2) Integral operators

Suppose $k : \Omega \times \Omega \to \mathbb{C}$ is Lebesgue measurable. For any $\psi \in \mathcal{H}$, let $\Xi_\psi \subset \Omega$ be the set of points in which $k(x,\cdot)\psi(\cdot) \in L^1(\Omega)$. For all ψ, for which Ξ_ψ^c has zero measure, we define

$$F_\psi(x) = \int_\Omega dy\, k(x,y)\psi(y)\,, \quad x \in \Xi_\psi$$

and set (arbitrarily) $F_\psi(x) = 0$ for $x \notin \Xi_\psi$. Then the integral operator I_k corresponding to integral kernel k is defined on

$$D(I_k) := \{\psi \in \mathcal{H} \mid \Xi_\psi^c \text{ has zero measure, } \int_\Omega |F_\psi|^2 < \infty\}$$

by $(I_k\psi)(x) = F_\psi(x)$.

* These are proper operators, but need not be densely defined or closed.

* Extremely nice special case:
  If $\int_\Omega dx \int_\Omega dy\, |k(x,y)|^2 < \infty$, then

  $I_k \in \mathcal{B}(\mathcal{H})$ and there is a sequence of finite-dimensional (rank) operators $F_k^{(n)}$

  $(\Leftrightarrow \dim(R(F_k^{(n)})) < \infty \quad \forall n)$

  s.t. $\lim_{n\to\infty} \| I_k - F_k^{(n)} \| = 0$.

  (Then I_k is a so called Hilbert-Schmidt operator.)

* If $k(x,y)^* = k(y,x)$ a.e. $x,y \in \Omega$ and $\exists\, C \geq 0$ s.t. $\int_\Omega dy\, |k(x,y)| \leq C$ a.e. $x \in \Omega$, then $I_k \in \mathcal{B}(\mathcal{H})$ and I_k is self-adjoint. (see Ex. 5.4.)

3) Differential operators

Let $(T\psi)(x) = \sum_{\alpha: |\alpha| \leq N} c_\alpha \partial^\alpha \psi(x)$

where $N > 0$, the sum goes over multi-indices α with degree up to N, and $c_\alpha \in \mathbb{C}$ $\forall |\alpha| \leq N$.

Then $T: D \to D$, at least for $D = C_c^\infty(\Omega) = \{ f: \Omega \to \mathbb{C} \mid f \text{ smooth and } \operatorname{supp} f \text{ compact} \}$.

Since D is dense in $L^2(\Omega)$, T is clearly a densely defined operator on $\mathcal{H}$. However, it is not closed, so it cannot be self-adjoint.

* Standard example: $(T\psi)(x) = -\nabla^2 \psi(x)$ (Laplacian).

* Closed extensions of differential operators is our next topic ...

5.17. Definition: Arithmetics of unbounded operators:

Let A, B be operators.
The natural domains for $A+B$ and AB are

1. $D(A+B) = D(A) \cap D(B)$ on which $(A+B)\psi = A\psi + B\psi$.

2. $D(AB) = \{ \psi \in D(B) \mid B\psi \in D(A) \}$ on which $AB = A \circ B$.

* To be used with care: for instance, $H_0 = -\frac{1}{2}\nabla^2$ and $V = M_V$ can separately be fairly easily defined as self-adjoint operators. However, "$H_0 + V$" as defined above is not necessarily self-adjoint, even though it might be essentially self-adjoint, i.e., the Schrödinger operator is then really $H = \overline{H_0 + V}$.

Appendix: Spectral representations

The definition of $U(t)$ in our version of the Stone's theorem (5.14) uses the following general result:

5.17. Theorem: Suppose A is a self-adjoint operator on a Hilbert space $\mathcal{H}$. Then there is a unique projection value measure E, on the Borel subsets of $\sigma(A)$, the spectrum of A, such that:

$$(\phi, A\psi) = \int_{\sigma(A)} E_{\phi,\psi}(d\lambda)\, \lambda \qquad \forall \psi \in D(A),\ \phi \in \mathcal{H}.$$

Moreover, then $\sigma(A)$ is a non-empty subset of $\mathbb{R}$.

Proof: Rudin, F.A., Theorem 13.30, or Teschl, Theorem 3.7. $\square$

* This generalization of diagonalization of Hermitean matrices is a central result of modern functional analysis. Its real mathematical content is hidden in the definitions:

5.18. Definition: Suppose T is an operator on a Hilbert space $\mathcal{H}$. Its spectrum $\sigma(T)$ is the collection of those $\lambda \in \sigma(T)$ for which $\lambda 1 - T$ is not invertible in $\mathcal{B}(\mathcal{H})$.

* In other words, $\lambda \notin \sigma(T)$ iff $R(\lambda 1 - T) = \mathcal{H}$, $\lambda 1 - T$ is one-to-one, and $\exists S \in \mathcal{B}(\mathcal{H})$ such that $S = (\lambda 1 - T)^{-1}$.

* If T is unbounded, it is possible that $\sigma(T) = \emptyset$. However, $\sigma(T)$ is always a closed subset of $\mathbb{C}$.

* The complement of $\sigma(T)$ is called the <u>resolvent set</u>, denoted by $\rho(T)$. To every $\lambda \in \rho(T)$ we know that $(\lambda - T)^{-1} \in \mathcal{B}(\mathcal{H})$. The corresponding map $\rho(T) \to \mathcal{B}(\mathcal{H})$ is called the <u>resolvent of T</u>.

* If T is <u>closed</u>, it suffices to check that $\lambda 1 - T$ is bijective (the first two items above). (By the closed graph theorem, then the inverse $(\lambda 1 - T)^{-1}$ is continuous, i.e., belongs to $\mathcal{B}(\mathcal{H})$)

* If $\lambda 1 - T$ is not one-to-one, then there is $x \in \mathcal{H}, x \neq 0$, st. $Tx = \lambda x$. Obviously, then $\lambda \in \sigma(T)$, and we say that λ is an <u>eigenvalue</u> of T and x is an <u>eigenvector</u> of T corresponding to λ.

* A subspace $M \subset \mathcal{H}$ is called an <u>invariant subspace</u> of T, if M is closed and $TM \subset M$. Clearly, if λ is an eigenvalue, then $\ker(\lambda 1 - T)$ is an invariant subspace, called the <u>eigenspace</u> of T corresponding to λ.

* We still need to define what is a projection valued measure, also called a resolution of the identity (e.g., Rudin). The terminology is not completely fixed (c.f. Teschl), so it is a good idea to always check them.
* We use the definition relevant to the general spectral decompositions, as in Rudin.
* As discussed during the lectures, there is some redundancy in the definition of PVMs below. For instance, item "c)" can be dropped. For more details, see Teschl, p. 88-89.

5.19. Definition: Suppose $\mathcal{M}$ is a σ-algebra in a set X, and $\mathcal{H}$ is a Hilbert space. A mapping $E: \mathcal{M} \to \mathcal{B}(\mathcal{H})$ is a projection valued measure (PVM) if it satisfies

a) $E(\emptyset) = 0$, $E(X) = 1 = \mathrm{id}_{\mathcal{H}}$

b) $E(\omega)$ is a self-adjoint projection $\forall \omega \in \mathcal{M}$

c) $E(\omega \cap \omega') = E(\omega)E(\omega') \quad \forall \omega, \omega' \in \mathcal{M}$

d) If $\omega, \omega' \in \mathcal{M}$ and $\omega \cap \omega' = \emptyset$, then $E(\omega \cup \omega') = E(\omega) + E(\omega')$.

e) $\forall \psi, \varphi \in \mathcal{H}$ the map $E_{\varphi,\psi}: \mathcal{M} \to \mathbb{C}$ defined by

$$E_{\varphi,\psi}(\omega) := (\varphi, E(\omega)\psi)$$

is a complex measure on $\mathcal{M}$.

If X = locally compact Hausdorff space and $\mathcal{M}$ = Borel σ-algebra on X, we say that E is a regular resolution of the identity, if every $E_{\varphi,\psi}$ is a regular Borel measure (see 2.15 and 6.19 in [RCA])

8.20. Proposition: Suppose $\mathcal{H}$ is a Hilbert space, $\mathcal{M}$ is a σ-algebra in X, and $E: \mathcal{M} \to \mathcal{B}(\mathcal{H})$ is a PVM. Define $E_{\varphi,\psi}$ by e) above for $\varphi, \psi \in \mathcal{H}$. Consider an arbitrary $\psi_0 \in \mathcal{H}$. Then

a) E_{ψ_0,ψ_0} is a bounded positive measure on $\mathcal{M}$ whose total variation is $\|\psi_0\|^2$, and $E_{\psi_0,\psi_0}(\omega) = \|E(\omega)\psi_0\|^2 \; \forall \omega \in \mathcal{M}$.

b) $E(\omega)$ and $E(\omega')$ commute $\forall \omega, \omega' \in \mathcal{M}$

c) If $\omega, \omega' \in \mathcal{M}$ are disjoint, then $R(E(\omega)) \perp R(E(\omega'))$.

d) E is finitely additive.

e) the map $\omega \mapsto E(\omega)\psi_0$ is a countably additive $\mathcal{H}$-valued measure on $\mathcal{M}$.

f) If $\omega_n \in \mathcal{M}$, $n \in \mathbb{N}_+$, all satisfy $E(\omega_n) = 0$, then $E(\bigcup_{n\in\mathbb{N}_+} \omega_n) = 0$.

Proof: "a)" If $\omega \in \mathcal{M} \Rightarrow E(\omega)^* = E(\omega) = E(\omega)^2 \Rightarrow$

$$E_{\psi_0,\psi_0}(\omega) = (\psi_0, E(\omega)\psi_0) = (\psi_0, E(\omega)^* E(\omega)\psi_0)$$
$$= (E(\omega)\psi_0, E(\omega)\psi_0) = \|E(\omega)\psi_0\|^2 \geq 0$$
$$\Rightarrow E_{\psi_0,\psi_0}(X) = \|\psi_0\|^2 < \infty.$$ Thus E_{ψ_0,ψ_0} is a bounded positive measure with $\|E_{\psi_0,\psi_0}\| = \|\psi_0\|^2$. ∎

"b)" If $\omega, \omega' \in \mathcal{M} \overset{c)}{\Rightarrow} E(\omega)E(\omega') = E(\omega\cap\omega') = E(\omega'\cap\omega) = E(\omega')E(\omega)$.

"c)" If $\omega \cap \omega' = \emptyset \Rightarrow 0 \overset{a)}{=} E(\emptyset) = E(\omega\cap\omega') \overset{c)}{=} E(\omega)E(\omega') =$

$\Rightarrow \forall \varphi, \psi \in \mathcal{H}: \; 0 = (\varphi, E(\omega)E(\omega')\psi) = (E(\omega)^*\varphi, E(\omega')\psi)$
$= (E(\omega)\varphi, E(\omega')\psi) \Rightarrow R(E(\omega)) \perp R(E(\omega'))$.

"d) & e)" If $\omega_n \in \mathcal{M}$, $n \in \mathbb{N}_+$, are disjoint, then $\forall N \in \mathbb{N}_+$
$$\omega_{N+1} \cap \left(\bigcup_{n=1}^{N} \omega_n\right) = \bigcup_{n=1}^{N} (\omega_{N+1} \cap \omega_n) = \emptyset \Rightarrow$$
$$E\left(\bigcup_{n=1}^{N+1} \omega_n\right) \overset{d)}{=} E(\omega_{N+1}) + E\left(\bigcup_{n=1}^{N} E_n\right).$$ Thus by induction
$$\Rightarrow E\left(\bigcup_{n=1}^{N} \omega_n\right) = \sum_{n=1}^{N} E(\omega_n) \quad \forall N \in \mathbb{N}_+.$$ Proves "d)".

(typically not countably additive, since by Ex. 3.4. here either $E(\omega_n) = 0$ or $\|E(\omega_n)\| = 1 \Rightarrow$ the sum is not norm-Cauchy unless $E(\omega_n) = 0 \; \forall n \geq n_0$.)

To prove "e)" it suffices to show that now
$$E\left(\bigcup_{n\in\mathbb{N}_+} \omega_n\right)\psi_0 = \sum_{n=1}^{\infty} E(\omega_n)\psi_0$$ as an $\mathcal{H}$-convergent sum.

For this, denote $\varphi_n := E(\omega_n)\psi_0 \in R(E(\omega_n))$. By "c)" $\Rightarrow \varphi_n \perp \varphi_m \; \forall n \neq m$. $\Rightarrow$ if $I \subset \mathbb{N}_+$ and $|I| < \infty$ then

$$\Big\| \sum_{n\in I} \varphi_n \Big\|^2 = \sum_{n',n\in I} (\varphi_{n'}, \varphi_n) = \sum_{n\in I} \|\varphi_n\|^2$$

$$= \sum_{n\in I} (E(\omega_n)\psi_0, E(\omega_n)\psi_0) = \sum_{n\in I} (\psi_0, E(\omega_n)\psi_0)$$

$$= \sum_{n\in I} E_{\psi_0,\psi_0}(\omega_n) = E_{\psi_0,\psi_0}\Big(\bigcup_{n\in I} \omega_n\Big) \overset{\text{"a)"}}{\leq} \|\psi_0\|^2$$

$\Rightarrow \sum_{n\in\mathbb{N}_+} \|\varphi_n\|^2 \leq \|\psi_0\|^2 \Rightarrow \forall \varepsilon > 0 \; \exists n_0$ s.t. $\forall m \geq 0$

$$\Big\| \sum_{n=n_0}^{n_0+m} \varphi_n \Big\|^2 = \sum_{n=n_0}^{n_0+m} \|\varphi_n\|^2 \leq \varepsilon^2 \Rightarrow \Big(\sum_{n=1}^{N} \varphi_n\Big)_{N\in\mathbb{N}_+} \text{ is}$$

Cauchy in $\mathcal{H}$ $\Rightarrow \exists \tilde{\psi} = \lim_{N\to\infty} \sum_{n=1}^{N} \varphi_n$. $\Rightarrow \forall \psi \in \mathcal{H}$:

$$(\psi, \tilde{\psi}) = \lim_{N\to\infty} \sum_{n=1}^{N} (\psi, E(\omega_n)\psi_0) = \sum_{n=1}^{\infty} E_{\psi,\psi_0}(\omega_n)$$

$$= E_{\psi,\psi_0}\Big(\bigcup_{n=1}^{\infty} \omega_n\Big) = (\psi, E(\cup\omega_n)\psi_0)$$

$$\Rightarrow \tilde{\psi} = \sum_{n=1}^{\infty} E(\omega_n)\psi_0 = E\Big(\bigcup_{n=1}^{\infty} \omega_n\Big)\psi_0 \;\blacksquare$$

"f)" Let $\omega := \bigcup_{n=1}^{\infty} \omega_n \in M$. Then $\forall \psi \in \mathcal{H}$, $E_{\psi,\psi}$ is a measure

$$\overset{\text{"a)"}}{\Rightarrow} \|E(\omega)\psi\|^2 = E_{\psi,\psi}(\omega) = \int E_{\psi,\psi}(d\lambda)\, \mathbb{1}(\lambda\in\omega)$$

$$\overset{\text{DCT}}{=} \lim_{N\to\infty} \int E_{\psi,\psi}(d\lambda)\, \underbrace{\mathbb{1}\Big(\lambda \in \bigcup_{n=1}^{N} \omega_n\Big)}_{\leq \sum_{n=1}^{N} \mathbb{1}(\lambda\in\omega_n)} \leq \sum_{n=1}^{\infty} \int E_{\psi,\psi}(d\lambda)\, \mathbb{1}(\lambda\in\omega_n)$$

$\Rightarrow \|E(\omega)\psi\|^2 \leq \sum_{n=1}^{\infty} E_{\psi,\psi}(\omega_n)$, where $E_{\psi,\psi}(\omega_n) = (\psi, E(\omega_n)\psi) = 0$ as $E(\omega_n) = 0$.

$\Rightarrow 0 \leq \|E(\omega)\psi\|^2 \leq 0 \Rightarrow E(\omega)\psi = 0$. $\therefore E(\omega) = 0 \;\square$

* The name "projection valued measure" is used since each $E(\omega)$ is a projection and, by "e)" above, each $\omega \mapsto E(\omega)\psi$ is an $\mathcal{H}$-valued measure.

* The above formulation of the spectral decomposition theorem is the one directly relevant to the Stone's theorem. There are many useful generalizations; three are listed below:

5.21. Definition: Suppose T is an operator on a Hilbert space $\mathcal{H}$. T is called normal, if it is densely defined, closed, and satisfies $T^*T = TT^*$.

* This obviously generalizes the definition of bounded normal operators, given in 3.4.

5.22. Theorem: Suppose T is a normal operator on $\mathcal{H}$. Then there is E, a unique PVM on $\sigma(T)$, called the spectral decomposition of T, which satisfies

$$(\phi, T\psi) = \int_{\sigma(T)} E_{\phi,\psi}(d\lambda)\,\lambda \quad \forall \psi \in D(T), \phi \in \mathcal{H}.$$

Moreover, if $S \in \mathcal{B}(\mathcal{H})$ commutes with T ($\Leftrightarrow ST \subset TS$), then $[S, E(\omega)] = 0$ for all Borel sets $\omega \subset \sigma(T)$.

Proof: Rudin, F. A., Theorem 13.33. □

* It is possible to "diagonalize" bounded normal operators simultaneously, if the operators commute. This is explained in the following theorem. In physics, one can think of the set "K" in the theorem as a collection of "quantum numbers" related to the family of normal operators (observables).