Self-Adjoint Operator

A *self-adjoint operator* $\hat{L}$ on domain $\mathscr{D}$ is *formally self-adjoint* ($\hat{L} = \hat{L}^\dagger$) and has *self-adjoint boundary condition* such that it satisfies the *Lagrange's Identity for ODE* and $Q(x)|_{\text{boundary}} = 0$

$$\boxed{w(u^*\hat{L}v - (\hat{L}^\dagger u)^* v) = \frac{d}{dx}Q(x)} \tag{1}$$

where $Q(u(x), u'(x), u''(x), \cdots, v(x), v'(x), v''(x), \cdots)$ is a bilinear function of $u(x), u'(x), \cdots,\ v(x), v'(x), \cdots$. $w(x)$ is a weight function. The boxed *Lagrange's Identity for ODE* is worth committing to memory.

Formally Self-Adjoint

Given the form of $\hat{L}$ and $w(x)$, the *formal adjoint* $\hat{L}^\dagger$ is defined to be the operator that completes Lagrange's Identity with $\hat{L}$ for any functions $u(x)$ and $v(x)$. Notice it's not an operator since no domain was specified. The operator $\hat{L}$ is said to be formally self-adjoint if it is equal to its adjoint $\hat{L} = \hat{L}^\dagger$ irrespective of their domains $\mathscr{D}$, $\mathscr{D}^\dagger$

$$w(u\hat{L}v - \hat{L}^\dagger u, v) = \frac{d}{dx}Q(u, v) \tag{2}$$

To find the formal adjoint of $\hat{L}$, one should start with $wu\hat{L}v$ and move all the differentials across u^* by using the commutation relation

$$[\frac{d}{dx}, f(x)] = f'(x) \Rightarrow f\frac{d}{dx} = \frac{d}{dx}f - f' \tag{3}$$

Example To find the formal adjoint of $\hat{L} = i\frac{d}{dx}$
Start with $wu^*\hat{L}v$ and move the $\frac{d}{dx}$ across u^*

$$wu^*\hat{L}v = wu^*iv' = w\frac{d}{dx}u^*vi - wu^{*\prime}vi \Rightarrow$$
$$wu\hat{L}v + wu^{*\prime}vi = w\frac{d}{dx}u^*vi \tag{4}$$

move $\frac{d}{dx}$ across w on the RHS to get Q

$$wu\hat{L}v + wu^{*\prime}vi = \frac{d}{dx}wu^*vi - w'u^*vi \Rightarrow$$
$$wu\hat{L}v - (-wu^{*\prime}vi - w'u^*vi) = \frac{d}{dx}wu^*vi = \frac{d}{dx}Q \tag{5}$$

Identify $\hat{L}^\dagger$

$$\begin{aligned} w(\hat{L}^\dagger u)^* v &= -wu^{*\prime} vi - w' u^* vi \Rightarrow \\ (\hat{L}^\dagger u)^* = -iu^{*\prime} - i\frac{w'}{w}u^* &= \left(i\frac{d}{dx} + i\frac{w'}{w}\right)^* \Rightarrow \\ \hat{L}^\dagger &= i\frac{d}{dx} + i\frac{w'}{w} \end{aligned} \tag{6}$$

Therefore $\hat{L}$ is formally adjoint when $\frac{w'}{w} = 0$.

Self-Adjoint Boundary Condition

For operator $\hat{L}$ on $\mathscr{D}$ to have *adjoint boundary condition*, the adjoint domain $\mathscr{D}^\dagger$ makes $Q|_a^b$ vanish. $\hat{L}$ on $\mathscr{D}$ is said to have self-adjoint boundary condition if $\mathscr{D} = \mathscr{D}^\dagger$

Example To find adjoint boundary condition for $\hat{L} = \frac{d^2}{dx^2}$ on $\mathscr{D} = \{v(x) \in L^2[0,1] | v(0) = 0, v'(0) = 1\}$, we first find its formal adjoint

$$\begin{aligned} u^* v'' = \frac{d}{dx}(u^* v') - u^{*\prime} v' &= \frac{d}{dx}(u^* v' - u^{*\prime} v) + u^{*\prime\prime} v \Rightarrow \\ u^* v'' - u^{*\prime\prime} v &= \frac{d}{dx}(u^* v' - u^{*\prime} v) \end{aligned} \tag{7}$$

We identify

$$\begin{cases} \hat{L}^\dagger = \frac{d^2}{dx^2} \\ Q = u^* v' - u^{*\prime} v \end{cases} \tag{8}$$

We thus need

$$\begin{aligned} Q|_0^1 = 0 \Rightarrow (u^*(1)v'(1) - u^{*\prime}(1)v(1)) - (u^*(0)v'(0) - u^{*\prime}(0)v(0)) = 0 \Rightarrow \\ u^*(1)v'(1) - u^{*\prime}(1)v(1) - u^*(0) = 0 \end{aligned} \tag{9}$$

Therefore

$$\mathscr{D}^\dagger = \{u(x) | u(1) = u'(1) = 0, u(0) = 0\} \tag{10}$$

$\mathscr{D}^\dagger \neq \mathscr{D}$, therefore $\hat{L}$ on $\mathscr{D}$ does not have self-adjoint boundary condition.