After our hard work in the setting of bounded operators, we can now easily prove:

Theorem (T.11) (Spectral Theorem for unbounded self-adjoint operators.)

Let H be a separable complex Hilbert space, and let $A: D(A) \subset H \to H$ be self-adjoint. Then there exist

- a finite measure space (M, μ),
- a measurable function $g: M \to \mathbb{R}$,
- a unitary map $U: H \to L^2(M, d\mu)$,

so that (i) $f \in D(A) \iff g \cdot Uf \in L^2(M, d\mu)$,

(ii) $\psi \in U(D(A)) \subset L^2(M, d\mu)$

$$\Rightarrow (UAU^{-1}\psi)(x) = g(x)\psi(x), \quad x \in M.$$

That is, $UAU^{-1} = T_g$.

Proposition (P.4) Let $A: D(A) \subset H \to H$ be densely defined and closed. Then $\rho(A) \ni z \mapsto R_z(A) = (z-A)^{-1} \in L(H)$ is analytic, and for $z, w \in \rho(A)$,

$$R_z(A) - R_w(A) = (w-z) R_z(A) R_w(A) \quad \circledast$$

In particular, $R_z(A) R_w(A) = R_w(A) R_z(A)$.

Proof Exercise. $\square$

Proof. Theorem (T.5) implies that $(A+i)^{-1}, (A-i)^{-1}: H \to D(A) \subset H$ are bounded. They commute by Proposition (P.4). Moreover,

$$((A+i)^{-1})^* = (A-i)^{-1}$$

since given $f, g \in H$, let $u = (A+i)^{-1} f$, $v = (A-i)^{-1} g \in D(A)$, then

$$((A+i)^{-1}f, g) = ((A+i)^{-1}(A+i)u, (A-i)v)$$
$$= (u, (A-i)v)$$
$$= ((A-i)^* u, v) = ((A+i)u, v) = (f, (A-i)^{-1}g).$$

- Since $(A+i)^{-1}: \mathcal{H} \longrightarrow \mathcal{D}(A) \subset \mathcal{H}$ is normal and bounded, we can apply Theorem (T.10). We get a finite measure space (M, μ), a bounded measurable function $\tilde{g}: M \to \mathbb{C}$, and a unitary map $\mathcal{U}: \mathcal{H} \to L^2(M, d\mu)$ s.t.

$$\mathcal{U}(A+i)^{-1}\mathcal{U}^{-1}f = \tilde{g}f, \quad f \in L^2(M, d\mu). \quad (*)$$

Plan: $(A+i)^{-1} \sim \tilde{g} \rightsquigarrow A \sim \frac{1}{\tilde{g}} - i$.

Since $(A+i)^{-1}$ is injective, $\tilde{g} \neq 0$ a.e. So $g = \frac{1}{\tilde{g}} - i : M \to \mathbb{C}$ is finite a.e.

- (i) - Suppose $f \in \mathcal{D}(A)$, then

and $\quad \mathcal{U}f = \mathcal{U}(A+i)^{-1}(A+i)f = \mathcal{U}(A+i)^{-1}\mathcal{U}^{-1}\mathcal{U}(A+i)f$
$$\overset{(*)}{=} \tilde{g}\,\mathcal{U}(A+i)f$$
$$\Rightarrow g \cdot \mathcal{U}f = g\tilde{g}\,\mathcal{U}(A+i)f = (1 - i\tilde{g})\mathcal{U}((A+i)f) \in L^2(M, d\mu).$$

- Conversely, if $f \in \mathcal{H}$ and $g \cdot \mathcal{U}f \in L^2(M, d\mu)$, then $\exists\, \varphi \in \mathcal{H}$ s.t. $\quad \mathcal{U}\varphi = (g+i)\mathcal{U}f$
$$\Rightarrow \mathcal{U}f = \tilde{g}(g+i)\mathcal{U}f = \tilde{g}\,\mathcal{U}\varphi \overset{(*)}{=} \mathcal{U}(A+i)^{-1}\mathcal{U}^{-1}\mathcal{U}\varphi$$
$$= \mathcal{U}(A+i)^{-1}\varphi$$
$$\Rightarrow f = (A+i)^{-1}\varphi \in \mathcal{D}(A).$$

- (ii) If $f \in \mathcal{D}(A)$, then $\mathcal{U}(Af) = \tilde{g}^{-1}\tilde{g}\,\mathcal{U}(Af) \overset{(*)}{=} \tilde{g}^{-1}\mathcal{U}(A+i)^{-1}Af$
$$= \tilde{g}^{-1}\mathcal{U}(f - i(A+i)^{-1}f) = (\tilde{g}^{-1} - i)\,\mathcal{U}f = g\,\mathcal{U}f.$$

· Finally, we prove that g is real-valued a.e. But this follows from the fact that

$$\mathbb{R} \underset{\text{Theorem (T.5)}}{\supset} \sigma(A) = \sigma(UAU^{-1}) = \sigma(T_g) \underset{\text{Proposition (P.2)}}{=} \operatorname{ess\,ran} g. \qquad \square$$

Example (E.14)

(i) Position operator. $H = L^2(\mathbb{R})$, $D(Q) = \{\psi \in L^2 : x\psi \in L^2\}$, $Q\psi(x) = x\psi(x)$. (So $Q = T_x$.) Then Theorem (T.11) is almost trivial for Q: take

$$(M,\mu) = (\mathbb{R}, \text{Lebesgue}),$$
$$g(x) = x$$
$$U = I.$$

If we want (M,μ) to be a finite metric space, use the unitary map

$$\begin{aligned} L^2(\mathbb{R}) &\longrightarrow L^2(\mathbb{R}, e^{-x^2}dx) \\ u &\longmapsto e^{x^2/2}u. \end{aligned}$$

(ii) $H = L^2(S^1)$, $A = D_\theta^2 : D(A) = H^2(S^1) \longrightarrow L^2(S^1)$.

Set $U : H \to \ell^2(\mathbb{Z})$, $U = \mathcal{F} : u \mapsto (\hat{u}(n))$,

$$\hat{u}(n) = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} e^{-inx} u(x)\,dx.$$

Then $UAU^{-1} =: B : U(D(A)) = h^2(\mathbb{Z}) \subset \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z})$,

$$(Bv)_n = n^2 v_n.$$

Note that $\ell^2(\mathbb{Z}) = L^2(M, d\mu)$ where $M = \mathbb{Z}$,

$$d\mu = \sum_{n\in\mathbb{Z}} \delta_n,$$

so in the notation of Theorem (T.11) $g(n) = n^2 : M \to \mathbb{R}$.

(To get a finite metric space, let $U : u \mapsto (e^{n^2/2}\hat{u}(n))$, $d\mu = \sum e^{-n^2}\delta_n$.)

(iii) $H = L^2(S^1)$, $V \in L^\infty(S^1)$ real-valued 'potential'. Then

$$A = D_\theta^2 + V : H^2(S^1) \subset L^2(S^1) \longrightarrow L^2(S^1)$$

is self-adjoint (Exercise). $\Rightarrow$ Theorem (T.11) applies.

But $\mathcal{U}$ is not "explicit" anymore. One can show that $\exists$ complete ONB (orthonormal basis) of eigenfunctions $\{u_n\} \subset H$ of A; and $\mathcal{U}f := \left((f, u_n)_{n \in \mathbb{N}} \right) \in \ell^2(\mathbb{Z})$ defines a unitary map as in Theorem (T.11) (modulo the finiteness of the measure space, which is easily arranged using the trick in example (i) here).

So: $\mathcal{U}$ decomposes H into eigenspaces of A.

(NB: this should be put in quotation marks in (i)!)

(iv) $H = L^2([0,1])$,

$$A = i\frac{d}{dt} : D(A) = \{ u \in H^1([0,1]) : u(0) = u(1) \} \subset H \longrightarrow H.$$

(See Example (E.8)(iii).) Theorem (T.11) decomposes H into the eigenspaces of A. (Exercise.)

We can use Theorem (T.11) to develop a Borel functional calculus much as in (the proof of) Theorem (T.9):

Theorem (T.12) (Borel functional calculus, unbounded operator case.)

Let $A : D(A) \subset H \to H$ be self-adjoint. Then there exists a unique continuous $*$-algebra-homomorphism $\phi : B^\infty(\sigma(A)) \to L(H)$ so that

(i) if $\{h_n\} \subset B^\infty(\sigma(A))$, $h_n(x) \xrightarrow{n\to\infty} x$ $\forall x$, and $\sup_{n,x} \left| \frac{h_n(x)}{1+|x|} \right| < \infty$ then $\phi(h_n)u \xrightarrow{n\to\infty} Au$ $\forall u \in D(A)$;

(ii) if $f_n(x) \to f(x)$ $\forall x \in \sigma(A)$ $(f_n, f \in B^\infty(\sigma(A))$ and $\|f_n\|_\infty$ is bounded, then $\phi(f_n) \to \phi(f)$ strongly in $L(H)$

Moreover, ϕ has the properties

(iii) $Au = \lambda u \Rightarrow \phi(f)u = f(\lambda)u$,

(iv) $f \geq 0 \Rightarrow \phi(f) \geq 0$.

Proof By Theorem (T.11), we may assume that $A = T_g$ on $D(T_g) \subset L^2(M, d\mu)$ where $g: M \to \mathbb{R}$ is measurable, and (M, μ) is a finite measure space.

- The existence of ϕ is proved as in the proof of Theorem (T.9): the definition $\phi(f) := T_{f \circ g}$ satisfies all properties, with (i) following from the Dominated Convergence Theorem.

- Uniqueness of ϕ is slightly more subtle. So suppose ϕ satisfies all properties up to (i) & (ii). We need to show that $\phi(f)u$ is uniquely determined by these properties for all $f \in B^\infty(\sigma(A))$, $u \in H$.

Step 1: For $N > 0$, $\phi(x \cdot 1_{[-N,N]}) = A$ on $\operatorname{ran} \phi(1_{[-N,N]})$.

Check: First, we check that $\phi(1_{[-N,N]})u \in D(A)$ for all $u \in H$.

We check membership in $D(A^*) = D(A)$: for all $v \in H$,

$$(Av, \phi(1_{[-N,N]})u) = (\phi(1_{[-N,N]})Av, u)$$

$$\overset{(i)}{=} \lim_{n \to \infty} (\phi(1_{[-N,N]})\phi(h_n)v, u)$$

$$= \lim_{n \to \infty} (\phi(h_n \cdot 1_{[-N,N]})v, u)$$

$$\overset{(ii)}{=} \lim_{n \to \infty} (\phi(x 1_{[-N,N]})v, u)$$

$$= \lim_{n \to \infty} (v, \phi(x 1_{[-N,N]})u).$$

$\Rightarrow \phi(1_{[-N,N]})u \in D(A^*) = D(A)$, and $A\,\phi(1_{[-N,N]})u = \phi(x 1_{[-N,N]})u$.

Since (by the algebra-homomorphism property)

$$\phi(1_{[-N,N]})^2 = \phi(1^2_{[-N,N]}) = \phi(1_{[-N,N]}),$$

this finishes the argument.

Step 2: Determine $\phi(f)u$ for $f \in B^\infty(\sigma(A))$ with $\operatorname{supp} f \subset [-N,N]$.

Well, * if $u \in \operatorname{ran} \phi(1_{[-N,N]})$, then Step 1 and the continuity and *-algebra homomorphism property of ϕ determine $\phi(f 1_{[-N,N]})u$ uniquely if f is a polynomial, hence (by continuity) if f is continuous, hence (by (ii)) if $f \in B^\infty(\sigma(A))$.

* For general $u \in H$, we have $u = \phi(1)u \overset{(ii)}{=} \lim_{N' \to \infty} \phi(1_{[-N',N']})u$,

and
$$\underbrace{\phi(f)}_{\in L(H)} u = \lim_{N' \to \infty} \phi(f)\,\phi(1_{[-N',N']})u$$
$$= \lim_{N' \to \infty} \phi(f 1_{[-N',N']})\, u \quad \text{independent of } N' \geq N$$
$$= \phi(f 1_{[-N,N]})\, u$$
$$= \phi(f 1_{[-N,N]})\big(\phi(1_{[-N,N]})u\big)$$

is therefore uniquely determined.

Step 3: conclusion. Given any $f \in B^\infty(\sigma(A))$, we have

$f_n := 1_{[-n,n]} f \longrightarrow f$ pointwise and boundedly, so

$\phi(f) = (\text{strong} \lim_{n \to \infty} \text{ of } \phi(f_n))$ is uniquely determined since all $\phi(f_n)$ are (by Step 2). $\square$

Remark (R.12): projection-valued measures. For $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ self-adjoint, let $P(\Omega) = 1_\Omega(A)$ for $\Omega \subset \mathbb{R}$ Borel. Then P is a projection-valued measure:

(i) $P(\Omega)$ is an orthogonal projection $\forall \Omega$

(ii) $P(\emptyset) = 0$, $P(\mathbb{R}) = I$

(iii) $\Omega = \bigcup_{n=1}^{\infty} \Omega_n$ where the Ω_n are pairwise disjoint

$$\Rightarrow \quad P(\Omega)u = \sum_{n=1}^{\infty} P(\Omega_n)u \quad \forall u \in \mathcal{H}$$

(iv) $P(\Omega_1 \cap \Omega_2) = P(\Omega_1)P(\Omega_2)$.

* Note that for $u \in \mathcal{H}$,

$$(P(\Omega)u, u) = (1_\Omega(A)u, u) = \int_{\sigma(A)} 1_\Omega \, d\mu_u = \mu_u(\Omega)$$

is the spectral measure of u.

Notation: $d\mu_u(\lambda) = d(P(\lambda)u, u)$. (Note: $P(\lambda)$ is not defined!)

* Given $g \in B^\infty(\sigma(A))$, $\quad (g(A)u, u) = \int_{\sigma(A)} g(\lambda) \, d(P(\lambda)u, u)$.

Formal way to write this: $\quad g(A) = \int_{\sigma(A)} g(\lambda) \, dP(\lambda)$

* One can also extend this to certain unbounded g, leading e.g. to the beautiful (formal...) $\quad A = \int_{\sigma(A)} \lambda \, dP(\lambda)$.

Example (E.15): spectral projectors.

(i) A = multiplication by x on $L^2(\mathbb{R})$. If $f \in B^\infty(\mathbb{R})$, then $f(A)$ = mult. by $f(x)$ simply.

Special case: $f = 1_\Omega$, $\Omega \subset \mathbb{R}$ Borel measurable

$\Rightarrow \quad 1_\Omega(A)$ = mult. by 1_Ω = spectral projector to $\Omega \subset \sigma(A) = \mathbb{R}$,

(ii) $A = D_\theta^2 : H^2(\mathbb{S}^1) \subset L^2(\mathbb{S}^1) \to L^2(\mathbb{S}^1)$

* Let $\Lambda > 0$, then $\mathbb{1}_{[0,\Lambda]}(A) = \sum_{\substack{n\in\mathbb{Z}\\ n^2 \le \Lambda}} P_n$, where $P_n u = \frac{1}{2\pi} e^{inx} \int_0^{2\pi} e^{-iny} u(y)\,dy$ projects onto the n^{th} Fourier mode of u.

Example (E.16): Schrödinger equation.

Let $V \in L^\infty(\mathbb{S}^1)$ and set $A = D_\theta^2 + V : H^2(\mathbb{S}^1) \subset L^2 \to L^2$.

Fix $u_0 \in H^2(\mathbb{S}^1)$ and set $u(t) = e^{-itA} u_0$.

Claim: $u \in C^0(\mathbb{R}; H^2(\mathbb{S}^1)) \cap C^1(\mathbb{R}; L^2(\mathbb{S}^1))$ satisfies

$$\begin{cases} i\frac{\partial u}{\partial t}(t) = Au(t) = (D_\theta^2 + V)u(t), & t \in \mathbb{R}, \quad \text{(Schrödinger eq.)} \\ u(0) = u_0 & \text{(initial condition)}, \end{cases}$$

and $\|u(t)\|_{L^2} = \|u_0\|_{L^2}$ $\forall t$ (unitarity of evolution).

Remark: $u(t) = e^{-itA} u_0$ is defined also for $u_0 \in L^2(\mathbb{S}^1)$, but it only satisfies the Schrödinger equation in a weak sense.
(Issue: what is $\frac{\partial u}{\partial t}$?)

Proof: Theorem (T.13) below. $\square$

Theorem (T.13) Let $A: D(A) \subset \mathcal{H} \to \mathcal{H}$ be self-adjoint, and set $\mathcal{U}(t) := e^{itA} \in L(\mathcal{H})$. Then:

(i) $\mathcal{U}(t)$ is unitary, and $\mathcal{U}(t+s) = \mathcal{U}(t)\mathcal{U}(s)$.

(ii) $t \mapsto \mathcal{U}(t)$ is strongly continuous, i.e. $\forall \psi \in \mathcal{H}$, $\mathbb{R} \ni t \mapsto \mathcal{U}(t)\psi \in \mathcal{H}$ is a continuous function.

(iii) For $\psi \in D(A)$, $\displaystyle\lim_{h\to 0} \frac{\mathcal{U}(h)\psi - \psi}{h} = iA\psi.$

More generally, $\displaystyle\lim_{h\to 0} \frac{\mathcal{U}(t+h)\psi - \mathcal{U}(t)\psi}{h} = iA\,\mathcal{U}(t)\psi \quad \forall t \in \mathbb{R}$

(iv) If $\psi \in \mathcal{H}$ and the limit $\displaystyle\lim_{h\to 0} \frac{\mathcal{U}(h)\psi - \psi}{h}$ exists, then $\psi \in D(A)$.

Example (E.16), continued. Part (i) of this result gives $\|u(t)\|_{L^2} = \|u_0\|_{L^2}\ \forall t$; part (ii) gives $u \in C^0(\mathbb{R}; L^2(\mathbb{S}^1))$; part (iii) shows that $\frac{\partial u}{\partial t} = -iAu$, and since $t \mapsto -iA\,u(t) = -iA\,e^{-itA}u_0 = -i\,e^{-itA}\underbrace{Au_0}_{\in L^2}$, we get $u \in C^1(\mathbb{R}; D(A)) = C^1(\mathbb{R}; H^2(\mathbb{S}^1))$.

Proof of Theorem (T.13). Write $\mathcal{U}(t) = \phi(f_t)$, $f_t(x) = e^{itx}$, in the notation of Theorem (T.12).

(i) follows from $\mathcal{U}(t)^*\mathcal{U}(t) = \phi(f_t)^*\phi(f_t) = \phi(\bar{f_t})\phi(f_t) = \phi(|f_t|^2)$

$$= \phi(1) = I,$$

and $\mathcal{U}(t+s) = \phi(f_{t+s}) = \phi(f_t f_s) = \phi(f_t)\phi(f_s) = \mathcal{U}(t)\mathcal{U}(s)$.

(ii) $\|f_t\|_\infty = 1\ \forall t$, and $f_{t+h} \xrightarrow{h\to 0} f_t$ pointwise; the claim thus follows from Theorem (T.12)(ii).

(iii). We have $\displaystyle\frac{\mathcal{U}(h) - \mathcal{U}(0)}{h}\psi = i\phi\left(\frac{e^{ihx}-1}{ihx}\,x\right)\psi$. Using Theorem (T.12)(i), we only need to observe that $a_h(x) := \dfrac{e^{ihx}-1}{ihx}$ satisfies

- $a_h(x) \xrightarrow{h\to 0} 1 \quad \forall x\in\mathbb{R}$ (ok by l'Hôpital);
- $|a_h(x)| \leq 1 \quad \forall h\neq 0,\ x\in\mathbb{R}$ (ok since $\forall s\in\mathbb{R}$, $|e^{is}-1| =$
$= \left|\int_0^1 \frac{d}{dt} e^{its}\,dt\right| = |s| \left|\int_0^1 e^{its}\,dt\right|$
$\leq |s| \int_0^1 |e^{its}|\,dt = |s|$.)

- The more general statement follows from $\frac{U(h)\psi - \psi}{h} \xrightarrow{h\to 0} iAu$ by applying $U(t)$.

(iv) Define an operator $B : D(B) \subset \mathcal{H} \to \mathcal{H}$ by

$$D(B) := \left\{ \psi\in\mathcal{H} : \lim_{h\to 0} \frac{U(h)\psi-\psi}{h} \text{ exists} \right\}, \quad B\psi = \frac{1}{i}\lim_{h\to 0}\frac{U(h)\psi-\psi}{h}.$$

By part (iii), $B\supset A$. We claim that B is symmetric: if $\varphi, \psi \in D(B)$, then

$$\begin{aligned}
(B\varphi, \psi) &= \lim_{h\to 0} \left(\frac{1}{i}\frac{U(h)-U(0)}{h}\varphi, \psi\right) \\
&= \lim_{h\to 0} \left(\varphi, \left(-\frac{1}{i}\right)\frac{U(h)^*-U(0)^*}{h}\psi\right) \\
&\overset{U(h)^* = U(h)^{-1} = U(-h)}{=} \lim_{h\to 0}\left(\varphi, \frac{1}{i}\frac{U(-h)-U(0)}{-h}\psi\right) \\
&= (\varphi, B\psi),
\end{aligned}$$

as claimed. Therefore, $B \subset B^* \subset A^* = A \subset B$, so $B = A$. This entails $D(B) = D(A)$, as was to be shown. $\square$

Definition (D.10) A function $\mathbb{R}\ni t \mapsto U(t) \in \mathcal{L}(\mathcal{H})$ so that

- $U(t)$ is unitary $\forall t$,
- $U(t+s) = U(t)U(s) \quad \forall t, s$,
- $\forall \psi\in\mathcal{H}, t\in\mathbb{R}, \lim_{t'\to t} U(t')\psi = U(t)\psi$

is called a *strongly continuous one-parameter unitary group*.

Theorem (T.13) produces all such groups:

Theorem (T.14) (Stone's theorem.) Let $t \mapsto U(t)$ be a strongly continuous one-parameter unitary group on the separable Hilbert space H. Then $\exists$ unique self-adjoint operator $A : D(A) \subset H \to H$ so that $U(t) = e^{itA}$ $\forall t \in \mathbb{R}$. (A is called the infinitesimal generator of U.) The domain of A is

$$D(A) = \left\{ \psi \in H : \exists \lim_{h \to 0} \frac{U(h)\psi - \psi}{h} \in H \right\}; \quad A\psi = i^{-1} \lim_{h \to 0} \frac{U(h)\psi - \psi}{h}.$$

Proof Omitted. See Theorem VIII.8 in Reed-Simon, vol. 1. $\square$

For example, $H = L^2(\mathbb{R})$, $(U(t)\psi)(x) = \psi(x-t)$, satisfies the assumptions of Theorem (T.14). The infinitesimal generator A has domain $D(A) = \{ \psi \in L^2(\mathbb{R}) : \exists \lim_{h \to 0} \frac{\psi(\cdot - h) - \psi}{h} \text{ in } L^2(\mathbb{R}) \}$, and one sensibly writes $A\psi = \frac{1}{i}(-\frac{d}{dx}\psi) = i \frac{d}{dx}\psi$.

We call $D(A)$ the Sobolev space $H^1(\mathbb{R})$.