ding, the statement of Theorem IX.41 and the general idea of its proof should be underod, but the gory details should be omitted.
Section 10 is intended as an introduction to wave front sets and oscillatory integrals, ɔ important tools for the study of partial differential equations with nonconstant coefficients. is theory can be used to give conditions on two distributions so that their product is well ined. The material in Section 10 is not used again in Volumes II and III.

X: Self-Adjointness and the Existence of Dynamics

People used to think that when a thing changes, it must be in a state of change and that when a thing moves, it is in a state of motion. This is now known to be a mistake. — *B. Russell*

X.1 Extensions of symmetric operators

We begin this chapter by studying symmetric operators and their extensions. Primarily, we wish to answer two questions: When do symmetric operators have self-adjoint extensions and, if they do, how can the extensions be characterized? These questions are answered by von Neumann's theory of deficiency indices which we will develop using many of the techniques we have already used in proving the basic criterion for self-adjointness (Theorem VIII.3) in Chapter VIII.

It is useful to begin by explaining why symmetric, non-self-adjoint operators are of interest in the first place. Typically, in quantum mechanics or quantum field theory, physical reasoning gives a formal expression for the Hamiltonian of the system; it is usually a partial differential operator on an appropriate L^2 space. We say "formal" when the domain of the Hamiltonian is not specified. It is usually easy to find a dense domain on which the formal Hamiltonian is a well-defined and symmetric operator H. The quantum dynamics should be given by a unitary group, and we know from Stone's theorem (Theorem VIII.8) that the infinitesimal generator of such a group must be self-adjoint. If $\bar{H}$, the closure of H, is self-adjoint, then we can use $\bar{H}$. But if $\bar{H}$ is not self-adjoint, then we must ask: Does $\bar{H}$ have self-adjoint extensions? And if it has several, which one shall we choose to generate the dynamics? In the case where there are several self-adjoint extensions, they are usually distinguished by the *physics* of the system being described. The problem of choosing the "right" self-adjoint extension is not just a mathematical "technicality" but is intimately related to the physics. For further discussion, see Examples 1 and 2 in this section.

We remark that throughout this section we discuss the extensions of *closed* symmetric operators. There is no loss of generality since every symmetric operator has a closure, and the operator and its closure have the same closed extensions.

Theorem X.1 Let A be a closed symmetric operator on a Hilbert space $\mathscr{H}$. Then

(1a) $\dim[\mathrm{Ker}(\lambda I - A^*)]$ is constant throughout the open upper half-plane.
(1b) $\dim[\mathrm{Ker}(\lambda I - A^*)]$ is constant throughout the open lower half-plane.

(2) The spectrum of A is *one* of the following:
(a) The closed upper half-plane
or (b) the closed lower half-plane
or (c) the entire plane
or (d) a subset of the real axis

(3) A is self-adjoint if and only if case (2d) holds.

(4) A is self-adjoint if and only if the dimensions in both (1a) *and* (1b) are zero.

Proof Let $\lambda = \nu + i\mu$, $\mu \neq 0$. Since A is symmetric,

$$\|(\lambda - A)\varphi\|^2 \geq \mu^2 \|\varphi\|^2 \tag{X.1}$$

for all $\varphi \in D(A)$. From this inequality and the fact that A is closed, it follows immediately that $\mathrm{Ran}(\lambda - A)$ is a closed subspace of $\mathscr{H}$. Furthermore,

$$\mathrm{Ker}(\lambda - A^*) = \mathrm{Ran}(\bar{\lambda} - A)^{\perp} \tag{X.2}$$

The proof of these statements are the same as the case $\lambda = i$ which is given in the proof of Theorem VIII.3.

We will show that if $\eta \in \mathbb{C}$ is small enough, $\mathrm{Ker}(\lambda - A^*)$ and $\mathrm{Ker}((\lambda + \eta) - A^*)$ have the same dimension. Let u in $D(A^*)$ lie in $\mathrm{Ker}((\lambda + \eta) - A^*)$ with $\|u\| = 1$. Suppose $(u, v) = 0$ for all $v \in \mathrm{Ker}(\lambda - A^*)$.

Then by (X.2) $u \in \mathrm{Ran}(\bar{\lambda} - A)$, so there is a $\varphi \in D(A)$ with $(\bar{\lambda} - A)\varphi = u$. Thus,

$$0 = (((\lambda + \eta) - A^*)u, \varphi) = (u, (\bar{\lambda} - A)\varphi) + \bar{\eta}(u, \varphi) = \|u\|^2 + \bar{\eta}(u, \varphi)$$

This is a contradiction if $|\eta| < |\mu|$ since by (X.1) $\|\varphi\| \leq \|u\|/|\mu|$. Thus for $|\eta| < |\mu|$, there is no $u \in \mathrm{Ker}((\lambda + \eta) - A^*)$ which is in $\mathrm{Ker}(\lambda - A^*)^{\perp}$. A short argument with projections (Problem 4) now shows that

$$\dim[\mathrm{Ker}((\lambda + \eta) - A^*)] \leq \dim[\mathrm{Ker}(\lambda - A^*)]$$

The same argument shows that if $|\eta| < |\mu|/2$, then $\dim[\mathrm{Ker}(\lambda - A^*)] \leq \dim[\mathrm{Ker}((\lambda + \eta) - A^*)]$, so we conclude that

$$\dim[\mathrm{Ker}(\lambda - A^*)] = \dim[\mathrm{Ker}((\lambda + \eta) - A^*)] \quad \text{if} \quad |\eta| < |\mu|/2$$

Since $\dim[\mathrm{Ker}(\lambda - A^*)]$ is locally constant, it equals a constant in the upper half-plane and equals a (possibly different) constant in the lower half-plane. This proves (1).

It follows from (X.1) that if $\mathrm{Im}\,\lambda \neq 0$, $\lambda - A$ always has a bounded left inverse and from (X.2) that the inverse is everywhere defined if and only if $\dim[\mathrm{Ker}(\bar{\lambda} - A^*)] = 0$. Thus it follows from part (1) that each of the open upper and lower half-planes is either entirely in the spectrum of A or entirely in the resolvent set. This, plus the fact that $\sigma(A)$ is closed proves (2). (3) and (4) are restatements of Theorem VIII.3. ∎

Corollary If A is a closed symmetric operator that is semibounded, i.e. $(A\varphi, \varphi) \geq -M\|\varphi\|^2$, then $\dim[\mathrm{Ker}(\lambda - A^*)]$ is constant for

$$\lambda \in \mathbb{C}\backslash[-M, \infty)$$

Proof This corollary follows from the proof of Theorem X.1. The same argument about the invariance of dimension can be carried out for real λ in $(-\infty, -M)$, thus connecting the upper and lower half-planes.

Corollary If a closed symmetric operator has at least one real number in its resolvent set, then it is self-adjoint.

Proof Since the resolvent set is open and contains a point on the real axis, it must contain points in both the upper and lower half-planes. The corollary now follows from part (3) of Theorem X.1.

Since the dimensions of the kernels of $i - A^*$ and $i + A^*$ play an important role, it is convenient to give them names.

Definition Suppose that A is a symmetric operator. Let

$$\mathscr{K}_+ = \mathrm{Ker}(i - A^*) = \mathrm{Ran}(i + A)^\perp$$
$$\mathscr{K}_- = \mathrm{Ker}(i + A^*) = \mathrm{Ran}(-i + A)^\perp$$

$\mathscr{K}_+$ and $\mathscr{K}_-$ are called the **deficiency subspaces** of A. The pair of numbers n_+, n_-, given by $n_+(A) = \dim[\mathscr{K}_+]$, $n_-(A) = \dim[\mathscr{K}_-]$ are called the **deficiency indices** of A.

We remark that it is possible for the deficiency indices to be any pair of nonnegative integers; and further it is possible for n_+ or n_- (or both) to equal infinity. The reader is asked to construct examples in Problem 1.

We now set about the task of constructing the closed symmetric extensions of A. Let B be such an extension. Then for $\varphi \in D(B^*)$, we have $(\psi, B^*\varphi) = (B\psi, \varphi) = (A\psi, \varphi)$ for all $\psi \in D(A)$. Thus $\varphi \in D(A^*)$ and $B^*\varphi = A^*\varphi$ so

$$A \subseteq B \subseteq B^* \subseteq A^* \tag{X.3}$$

We introduce two new sesquilinear forms on $D(A^*)$:

$$(\varphi, \psi)_A = (\varphi, \psi) + (A^*\varphi, A^*\psi)$$
$$[\varphi, \psi]_A = (A^*\varphi, \psi) - (\varphi, A^*\psi)$$

A subspace of $D(A^*)$ such that $[\varphi, \psi]_A = 0$ for all φ and ψ in the subspace will be called ***A*-symmetric**. When we refer to subspaces of $D(A^*)$ as ***A*-closed** or ***A*-orthogonal** we mean in the inner product given by the graph inner product $(\cdot, \cdot)_A$.

Lemma Let A be a closed symmetric operator. Then

(a) The closed symmetric extensions of A are the restrictions of A^* to A-closed, A-symmetric subspaces of $D(A^*)$.

(b) $D(A)$, $\mathscr{K}_+$, and $\mathscr{K}_-$ are A-closed, mutually A-orthogonal subspaces of $D(A^*)$ and

$$D(A^*) = D(A) \oplus_A \mathscr{K}_+ \oplus_A \mathscr{K}_-$$

(c) There is a one-to-one correspondence between A-closed, A-symmetric subspaces S of $D(A^*)$ which contain $D(A)$ and the A-closed, A-symmetric subspaces S_1 of $\mathscr{K}_+ \oplus_A \mathscr{K}_-$ given by $S = D(A) \oplus_A S_1$.

Proof To prove (a), notice that (X.3) implies that every symmetric extension of A is contained in A^*. Further, the extension is closed if and only if its domain is A-closed and the extension is symmetric if and only if its domain is A-symmetric.

To prove (b), notice that $D(A)$ is A-closed since A is closed, and $\mathscr{K}_+$ and $\mathscr{K}_-$ are A-closed since they are already closed in the weaker topology given by the usual inner product. The fact that the three subspaces are orthogonal is a straightforward calculation which we omit. Suppose $\psi \in D(A^*)$ and $\psi \perp_A D(A) \oplus_A \mathscr{K}_+ \oplus_A \mathscr{K}_-$. For $\varphi \in D(A)$, we have $(\varphi, \psi) + (A^*\varphi, A^*\psi) = (\varphi, \psi)_A = 0$, so

$$(\varphi, \psi) = -(A\varphi, A^*\psi)$$

Thus, $A^*\psi \in D(A^*)$ and $A^*A^*\psi = -\psi$. Since

$$(A^* + i)(A^* - i)\psi = (A^*A^* + I)\psi = 0,$$

we conclude that $(A^* - i)\psi \in \mathscr{K}_-$. But if $\varphi \in \mathscr{K}_-$, then

$$\begin{aligned} i(\varphi, (A^* - i)\psi) &= (\varphi, \psi) + (A^*\varphi, A^*\psi) \\ &= (\varphi, \psi)_A = 0 \end{aligned}$$

since $\psi \perp_A \mathscr{K}_-$. Thus, we must have $(A^* - i)\psi = 0$, which implies that $\psi \in \mathscr{K}_+$. Since $\psi \perp_A \mathscr{K}_+$, we conclude that $\psi = 0$ which completes the proof of (b).

Let S_1 be an A-closed, A-symmetric subspace of $\mathscr{K}_- \oplus_A \mathscr{K}_-$. Suppose that $\varphi = \varphi_0 + \varphi_1$, $\psi = \psi_0 + \psi_1$ with $\varphi_0, \psi_0 \in D(A)$; $\varphi_1, \psi_1 \in S_1$. Then $[\varphi_0, \psi_0]_A = 0$ since A is symmetric and $[\varphi_1, \psi_1]_A = 0$ since S_1 is A-symmetric. Further,

$$\begin{aligned} [\varphi_0, \psi_1]_A &= (A^*\varphi_0, \psi_1) - (\varphi_0, A^*\psi_1) \\ &= (A\varphi_0, \psi_1) - (\varphi_0, A^*\psi_1) \\ &= 0 \end{aligned}$$

since $\varphi_0 \in D(A)$ and $\psi_1 \in D(A^*)$. A similar proof shows that $[\varphi_1, \psi_0]_A = 0$. Thus,

$$[\varphi, \psi]_A = [\varphi_0, \psi_0]_A + [\varphi_1, \psi_0]_A + [\varphi_0, \psi_1]_A + [\varphi_1, \psi_1]_A = 0$$

so $S = D(A) \oplus_A S_1$ is an A-symmetric subspace. S is A-closed since $D(A)$ and S_1 are A-closed and A-orthogonal.

Conversely, let S be an A-closed, A-symmetric subspace of $D(A^*)$ containing $D(A)$. Let $S_1 = S \cap (\mathscr{K}_+ \oplus_A \mathscr{K}_-)$. Then S_1 is clearly A-closed and A-symmetric. Now suppose that $\varphi \in S$. Then φ can be uniquely expressed $\varphi = \varphi_0 + \varphi_1$ where $\varphi_0 \in D(A)$ and $\varphi_1 \in \mathscr{K}_+ \oplus_A \mathscr{K}_-$. Since $D(A) \subset S$, we have $\varphi_0 \in S$ which implies $\varphi_1 \in S$ also. Thus $\varphi_1 \in S_1$ so $S = D(A) \oplus_A S_1$. This proves (c). ∎

We are now ready to prove the main theorem of this section.

Theorem X.2 Let A be a closed symmetric operator. The closed symmetric extensions of A are in one-to-one correspondence with the set of partial isometries (in the usual inner product) of $\mathscr{K}_+$ into $\mathscr{K}_-$. If U is such an isometry with initial space $I(U) \subseteq \mathscr{K}_+$, then the corresponding closed symmetric extension A_U has domain

$$D(A_U) = \{\varphi + \varphi_+ + U\varphi_+ \mid \varphi \in D(A), \varphi_+ \in I(U)\}$$

and

$$A_U(\varphi + \varphi_+ + U\varphi_+) = A\varphi + i\varphi_+ - iU\varphi_+$$

If $\dim I(U) < \infty$, the deficiency indices of A_U are

$$n_\pm(A_U) = n_\pm(A) - \dim[I(U)]$$

Proof Let A_1 be a closed symmetric extension of A. From the lemma we know that $D(A_1) = D(A) \oplus_A S_1$ where S_1 is an A-closed A-symmetric subspace of $\mathscr{K}_+ \oplus \mathscr{K}_-$. If $\varphi \in S_1$, it can be written uniquely as $\varphi = \varphi_+ + \varphi_-$. Since S_1 is A-symmetric

$$\begin{aligned} 0 &= (A^*\varphi, \varphi) - (\varphi, A^*\varphi) \\ &= 2i(\varphi_-, \varphi_-) - 2i(\varphi_+, \varphi_+) \end{aligned}$$

which implies that

$$\|\varphi_+\|^2 = \|\varphi_-\|^2 \tag{X.4}$$

Since S_1 is a subspace of $\mathscr{K}_+ \oplus_A \mathscr{K}_-$, (X.4) shows that $\varphi_+ \mapsto \varphi_-$ is a well-defined isometry from a subspace of $\mathscr{K}_+$ into $\mathscr{K}_-$. Call the corresponding partial isometry U. Then

$$D(A_1) = \{\varphi + \varphi_+ + U\varphi_+ \mid \varphi \in D(A), \varphi_+ \in I(U)\} \tag{X.5}$$

and

$$A_1(\varphi + \varphi_+ + U\varphi_+) = A^*(\varphi + \varphi_+ + U\varphi_+) = A\varphi + i\varphi_+ - iU\varphi_+ \tag{X.6}$$

Conversely, let U be an isometry from a subspace of $\mathscr{K}_+$ into $\mathscr{K}_-$ and define $D(A_1)$ and A_1 by (X.5) and (X.6). Then $D(A_1)$ is an A-closed, A-symmetric subspace of $D(A^*)$, so by the lemma, A_1 is a closed symmetric extension of A.

The statement about deficiency indices follows by looking at the ranges of $i + A_1$ and $i - A_1$ on $D(A_1)$. ▮

Corollary Let A be a closed symmetric operator with deficiency indices n_+ and n_-. Then,

(a) A is self-adjoint if and only if $n_+ = 0 = n_-$.
(b) A has self-adjoint extensions if and only if $n_+ = n_-$. There is a one–one correspondence between self-adjoint extensions of A and unitary maps from $\mathscr{K}_+$ onto $\mathscr{K}_-$.
(c) If either $n_+ = 0 \neq n_-$ or $n_- = 0 \neq n_+$, then A has no nontrivial symmetric extensions (such operators are called **maximal symmetric**).

Example 1 We will consider the example introduced in Section VIII.2 from several points of view. Let T be the operator $i\,d/dx$ on $L^2(0, 1)$ with the domain $D(T) = \{\varphi \mid \varphi \in AC[0, 1], \varphi(0) = 0 = \varphi(1)\}$. We showed in Section VIII.2 that T^* is the operator $i\,d/dx$ with domain $D(T^*) = AC[0, 1]$.

Since the operator T is so simple and since we know the domain of its adjoint explicitly, we can determine the self-adjoint extensions of T without using the machinery developed in this section. It is instructive to do that first. Suppose S is a symmetric extension of T. Since $D(S^*) \subset D(T^*)$, we know that the functions in $D(S^*)$ are absolutely continuous and $S^*\varphi = i\,d\varphi/dx$. Thus for $\varphi \in D(S)$ and $\psi \in D(S^*)$, integration by parts shows that

$$(S\varphi, \psi) - (\varphi, S^*\psi) = \overline{\varphi(1)}\psi(1) - \overline{\varphi(0)}\psi(0) = 0 \tag{X.7}$$

In the case $S = T$ we can see why T is not self-adjoint. The boundary conditions on the functions in $D(T)$ are so strong that no boundary conditions on the functions in $D(T^*)$ are necessary in order to ensure that the right-hand side of (X.7) equals zero. What is necessary is to extend the set of functions in $D(S)$ by allowing more general boundary conditions so that the equality (X.7) requires the *same* boundary conditions on the functions in $D(S^*)$. We now do this. Let S be a self-adjoint extension of T and suppose that $\varphi \in D(S)\backslash D(T)$. Then (X.7) requires that $|\varphi(1)|^2 = |\varphi(0)|^2$ and since $\varphi \notin D(T)$, $\varphi(0) \neq 0$, so there is an α with $|\alpha| = 1$ so that $\varphi(1) - \alpha\varphi(0) = 0$. If ψ is any other function in $D(S)$, then (X.7) requires that $\psi(1) = \alpha\psi(0)$ with the *same* α. Thus, $S \subset T_\alpha$ where $T_\alpha = i\,d/dx$ on

$$D(T_\alpha) = \{\varphi \mid \varphi \in AC[0, 1], \varphi(1) = \alpha\varphi(0)\}$$

Since T_α is symmetric and S is self-adjoint, $S = T_\alpha$ for some α.

Next, we determine which T_α are self-adjoint. Choose $\varphi \in D(T_\alpha)$ and $\psi \in D(T_\alpha^*)$. Then (X.7) requires that

$$\bar{\alpha}\,\overline{\varphi(0)}\psi(1) - \overline{\varphi(0)}\psi(0) = 0$$

so that $\psi(1) = \alpha\psi(0)$. Thus $\psi \in D(T_\alpha)$, so $D(T_\alpha^*) = D(T_\alpha)$, i.e. T_α is self-adjoint for each α. Thus, the set of self-adjoint extensions of T consists of the collection of operators $\{T_\alpha | \alpha \in \mathbb{C}, |\alpha| = 1\}$.

We now show how the machinery of this section leads to the same result. To determine $\mathscr{K}_+$, we must find the solutions of $T^*\psi = i\psi$. If $\psi \in D(T^*)$, then $\psi \in AC[0, 1]$, and the equality $i\, d\psi/dx = i\psi$ shows that ψ' is also absolutely continuous. Repeating this argument shows that any solution of $T^*\psi = i\psi$ is in fact infinitely differentiable and satisfies $\psi' = \psi$. Thus $\mathscr{K}_+ = \{ce^x | c \in \mathbb{C}\}$, and similarly $\mathscr{K}_- = \{ce^{-x} | c \in \mathbb{C}\}$. Therefore, the deficiency indices of T are $\langle 1, 1\rangle$. Let

$$\varphi_+ = \frac{\sqrt{2}}{\sqrt{e^2 - 1}}\, e^x \qquad \text{and} \qquad \varphi_- = \frac{\sqrt{2}\, e}{\sqrt{e^2 - 1}}\, e^{-x}$$

be normalized vectors from $\mathscr{K}_\pm$. Then the only partial isometries of $\mathscr{K}_+$ into $\mathscr{K}_-$ are the maps $\varphi_+ \mapsto \gamma\varphi_-$ where $|\gamma| = 1$. By Theorem X.2, the only symmetric extensions of T are the operators $A_\gamma = i\, d/dx$ with domain

$$D(A_\gamma) = \{\varphi + \beta\varphi_+ + \gamma\beta\varphi_- \mid \varphi \in D(T), \beta \in \mathbb{C}\}$$

By the last statement of Theorem X.2, each A_γ has zero deficiency indices and is therefore self-adjoint. To see that these are the same operators we got before, notice that if $\psi \in D(A_\gamma)$, then

$$\psi(0) = \frac{\beta(1 + \gamma e)\sqrt{2}}{\sqrt{e^2 - 1}} \qquad \text{and} \qquad \psi(1) = \frac{\sqrt{2}\,\beta(\gamma + e)}{\sqrt{e^2 - 1}}$$

so

$$\psi(1) = \frac{\gamma + e}{1 + \gamma e}\, \psi(0) = \alpha\psi(0) \qquad \text{where} \quad |\alpha| = \left|\frac{\gamma + e}{1 + \gamma e}\right| = 1$$

Conversely, if $\psi(1) = \alpha\psi(0)$, then ψ can be written $\psi = \varphi + \beta\varphi_+ + \gamma\beta\varphi_-$ for some β where $\gamma = (\alpha - e)/(1 - \alpha e)$. Thus, $A_\gamma = T_\alpha$.

We now examine the same problem from a "physical" point of view. Suppose that we have a smooth wave packet $\varphi(x)$ on $[0, 1]$ which is zero near the end points and which is being translated to the right (Figure X.1). For small enough y (so that the packet does not get to the end), the translations are given by the family of operators $U(y)$: $\varphi(x) \to \varphi(x - y)$. In quantum mechanics, translation should be represented by a unitary group whose generator is the momentum operator. For the wave packet $\varphi(x)$, this is the case:

$$\lim_{y\to 0} \frac{U(y)\varphi - \varphi}{iy} = \lim_{y \to 0} \frac{\varphi(x - y) - \varphi(x)}{iy} = i\, \frac{d}{dx}\, \varphi$$

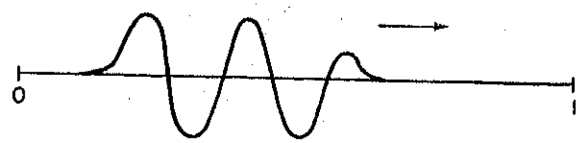

FIGURE X.1 The wave packet $\varphi(x)$.

So, the generator of translation acts like $i\, d/dx$ on the functions with support away from the end points. In fact, $i\, d/dx$ is symmetric on $C_0^1(0, 1)$, the C^1 functions of compact support on $(0, 1)$, and its closure is just our operator T. But T is not self-adjoint and the reason is clear: We have specified the translation $U(y)$ only for functions whose support does not contain zero or one and then only for sufficiently small y (depending on the support). We must specify what happens when the wave packet gets to the end! If we want translation to be represented by a unitary group, then what goes out at one end must come in at the other (as though the interval [0, 1] were bent into a circle). That is, unitarity requires

$$\int_0^1 |\varphi(x - y)|^2\, dx = \int_0^1 |\varphi(x)|^2\, dx$$

where $x - y$ means translation mod 1. However, we still have the freedom of choosing the phase of the wave packet as it comes in at zero. By the superposition principle all functions must change by the same phase when they come back in. Thus the different "translations" are just given by specifying α, $|\alpha| = 1$ and by requiring that all reasonable wave packets $\psi_y \equiv \varphi(\cdot + y)$ satisfy $\psi_y(1) = \alpha\psi_y(0)$ for *all* times y. This motion is just given by e^{iyT_α} where T_α is the operator described above. Thus, even in this physically trivial situation we see that *different* self-adjoint extensions correspond to *different physics*.

A simple and useful criterion for a symmetric operator to have self-adjoint extensions is given by the following theorem.

Definition An antilinear map C: $\mathscr{H} \to \mathscr{H}$ $(C(\alpha\varphi + \beta\psi) = \bar{\alpha}C\varphi + \bar{\beta}C\psi)$ is called a **conjugation** if it is norm-preserving and $C^2 = I$.

Theorem X.3 (von Neumann's theorem) Let A be a symmetric operator and suppose that there exists a conjugation C with C: $D(A) \to D(A)$ and $AC = CA$. Then A has equal deficiency indices and therefore has self-adjoint extensions.