-V) = D(-V) = D(V) = D(1+V).$$

Thus we can define

$$T := i(1+V)(1-V)^{-1} : R(1-V) \to R(1+V).$$

Since $R(1\pm V)$ are subspaces and T is linear, (see the proof of Prop. 9.2.), T is an operator. Suppose $\psi, \phi \in D(T)$.

$\Rightarrow$ $\exists\, \psi', \phi' \in D(V)$ s.t. $\psi = \psi' - V\psi'$
$\phi = \phi' - V\phi'$

In addition, $T\psi = i(\psi' + V\psi')$,
$T\phi = i(\phi' + V\phi')$.

$$\Rightarrow (\phi, T\psi) = (\phi' - V\phi', i(\psi' + V\psi'))$$
$$= i\left[(\phi', \psi') + (\phi', V\psi') - (V\phi', \psi') - (V\phi', V\psi')\right]$$

and
$$(T\phi, \psi) = -i(\phi' + V\phi', \psi' - V\psi')$$
$$= -i\left[(\phi', \psi') - (\phi', V\psi') + (V\phi', \psi') - (V\phi', V\psi')\right]$$

Therefore,

$$(\phi, T\psi) - (T\phi, \psi) = 2i\left[(\phi', \psi') - (V\phi', V\psi')\right].$$

However, by the polarization identity (Exercise 3.7.),

$$(\phi', \psi') = \frac{1}{4}\Big(\|\phi'+\psi'\|^2 - \|\phi'-\psi'\|^2 - i\|\phi'+i\psi'\|^2 + i\|\phi'-i\psi'\|^2\Big).$$

Since V is an isometric operator, we have $\forall \alpha \in \mathbb{C}$: $\phi' + \alpha\psi' \in D(V)$ and $\|\phi'+\alpha\psi'\| = \|V(\phi'+\alpha\psi')\| = \|V\phi' + \alpha V\psi'\|$. Then a second application of the polar. identity shows that $(\phi', \psi') = (V\phi', V\psi')$.
Therefore, $(\phi, T\psi) = (T\phi, \psi)$ $\forall \phi, \psi \in D(T)$, and T is a symmetric operator.
For any $\psi \in D(T)$, $\exists \phi \in D(V)$ s.t.
$\psi = \phi - V\phi$ and $T\psi = i(\phi + V\phi)$.

$$\Rightarrow \quad T\psi + i\psi = i(\phi + V\phi + \phi - V\phi) = 2i\phi \in D(V)$$
$$T\psi - i\psi = i(\phi + V\phi - \phi + V\phi) = 2iV\phi \in R(V)$$

Thus $T\psi - i\psi = V(2i\phi) = V(T\psi + i\psi)$ $\forall \psi \in D(T)$, and $R(T+i) \subset D(V)$. Also $\phi \in D(V) \Rightarrow \psi := (1-V)\phi \in D(T)$ and $\phi = (T+i)(\frac{1}{2i}\psi) \Rightarrow \phi \in R(T+i)$. Thus $R(T+i) = D(V)$ and we can conclude that $V = C_T$. This proves the "converse".
Let then T', T be symmetric operators. By o), we can apply the converse to the isometries C_T and $C_{T'}$. If $C_{T'} = C_T$, by o), $D(T') = R(1 - C_{T'}) = R(1 - C_T) = D(T)$, and

$$T' = i(1 + C_{T'})(1 - C_{T'})^{-1} = i(1 + C_T)(1 - C_T)^{-1} = T.$$

This proves a).
For b), assume first $T \subset T'$. Then $\psi \in D(C_T) \Rightarrow \exists \phi \in D(T) \subset D(T')$ s.t.

$$\psi = T\phi + i\phi = T'\phi + i\phi \Rightarrow \psi \in D(C_{T'}).$$

Also $C_{T'}\psi = C_{T'}(T'\phi + i\phi) = T'\phi - i\phi$
$= T\phi - i\phi = C_T(T\phi + i\phi) = C_T\psi$.
Therefore, $C_T \subset C_{T'}$. For the converse, assume $C_T \subset C_{T'}$. Then $\psi \in D(T) = R(1 - C_T)$
$\Rightarrow \exists \phi \in D(C_T) \subset D(C_{T'})$ s.t. $\psi = \phi - C_T\phi$
$= \phi - C_{T'}\phi \Rightarrow \psi \in R(1 - C_{T'}) = D(T')$.

In addition, by the "Converse", then

$$T'\psi = i(1+\mathcal{C}_{T'})(1-\mathcal{C}_{T'})^{-1}\psi$$
$$= i(1+\mathcal{C}_{T'})\phi = i(1+\mathcal{C}_T)\phi$$
$$= i(1+\mathcal{C}_T)(1-\mathcal{C}_T)^{-1}\psi = T\psi.$$

Therefore, then $T \subset T'$. This concludes the proof of b).

For c) and d), let us first note that, since $\mathcal{C}_T$ is an isometric operator, by Exercise 7.2.a) it has unique continuous extension $V : \overline{D(\mathcal{C}_T)} \to \overline{R(\mathcal{C}_T)}$ which is also an isometry. Clearly, $G(V) = \overline{G(\mathcal{C}_T)}$, and thus $\mathcal{C}_T$ is always closable, and $V = \overline{\mathcal{C}_T}$.

Assume first that $\mathcal{C}_T$ is closed $\Rightarrow V = \mathcal{C}_T$. As in (cc) on p. 43, let $\psi_n \in D(T)$ be a sequence for which $\psi_n \to \psi$ and $T\psi_n \to \phi$. Then $\phi_n := T\psi_n + i\psi_n \in D(\mathcal{C}_T)$ and $\phi_n \to \phi + i\psi$, and thus $\phi + i\psi \in \overline{D(\mathcal{C}_T)} = D(\mathcal{C}_T)$ and $\mathcal{C}_T\phi_n \to \mathcal{C}_T(\phi + i\psi)$.
But $\mathcal{C}_T\phi_n = \mathcal{C}_T(T\psi_n + i\psi_n) = T\psi_n - i\psi_n$
$\to \phi - i\psi$. Therefore,
$\mathcal{C}_T(\phi + i\psi) = \phi - i\psi$
$\Rightarrow 2i\psi = (1-\mathcal{C}_T)(\phi + i\psi) \in R(1-\mathcal{C}_T) \overset{a)}{=} D(T)$
$\Rightarrow \psi \in D(T)$ and

$$T\psi = i(1+\mathcal{C}_T)(1-\mathcal{C}_T)^{-1}\psi$$
$$= \frac{i}{2i}(1+\mathcal{C}_T)(\phi + i\psi) = \frac{1}{2}(\phi + i\psi + \phi - i\psi)$$
$$= \phi.$$

Thus T satisfies (cc), and is closed.
For the converse, suppose T is closed. Consider $\phi \in \overline{D(\mathcal{C}_T)}$. Then there are $\phi_n \in D(\mathcal{C}_T)$ s.t. $\phi_n \to \phi$. $\Rightarrow \exists \psi_n \in D(T)$ s.t. $\phi_n = T\psi_n + i\psi_n$ and $\mathcal{C}_T\phi_n = T\psi_n - i\psi_n$. Thus

$$\psi_n = \frac{1}{2i}(\phi_n - \mathcal{C}_T\phi_n) \to \frac{1}{2i}(\phi - V\phi)$$

and $T\psi_n = \frac{1}{2}(\phi_n + \mathcal{C}_T\phi_n) \to \frac{1}{2}(\phi + V\phi)$.

Since T is closed, (cc) implies that

$$\frac{1}{2i}(\phi - V\phi) \in D(T) \ \& \ \frac{1}{2i}T(\phi - V\phi) = \frac{1}{2}(\phi + V\phi).$$

$\Rightarrow \phi - V\phi \in D(T)$ & $T(\phi - V\phi) = i(\phi + V\phi)$.
$\Rightarrow (T+i)(\phi - V\phi) = i(\phi + V\phi + \phi - V\phi) = 2i\phi$
$\Rightarrow \phi \in R(T+i) = D(C_T)$.
therefore, then $\overline{D(C_T)} = D(C_T) \Rightarrow V = C_T$ and C_T is closed. This proves c).

For d), assume T is symmetric and densely def. $\Rightarrow$ T is closable, and $\overline{T}$ is symmetric (Thm. 5.10, c)).
Thus by the above results $C_{\overline{T}}$ is closed and by b): $T \subset \overline{T} \Rightarrow C_T \subset C_{\overline{T}}$. $\Rightarrow$ $\overline{C_T} \subset C_{\overline{T}}$.
On the other hand, $V = \overline{C_T}$ is an isometry, and if $\psi \in D(V)$ s.t. $(1-V)\psi = 0$
$\Rightarrow \psi \in D(C_{\overline{T}})$ and $(1 - C_{\overline{T}})\psi = 0 \Rightarrow \psi = 0$.
Thus $\exists \tilde{T} := i(1+V)(1-V)^{-1}$ which is a closed symmetric operator. Since $C_T \subset \overline{C_T} = C_{\tilde{T}} \subset C_{\overline{T}}$
$\overset{b)}{\Rightarrow} T \subset \tilde{T} \subset \overline{T}$. Therefore, $\tilde{T} = \overline{T}$
$\Rightarrow \overline{C_T} = C_{\tilde{T}} = C_{\overline{T}}$. This proves d). $\square$

9.5. Definition Let S be densely defined and symmetric. Its <u>deficiency spaces</u> are $\mathcal{K}_+$ and $\mathcal{K}_-$, defined by

$$\mathcal{K}_+ := R(S+i)^{\perp}, \quad \mathcal{K}_- := R(S-i)^{\perp}.$$

The <u>deficiency indices</u> of S are

$$n_+ := \dim \mathcal{K}_+, \quad n_- := \dim \mathcal{K}_-$$

(Reminder: For a Hilbert space $\mathcal{H}$, $\dim \mathcal{H} = \mathrm{card}(\mathrm{ONB})$.)