Some references on self-adjoint extensions:

N. I. Akhiezer & I. M. Glazman, Theory of Linear Operators in Hilbert Space
Volume II, Ch VII, somewhat terse but an excellent reference. Note the unconventional definition of point and continuous spectrum.

M. A. Naimark. Linear Differential Operators

Volume II, Ch IV.14 for self-adjoint extensions, Ch V for the specific application to differential operators

R. T. W. Martin. Bandlimited functions, curved manifolds, and self-adjoint extensions of symmetric operators. https://uwspace.uwaterloo.ca/handle/10012/3698

Part 2 Ch 4 for a self-contained account of the theory of self-adjoint extensions, Part 3 Ch 9 for a discussion of Krein's formula

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Journal Club: Self-Adjoint Extensions

1. Introduction: the Momentum Operator

- consider the momentum operator for a 1D particle in QM

$$p = -i \frac{d}{dx}$$

Q: Is the momentum op. self-adjoint?

a) yes

b) no

c) maybe ← depends on the domain

Physical Intuition:

- if self-adjoint → $\exists$ momentum eigenstates, observable
  → states of definite momentum

ex 1 real line $(-\infty, \infty)$: $\exists$? states of definite p?
→ yes: plane waves

ex 2 (a, ∞) : · only states of definite p in one direction
· not self-adjoint

ex 3 (a, b) : · sometimes $\exists$ states of definite p
· depends on boundary conditions

- cheated a bit. p above is not an operator per se
- need to specify domain and $\mathcal{H}$
- an op is self-adjoint if $D(T) = D(T^*)$

Theory of Self-Adjoint Extensions

- tells you under what circumstances $\exists$ self-adjoint realizations
- tells you how to construct self-adjoint operators
- formal theory of boundary conditions

1. Basic Notions

Def^n Let $T : D(T) \subset \mathcal{H} \longrightarrow R(T) \subset \mathcal{H}$ be a linear operator. The domain of its adjoint T^* is

$$D(T^*) = \{ g \in \mathcal{H} : \exists\, h_g \text{ s.t. } \langle Tf | g \rangle = \langle f | h_g \rangle \ \forall f \in D(T) \}$$

and $T^* : g \longmapsto T^* g = h_g$

Def^n T is Hermitian if $\langle Tf | g \rangle = \langle f | Tg \rangle \quad \forall f, g \in D(T)$

Def^n T is symmetric if it is Hermitian & densely defined

Def^n A symm. op. T is self-adjoint if $T = T^*$, i.e., $D(T) = D(T^*)$

ex Momentum operator on the interval (a,b),

$$\mathcal{H} = L^2(a,b), \qquad \langle f | g \rangle = \int_a^b f^*(x) g(x)\, dx$$

Q: largest domain on which $p = -i\partial_x$ may act?

$$D(P_{max}) = \{ \psi \in L^2(a,b) \mid \psi \in AC(a,b),\ \psi' \in L^2(a,b) \}$$

- let $f, g \in D(P_{max})$

$$\langle P_{max} f | g \rangle = \int_a^b (-if'(x))^* g(x)\, dx$$

$$= i f^*(x) g(x) \Big|_a^b - \int_a^b f^*(x) \cdot i g'(x)\, dx$$

$$= i[f^*(b) g(b) - f(a) g(a)] + \underbrace{\int_a^b f^*(x) (-ig'(x))\, dx}_{\langle f | P_{max} g \rangle}$$

note: if $f(a) = f(b) = 0$

this vanishes!

Define the symm. op. P_o : $D(P_o) = \{ \psi \in D(P_{max}) \mid \psi(a) = \psi(b) = 0 \}$

✓ Hermitian

✓ Densely-defined (e.g. square-well NRIG eigenbasis)

- $\mathcal{D}(P_0)$ is smallest possible domain of def^n for a symm. realization of $p = -i\partial_x$
- $(P_0)^* = P_{max}$ the adjoint
- $P_0 \neq P_{max}$ (since $\mathcal{D}(P_0) \neq \mathcal{D}(P_{max})$) $\square$

Def^n T' is an extension of T if $\mathcal{D}(T) \subseteq \mathcal{D}(T')$ and $T'f = Tf$ for $f \in \mathcal{D}(T)$.
We write $T \subset T'$

Prop^n $T \subset T^*$

ex Momentum operator
- need $f^*(b)g(b) - f^*(a)g(a)$ to vanish
- sps. $f(a) = f(b)$ $\Rightarrow$ $f^*(a)\,(g(b) - g(a)) \overset{?}{=} 0$
  $\Rightarrow$ also need $g(b) = g(a)$

Define P' : $\mathcal{D}(P') = \{ \psi \in \mathcal{D}(P_{max}) \mid \psi(a) = \psi(b) \}$
Note: - $P_0 \subset P'$
- $\mathcal{D}(P'^*) = \mathcal{D}(P')$ $\Rightarrow$ P' is a self-adjoint extension of P_0

- all s.adj. exts. parametrized by $\theta \in [0, 2\pi)$
$$\mathcal{D}(P'_\alpha) = \{ \psi \in \mathcal{D}(P_{max}) \mid \psi(a) = e^{i\theta}\psi(b) \}$$ $\square$

Prop^n If $T \subset T'$, then $(T')^* \subset T^*$ for T symm.

$\Rightarrow$ $T \subset T' \subset (T')^* \subset T^*$
constructing s.adj. exts $\longleftrightarrow$ "borrowing" from $\mathcal{D}(T^*)$ so that $\mathcal{D}(T') = \mathcal{D}(T'^*)$

3. Von Neumann Formulas & Cayley Transform

Thm I Let S: closed symm. op. Then $\mathcal{D}(S^*) = \mathcal{D}(S) + N_+ + N_-$

where $N_\pm := \ker(S^* \mp i) = (\mathcal{R}(S \pm i))^\perp$

Note: · $N_\pm$ are the deficiency spaces of S

· eigenspaces of S^* to eigenvalue $\pm i$,

i.e. $\phi \in N_\pm \iff S^*\phi = \pm i \phi$

· Thm I tells us $\mathcal{D}(S^*)$, $\mathcal{D}(S)$ differ only by vectors in the deficiency spaces

Thm II Let S: closed symm. op

a) S' is a closed symm. ext. of S iff $\exists$ closed subspaces $F_\pm \subseteq N_\pm$ and an isometry $\tilde{V}: F_- \to F_+$ such that

$$\mathcal{D}(S') = \mathcal{D}(S) + \{ g + Vg : g \in F_- \}$$

b) S' is self-adjoint iff $F_+ = N_+$, $F_- = N_-$

Def^n $n_\pm := \dim N_\pm$ are the deficiency indices of S

Thm II $\Rightarrow$ self-adjoint extensions only exist if $n_+ = n_-$

(why? need isometry $\tilde{V}: N_- \to N_+$)

· Thms I, II are in principle constructive, but rather unwieldy...

· More algorithmic: Cayley transform

· Let S: closed symm. op.

· Define $V := (S - i)(S + i)^{-1}$

· Can show that V is an isometry on its domain

· Idea: construct unitary extensions of V

// usually, isometries & unitaries easier to work with than sym. & s.-adj.

// ops since unitaries act on all of $\mathcal{H}$

- heuristic: V is "missing" the dimensions spanned by N_- from its domain, N_+ from its range
- if we can find an isometry $\tilde{V}: N_- \to N_+$

Define $U: \begin{cases} \psi \to V\psi & \psi \in \mathcal{H} \ominus N_- \\ \psi \to \tilde{V}\psi & \psi \in N_- \end{cases}$ rest by linearity

$\to$ U is now unitary

Inverse transform gives $T = -i(U+1)(U-1)^{-1}$ self-adjoint ($U(n_\pm)$-param.)

Example: Momentum operator on $L^2(0,1)$

① Deficiency spaces: $P_0^* \phi = \pm i\phi \Rightarrow -i\phi'(x) = \pm i\phi$

$\phi'(x) = \mp\phi \Rightarrow \phi(x) = Ce^{\mp x}$

$\to$ both are square-integrable on $(0,1)$, i.e. in $\mathcal{H} = L^2(0,1)$

$\to$ choose deficiency vectors $v_+(x) = e^{1-x}$ (chosen so $\|v_+\| = \|v_-\|$)

$v_-(x) = e^{x}$

$\Rightarrow$ $N_+ = \mathbb{C}v_+$, $N_- = \mathbb{C}v_-$ $n_+ = n_- = 1$

$\Rightarrow$ self-adjoint extensions exist, $U(1)$ family

② Cayley transform: $V := (P_0 - i)(P_0 + i)^{-1}$

- let $f \in \mathcal{D}(P_0)$, $(P_0 + i)f = g \Rightarrow -if'(x) + if(x) = g(x)$

$(\ldots)$

$f(x) = ie^{x}\int_0^x e^{-y} g(y)\, dy$

So $V: g \longmapsto (-i\partial_x - i)\left(ie^x \int_0^x e^{-y} g(y)\, dy\right) = 2e^x \int_0^x e^{-y} g(y)\, dy + g(x)$

(not too illuminating, but want to demonstrate calculations)

- isometries b/w $N_- \to N_+$ given by $e^x \longrightarrow e^{i\alpha} e^{1-x}$ $\alpha \in [0, 2\pi)$

(clear from def^{n} of V that dimension $\ker(P_0^* + i) = N_-$ is missing, restored here)

$\Rightarrow$ $U(1)$ family of self-adjoint ops $P_\alpha := -i(U_\alpha + 1)(U_\alpha - 1)^{-1}$

From def^{n}, $\mathcal{D}(P_\alpha) = \mathcal{R}(U_\alpha - 1) = \mathcal{H}$

$\mathcal{R}(P_\alpha) = \mathcal{R}(U_\alpha + 1) = \mathcal{H}$ ✓

How to relate to boundary condition?

consider, sps. $g \in \mathcal{D}(P_\alpha)$, i.e. $g = (U_\alpha - 1)f$ for some $f \in \mathcal{H}$

$$\Rightarrow \quad g = \begin{cases} Vf - f & \text{if } f \in \mathcal{H} \ominus N_- \longrightarrow \text{trivial B.C.} \\ \alpha \, e^{i\alpha} e^{1-x} - e^{x} & \text{if } f \in N_- \end{cases}$$

$$g(0) = e\,e^{i\alpha} - 1 \qquad \Rightarrow \qquad \frac{g(1)}{g(0)} = \frac{e^{i\alpha} - e}{e\,e^{i\alpha} - 1}$$

$$g(1) = e^{i\alpha} - e$$

$\therefore$ can check $\left| \frac{g(1)}{g(0)} \right| = 1$, i.e. $g(1) = g(0) \cdot e^{i\theta(\alpha)}$