Self-adjoint extensions of symmetric operators

Theorem (Reed/Simon I, Thm VIII.3) If A is a closed symmetric operator in $\mathcal{H}$, the following are equivalent:

(a) A is self-adjoint,

(b) $\operatorname{Ker}(A^* \pm i) = \{0\}$, ($A^* \pm i$ are injective)

(c) $\operatorname{Ran}(A \pm i) = \mathcal{H}$. ($A \pm i$ are surjective)

The spaces $K_+ = \operatorname{Ker}(A^* - i)$ and $K_- = \operatorname{Ker}(A^* + i)$ are called the deficiency subspaces of A, and $n_+(A) = \dim K_+$, $n_-(A) = \dim K_-$ are the deficiency indices of A.

Lemma (R/S II §X.1) If A is a closed symmetric operator in $\mathcal{H}$, then

$$\mathcal{D}(A^*) = \mathcal{D}(A) \oplus_A K_+ \oplus_A K_-,$$

in which $\oplus_A$ indicates a Hilbert-space direct sum in $\mathcal{D}(A^*)$, with respect to the inner product $(u,v)_A = (A^* u, A^* v) + (u,v)$.
In particular, the three subspaces in this sum are closed and mutually orthogonal in the Hilbert space $(\mathcal{D}(A^*), (\cdot,\cdot)_A)$.

$\boxed{\text{Theorem}}$ (R/S, Cor. to Thm X.2) Let A be a closed symmetric operator in $\mathcal{H}$:

(a) A has self-adjoint extensions if and only if $n_+ = n_-$, and
A is self-adjoint if and only if $n_+ = n_- = 0$.

(b) If $n_+ = n_-$, there is a one-to-one correspondence between self-adjoint extensions of A and unitary operators $U : K_+ \to K_-$. The extension A_U corresp. to U is

$$\begin{cases} \mathcal{D}(A_U) = \{ v + v_+ + Uv_+ : v \in \mathcal{D}(A),\ v_+ \in K_+ \}, \\ A_U v = A^* v \quad \text{for } u \in \mathcal{D}(A_U). \end{cases}$$

The Friedrichs Extension (See R/S II Thm X.23)

We have mentioned the one-to-one correspondence between positive self-adjoint operators and positive closed quadratic forms. In fact, each positive symmetric operator A_0 gives rise to a quadratic form q through $Q(q) = \mathcal{D}(A)$, $q(u,v) = (Au,v)$, and this form has a closure $\hat{q}$, which is positive. To $\hat{q}$, there corresponds a self-adjoint extension $\hat{A}$ of A_0, called the Friedrichs extension of A_0.

The Friedrichs extension has the property (among others), that it is the unique self-adjoint extension A of A_0 such that $\mathcal{D}(A) \subset Q(\hat{q})$.

Let us place the operators associated with $\varepsilon^{-1}\nabla\cdot\sigma\nabla$ into the context of self-adjoint extensions and quadratic forms.

The relevant closed symmetric operator is $A_0 = T^* T_0$ in $L^2(\Omega,\varepsilon)$:

$$\begin{cases} \mathcal{D}(A_0) = \{u \in H^1(\Omega) : \sigma\nabla u \in \mathcal{D}(\nabla\cdot),\ u|_{\partial\Omega} = 0,\ \sigma\nabla u\cdot n = 0\}, \\ A_0 u = \varepsilon^{-1}\nabla\cdot\sigma\nabla u \quad \text{for } u \in \mathcal{D}(A_0). \end{cases}$$

The adjoint A_0^* of A_0 is $T_0^* T$:

$$\begin{cases} \mathcal{D}(A_0^*) = \{u \in H^1(\Omega) : \sigma\nabla u \in \mathcal{D}(\nabla\cdot)\}, \\ A_0^* u = \varepsilon^{-1}\nabla\cdot\sigma\nabla u \quad \text{for } u \in \mathcal{D}(A_0^*). \end{cases}$$

The closed quadratic form $\hat{q}$ corresponding to A_0 is

$$\begin{cases} Q(\hat{q}) = H^1_0(\Omega) \subset L^2(\Omega,\varepsilon), \\ \hat{q}(u,v) = \int_\Omega \sigma \nabla u \cdot \nabla \bar{v} \quad , \end{cases}$$

and the Friedrichs extension $\hat{A}$ of A_0 is the Dirichlet operator $A_D = T_0^* T_0$:

$$\begin{cases} \mathcal{D}(A_D) = \{ u \in H^1(\Omega) : \sigma \nabla u \in \mathcal{D}(\nabla\cdot),\ u|_{\partial\Omega} = 0 \}, \\ A_D u = \varepsilon^{-1} \nabla \cdot \sigma \nabla u \ . \end{cases}$$

Notice that the Neumann extension A_N, for example, has $\mathcal{D}(A_N) \not\subset Q(q)$, for

$$\mathcal{D}(A_N) = \{ u \in H^1(\Omega) : \sigma \nabla u \in \mathcal{D}(\nabla\cdot),\ \sigma \nabla u \cdot n = 0 \},$$

and thus includes functions with nonzero boundary values, such as nonzero constant functions.

A one-dimensional example (in ODEs) provides an excellent and important illustration of self-adjoint extensions of a symmetric operator and the corresponding quadratic forms.

The Hilbert space is $L^2(0,1)$, and we begin with the closed operator ∂_x° :

$$\begin{cases} \mathcal{D}(\partial_x^\circ) = H^1_0(0,1), \\ \partial_x^\circ u = \partial_x u \ \left(= \frac{\partial u}{\partial x} = u' \right) \quad \text{for } u \in H^1_0(0,1). \end{cases}$$

The adjoint of ∂_x° is given by

$$\begin{cases} \mathcal{D}(\partial_x^{\circ *}) = H^1(0,1), \\ \partial_x^{\circ *} u = -\partial_x u \quad \text{for} \quad u \in H^1(0,1). \end{cases}$$

This is just the definition of $-\partial_x$, so we have

$$\partial_x^{\circ *} = -\partial_x .$$

So ∂_x° and $-\partial_x$ are mutually adjoint.

Our closed symmetric operator in $L^2(0,1)$ is $(\partial_x^\circ)^2 = A_0$:

$$\begin{cases} \mathcal{D}(A_0) = \{ u \in H_0^1(0,1) : \partial_x u \in H_0^1(0,1) \}, \\ A_0 u = \partial_{xx} u . \end{cases}$$

The adjoint A_0^* of A_0 is

$$\begin{cases} \mathcal{D}(A_0^*) = \{ H^1(0,1) : \partial_x u \in H^1(0,1) \}, \\ A_0^* u = \partial_{xx} u . \end{cases}$$

In fact, A_0^* is the second derivative, defined on its maximal domain in the L^2 sense. It is denoted simply by ∂_{xx}, and its domain is $H^2(0,1)$. The domain of A_0 is $H_0^2(0,1)$, consisting of all L^2 functions with first and second derivatives having vanishing trace on $(0,1)$:

$$\mathcal{D}(\partial_{xx}^\circ) = H_0^2(0,1) = \{ u \in L^2 : u' \in L^2,\ u'' \in L^2,\ u(0) = u(1) = 0,\ u'(0) = u'(1) = 0 \},$$

$$\mathcal{D}(\partial_{xx}) = H^2(0,1) = \{ u \in L^2 : u' \in L^2,\ u'' \in L^2 \}.$$

We will use the notation $A_0 = \partial_{xx}^{\circ}$ and $A_0^* = \partial_{xx}$, and we have

$$\mathcal{D}(\partial_{xx}^{\circ}) = H_0^2(0,1) \subsetneq H^2(0,1) = \mathcal{D}(\partial_{xx}) ,$$

Thus ∂_{xx}° is closed and symmetric but not self-adjoint, and

$$\mathrm{Ker}(\partial_{xx} - i) = \mathrm{span}\{e^{\sqrt{i}\,x}, e^{-\sqrt{i}\,x}\} \cong \mathbb{C}^2 ,$$

$$\mathrm{Ker}(\partial_{xx} + i) = \mathrm{span}\{e^{\sqrt{-i}\,x}, e^{-\sqrt{-i}\,x}\} \cong \mathbb{C}^2 ,$$

and $n_+ = n_- = 2$, that is, ∂_{xx}° has deficiency index 2. This means that there is a one-to-one correspondence between unitary 2×2 matrices and self-adjoint extensions of ∂_{xx}°. The group of 2×2 unitary matrices is a <u>fine-dimensional</u> Lie group.

Each self-adjoint extension of ∂_{xx}° is characterized by homogeneous boundary-value conditions, as manifested by the relation

$$(A^* u, v) - (u, A^* v) = \int_0^1 (u'' \bar{v} - u \bar{v}'') =$$

$$= \left[u'(1)\bar{v}(1) - u(1)\bar{v}'(1)\right] - \left[u'(0)\bar{v}(0) - u(0)\bar{v}'(0)\right] .$$

The domain of a self-adjoint extension is a maximal sub-Hilbert space of $H^2(0,1)$ for which this expression vanishes.

These are some of the common extensions of ∂_{xx}° with corresponding quad. forms:

- The Friedrichs extension, which is the Dirichlet second derivative operator:

$$\mathcal{D}(\partial_{xx}^{D}) = \{ u \in H^2(0,1) : u(0) = u(1) = 0 \},$$

$$Q(\partial_{xx}^{D}) := Q(q^{D}) = H_0^1(0,1) \quad ; \quad q^{D}(u,v) = \int_0^1 u' \bar{v}' .$$

- The Neumann extension:

$$\mathcal{D}(\partial_{xx}^{N}) = \{ u \in H^2(0,1) : u'(0) = u'(1) = 0 \},$$

$$Q(\partial_{xx}^{N}) := Q(q^{N}) = H^1(0,1) \quad ; \quad q^{N}(u,v) = \int_0^1 u' \bar{v}' .$$

- The Robin extensions:

$$\mathcal{D}(\partial_{xx}^{R}) = \{ u \in H^2(0,1) : \alpha_0 u(0) + u'(0) = 0, \ \alpha_1 u(1) + u'(1) = 0, \ \alpha_0, \alpha_1 > 0 \},$$

$$Q(\partial_{xx}^{R}) := Q(q^{R}) = H^1(0,1) \quad ; \quad q^{R}(u,v) = \int_0^1 u' \bar{v}' + \alpha_0 |u(0)|^2 + \alpha_1 |u(1)|^2 .$$

- The κ-pseudo-periodic extensions ($\kappa = 0 \rightsquigarrow$ periodic extension):

$$\mathcal{D}(\partial_{xx}^{\kappa}) = \{ u \in H^2(0,1) : u(1) = e^{i\kappa} u(0), \ u'(1) = e^{i\kappa} u'(0) \},$$

$$Q(\partial_{xx}^{\kappa}) := Q(q^{\kappa}) = H_{\kappa}^1(0,1) = \{ u \in H^1(0,1) : u(1) = \kappa u(0) \}.$$

The minimum and minimax principles (Reed/Simon IV, Weinstein/Stenger, for ex.)

Suppose that the self-adjoint operator A in $\mathcal{H}$ is such that $(A-\lambda)$ has a bounded inverse for all $\lambda < \lambda_+ \leq \infty$, except for a set $\{\lambda_i\}_{i=0}^{N}$ $(N \leq \infty)$ of eigenvalues with $\lambda_i \leq \lambda_{i+1} < \lambda_+$ with corresponding eigenvectors $\{u_i\}_{i=0}^{N}$.

If q is the associated quadratic form with domain $Q(q)$, denote $Q(A) = Q(q)$. We have $\mathcal{D}(A) \subset Q(A)$. The Rayleigh quotient is defined by

$$R(u) = \frac{q(u,u)}{(u,u)} \quad \text{for} \quad u \in Q(A),$$

so $R(u) = \dfrac{(Au,u)}{(u,u)}$ for $u \in \mathcal{D}(A)$. Then we have

$$\lambda_0 = \inf_{\substack{\psi \in Q(A) \\ \psi \neq 0}} R(\psi) = \inf_{\substack{\psi \in \mathcal{D}(A) \\ \psi \neq 0}} R(\psi)$$

$$\lambda_n = \inf_{\substack{\psi \in Q(A) \\ \psi \neq 0,\, \psi \perp \{u_i\}_{i=1}^{n-1}}} R(\psi) = \inf_{\substack{\psi \in \mathcal{D}(A) \\ \psi \neq 0,\, \psi \perp \{u_i\}_{i=1}^{n-1}}} R(\psi), \quad n > 0.$$

Also, we have

$$\lambda_n = \sup_{\varphi_1 \cdots \varphi_{n-1}} \inf_{\substack{\psi \in \mathcal{D}(A) \\ \psi \in \{\varphi_1, \ldots, \varphi_{n-1}\}^{\perp} \\ \psi \neq 0}} R(\psi)$$

$$= \sup_{\varphi_1 \cdots \varphi_{n-1}} \inf_{\substack{\psi \in Q(A) \\ \psi \in \{\varphi_1 \ldots \varphi_{n-1}\}^{\perp} \\ \psi \neq 0}} R(\psi).$$

There is also a inf-sup, or min-max, formulation of this principle.

Time evolution by self-adjoint operators : unitary groups.

A typical time-dependent problem in physics involves a differential operator as the propagator and some physical boundary conditions. In systems in which energy is conserved in some way, the problem can often be posed as one of the following; where A is a self-adjoint operator (taking boundary conditions into account) in a Hilbert space $\mathcal{H}$, typically $L^2(\Omega)$.

(1) $u_t = -Au$, $u(0) = u_0 \in \mathcal{H}$, A positive $[(Au,u) \geq 0 \ \forall u \in \mathcal{D}(A)]$

(2) $iu_t = Au$, $u(0) = u_0 \in \mathcal{H}$,

(3) $u_{tt} = Au$, $u(0) = u_0$, $u_t(0) = v_0$.

The third of these can be cast in first order as follows.
Suppose that $A = T^*T$, where $T : \mathcal{D}(T) \subset \mathcal{H} \longrightarrow K$, and define a new operator $\mathcal{A}$ in $\mathcal{D}(T) \oplus \mathcal{H}$ by

$$\begin{cases} \mathcal{D}(\mathcal{A}) = \mathcal{D}(T^*T) \oplus \mathcal{D}(T) \subset \mathcal{D}(T) \oplus \mathcal{H} \\ \mathcal{A} = \begin{bmatrix} 0 & I \\ -T^*T & 0 \end{bmatrix}, \text{ that is,} \end{cases}$$

$$\mathcal{A}\begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} v \\ -T^*Tu \end{bmatrix} \quad \text{for} \quad \begin{bmatrix} u \\ v \end{bmatrix} \in \mathcal{D}(\mathcal{A}).$$

One can show that $i\mathcal{A}$ is self-adjoint in $\mathcal{D}(T) \oplus \mathcal{H}$.

Equation (3) no becomes

$$(3') \quad \begin{pmatrix} u_t \\ v_t \end{pmatrix} = \mathcal{A} \begin{pmatrix} u \\ v \end{pmatrix}, \quad \begin{pmatrix} u(0) \\ v(0) \end{pmatrix} = \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} \in \mathcal{D}(T) \oplus \mathcal{H}$$

Notice that the initial condition is not in $\mathcal{D}(A)$ (or $\mathcal{D}(\mathcal{A})$ for (3')) but in $\mathcal{H}$ (or $\mathcal{D}(T) \oplus \mathcal{H}$ for (3')), so the equation does not make sense as written. However, there is a natural way to define the dynamics for all initial conditions in the underlying Hilbert space. For $u_0 \in \mathcal{D}(A)$, there is a unique solution $u(t)$, which, for each t, is a bounded function of the initial condition u_0 in the $\mathcal{H}$ norm. The solution can thus be extended to initial conditions in $\mathcal{H}$.

Let us deal with problem (2), which subsumes (3').

<u>Defn</u> A <u>strongly continuous</u> <u>one-parameter</u> <u>unitary group</u> of operators $U(t)$ in $\mathcal{H}$ is a map from $\mathbb{R}$ to the space of unitary (i.e., norm-preserving) operators on $\mathcal{H}$ such that

(a) $U(t+s) = U(t)U(s) \quad \forall \; s,t \in \mathbb{R}$ (homomorphism)

(b) If $v \in \mathcal{H}$, then $U(t)v \to U(t_0)v$ as $t \to t_0$. (str. cont.)

<u>Stone's Theorem</u> There is a one-to-one correspondence between self-adjoint operators in $\mathcal{H}$ and strongly continuous one-parameter unitary groups in $\mathcal{H}$ that satisfies the following conditions.
If $U(t)$ is the unitary group corresponding to the self-adjoint operator A,

(i) For $u \in \mathcal{D}(A)$, $\frac{1}{t}(U(t)u - u) \longrightarrow iAu$ as $t \to 0$;

(ii) If $\lim_{t\to 0} \frac{1}{t}(U(t)u - u)$ exists, then $u \in \mathcal{D}(A)$.

See, for example, Reed/Simon I, Theorems VIII.7 and VIII.8 for a proof. The more difficult direction, that each $U(t)$ corresponds to some A is what is called Stone's Theorem. This theorem gives meaning to the equation

(*) $$u_t = iAu, \quad u(0) = u_0$$

and its solution $U(t)u_0$. $U(t)$ is commonly denoted by e^{iAt}.

$$u(t) = U(t)u_0 = e^{iAt}u_0 .$$

Condition (i) in the theorem and property (a) of the definition of a unitary group justify (*), and the notation e^{iAt} is well defined in the functional calculus associated with self-adjoint operators. It has a very concrete realization in the context of the spectral theory, which the following examples demonstrate.

Condition (ii) is actually used to <u>define</u> the operator A, given the unitary group $U(t)$. The operator iA is called the <u>generator</u> of $U(t)$.

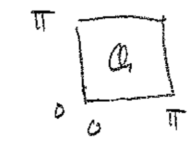
For problem (1), there is also a unique solution defined $\forall\, u_0 \in \mathcal{H}$ by

$$u(t) = e^{-At} u_0 \,,$$

where $U(t) = e^{-At}$, $t > 0$, is the <u>semigroup</u> associated to its generator, the self-adjoint operator $-A$, which is negative.

<u>Example</u> Vibration of a square membrane, an IBVP (init. bound-val. prob)

$$\begin{cases} \partial_{tt} u = \Delta u \\ u\big|_{\partial\Omega} = 0 \end{cases}, \quad \begin{cases} u(x,y;0) = u_0(x,y) \\ u_t(x,y;0) = v_0(x,y) \end{cases}$$



The rigorous context for this problem is the anti-self-adjoint

$$\begin{cases} \mathcal{A} = \begin{bmatrix} 0 & I \\ -\Delta & 0 \end{bmatrix} \\ \mathcal{D}(\mathcal{A}) = \mathcal{D}(\Delta_0) \oplus H^1(\Omega) \subset H^1(\Omega) \oplus L^2(\Omega) \end{cases}$$

in the Hilbert space $H^1(\Omega) \oplus L^2(\Omega)$, where Δ_0 is the Dirichlet Laplacian in Ω:

$$\mathcal{D}(\Delta_0) = \{ u \in H^1_0(\Omega) : \nabla \cdot \nabla u \in L^2 \}.$$

$$= \{ u : u \in L^2,\ \nabla u \in L^2,\ \nabla \cdot \nabla u \in L^2 \}.$$

The equation is well formed as

$$\begin{pmatrix} u_t \\ v_t \end{pmatrix} = \mathcal{A} \begin{pmatrix} u \\ v \end{pmatrix}, \quad \begin{pmatrix} u(0) \\ v(0) \end{pmatrix} = \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} \in H^1(\Omega) \oplus L^2(\Omega),$$

Since $i\mathcal{A}$ is self-adjoint, there is a unique unitary group $\mathcal{U}(t) = e^{\mathcal{A}t}$ such that the solution is given by

$$\begin{pmatrix} u(t) \\ v(t) \end{pmatrix} = e^{\mathcal{A}t} \begin{pmatrix} u_0 \\ v_0 \end{pmatrix} .$$

This solution can be expressed very explicitly in terms of the eigenfunctions and eigenvalues of $-\Delta_0$, which are

$$\begin{cases} \lambda_{mn} = m^2 + n^2 \\ u_{mn} = \sin mx \sin ny \end{cases} , \quad m, n \geq 1 \quad \text{integers} .$$

The general solution of the BVP is

$$u(x,t) = \sum_{n,m=1}^{\infty} \left(a_{mn} \cos \lambda_{mn} t + b_{mn} \sin \lambda_{mn} t \right) \sin mx \sin ny ,$$

where $\{a_{mn}\}$ and $\{\lambda_{mn} b_{mn}\}$ are in ℓ^2. The initial condition is satisfied by putting

$$u(x,y;0) = \sum_{n,m=1}^{\infty} a_{mn} \sin mx \sin ny = u_0(x) ,$$
$$v(x,y;0) = \sum_{n,m=1}^{\infty} \lambda_{mn} b_{mn} \sin mx \sin ny = v_0(x) ,$$

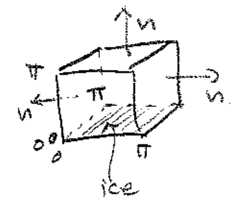
and solving for the coefficients by

$$a_{mn} = \frac{1}{4} \int_0^{\pi}\!\!\int_0^{\pi} u_0(x,y) \sin mx \sin ny \, dx dy ,$$

$$b_{mn} = \frac{1}{4\lambda_{mn}} \int_0^{\pi}\!\!\int_0^{\pi} v_0(x,y) \sin mx \sin ny \, dx dy .$$

Details need to be filled in, but all of this is rigorous in the framework we have described.

<u>Example</u> The heat equation in a box insulated on all sides except the bottom, which is set upon ice.



PDE $\quad u_t = \Delta u \, , \quad (x,y,z) \in \Omega = [0,\pi]^3$

BV $\quad \begin{cases} \partial_n u(x,y,z;t) = 0 & \text{for } x=0,\ x=\pi;\ y=0,\ y=\pi,\ z=\pi \\ u(x,y,0;t) = 0 \end{cases}$

IV $\quad u(x,y,z;0) = u_0(x,y,z)$

The correct extension of the symmetric operator Δ_0,

$$\mathcal{D}(\Delta_0) = \{ u \in L^2 : \nabla u \in L^2, \nabla\cdot\nabla u \in L^2;\ u|_{\partial\Omega} = 0,\ \partial_n u|_{\partial\Omega} = 0 \}$$

$$\Delta_0 u = \nabla\cdot\nabla u \quad \text{for } u \in \mathcal{D}(\Delta_0)$$

is the self-adjoint operator $\tilde{\Delta}$, given by

$$\mathcal{D}(\tilde{\Delta}) = \left\{ u \in L^2 : \nabla u \in L^2, \nabla\cdot\nabla u \in L^2,\ \begin{array}{l} \partial_n u = 0 \text{ on } \partial\Omega \text{ for } z \neq 0 \\ u = 0 \text{ on } \partial\Omega \text{ for } z = 0 \end{array} \right\}$$

$$\tilde{\Delta} u = \nabla\cdot\nabla u \quad \text{for } u \in \mathcal{D}(\tilde{\Delta}).$$

The solution $u(x,y,z;t) = e^{\tilde{\Delta} t} u_0(x,y,z)$ can be expressed using the eigenvalues and eigenfunctions of $\tilde{\Delta}$:

$$\lambda_{mn} = -\left(l^2 + m^2 + (n+\tfrac{1}{2})^2\right), \qquad m, n, l \text{ integers, } m,n \geq 0,$$
$$u_{mn} = \cos lx \cos my \sin(n+\tfrac{1}{2})z. \qquad l \geq 1$$

The general solution is

$$u(x,y,z;t) = \sum_{lmn} a_{lmn}\, e^{-(l^2+m^2+(n+\frac{1}{2})^2)\,t} \cos lx \cos my \sin(n+\tfrac{1}{2})z,$$

with $u_0(x,y,z) = \sum_{lmn} a_{lmn} \cos lx \cos my \sin(n+\tfrac{1}{2})z$,

$\{a_{lmn}\} \in l^2$