5.13. Suppose the map $Q: I \to \mathcal{B}(\mathcal{H})$, $I \subset \mathbb{R}$ interval, is strongly continuous. $Q(t)$ is said to be strongly differentiable at t_0 for $\psi_0 \in \mathcal{H}$, if the following norm-lim. exists

$$\exists \lim_{\substack{t \to t_0 \\ t \in I}} \frac{1}{t-t_0}\left(Q(t)\psi_0 - Q(t_0)\psi_0\right) =: \frac{d}{dt} Q(t)\psi_0\Big|_{t=t_0}$$

Defn. Suppose $(U(t))_{t\geq 0}$ is a strongly continuous unitary semi-group. Its infinitesimal generator is a map $A : D(A) \to \mathcal{H}$ defined using

$$D(A) := \{\psi \in \mathcal{H} \mid U(t) \text{ is strongly differentiable at } t=0 \text{ for } \psi\}$$

and for any $\psi \in D(A)$

$$A\psi := \lim_{\varepsilon \to 0^+} \frac{i}{\varepsilon}\left(U(\varepsilon)\psi - \psi\right) = i \frac{d}{dt} U(t)\psi\Big|_{t=0}$$

5.14. Theorem (Stone)

Suppose $(U(t))_{t\geq 0}$ is a strongly continuous unitary semigroup, and let A denote its infinitesimal generator, defined as above. Then A is a densely defined self-adjoint operator on $\mathcal{H}$ and $\forall t \geq 0$:

(Exp) $\quad U(t) = e^{-itA}$ (defined via spectral decomposition of A)

Denote $\psi(t) := U(t)\psi$ for $\psi \in \mathcal{H}$, $t \geq 0$.

Then a) $t \mapsto \psi(t)$ is norm-continuous.

b) If $\psi(0) \in D(A)$, then $\psi(t) \in D(A)$ $\forall t \geq 0$ and

$$i \frac{d}{dt}\psi(t) = A\psi(t) = U(t)A\psi(0).$$

c) $\forall \psi(0) \in \mathcal{H}$: $\psi(t) = \lim_{\varepsilon \to 0^+} \exp\left(-it \frac{i}{\varepsilon}(U(\varepsilon)-1)\right)\psi(0)$.

Conversely, if A is self-adjoint, and $U(t) = e^{-itA}$, then $(U(t))_{t\geq 0}$ is a strongly continuous semigroup and A is its infinitesimal generator.

Proof : Functional calculus with spectral representations. (See the Appendix on page 55.) . For complete proofs, see Rudin, Funct. Anal., Th. 13.35 and Th. 13.37 or Reed & Simon I, chapter VIII.4. or Teschl, chapter 3. $\square$

Remarks: * The spectrum of a self-adjoint operator A, is a set $\sigma(A) \subset \mathbb{R}$. The spectral representation assigns to every Borel subset $\omega \subset \sigma(A)$ an orthogonal projection P_ω. so that for any $\phi, \psi \in \mathcal{H}$ the map $\mu_{\phi,\psi} : \omega \mapsto (\phi, P_\omega \psi)$ is a Borel measure, and $\forall \phi \in \mathcal{H}$, $\psi \in D(A)$

$$(\phi, A\psi) = \int_{\sigma(A)} \lambda \, \mu_{\phi,\psi}(d\lambda)$$

$$=: \int_{\sigma(A)} \lambda \, d(\phi, P_\lambda \psi)$$

The definition in (Exp) means

$\forall t \in \mathbb{R}, \phi, \psi \in \mathcal{H}$:

$$(\phi, e^{-itA}\psi) := \int_{\sigma(A)} e^{-it\lambda} \, d(\phi, P_\lambda \psi)$$

and the basic results of functional calculus show that then $D(e^{-itA}) = \mathcal{H}$ and e^{-itA} is unitary operator.

* If $\mathcal{H} = \mathbb{C}^N$, A is a self-adjoint matrix, with eigenvalues $\lambda_n \in \mathbb{R}$ and (orthonormal) collection of eigenvectors $e_n \in \mathbb{C}^N$ ...

$\longrightarrow$

... and the spectral definition means

$$(\phi, e^{-itA}\psi) := \sum_{n=1}^{N} e^{-it\lambda_n} (\phi, e_n)(e_n, \psi).$$

* If A is a bounded operator,

$$e^{-itA} = \sum_{n=0}^{\infty} \frac{1}{n!} (-itA)^n, \qquad (*)$$

but for unbounded operators, using the sum is usually not a good idea. For instance, if A is self-adj, usually $D(A^2) \subset D(A)$ is a proper subset, and the sum in $(*)$ makes sense only for so called analytic vectors; for ψ s.t.

$$\psi \in C^\infty(A) := \bigcap_{n=1}^{\infty} D(A^n) \quad \text{and}$$

$$\sum_{n=0}^{\infty} \frac{1}{n!} \|A^n \psi\| \, t^n < \infty \quad \text{for some } t > 0.$$

* It is possible, that S is essentially self-adjoint, i.e., S is symmetric and $\bar{S}$ is self-adjoint, but although $C^\infty(\bar{S})$ is dense, $C^\infty(S)$ is empty.

* However, by c), e^{-itA} is a strong limit of

$$\sum_{n=0}^{\infty} \frac{1}{n!} (-itA_\varepsilon)^n \quad \text{where } A_\varepsilon = \frac{i}{\varepsilon}(U(\varepsilon) - I) \text{ is a bounded operator.}$$

5.15 Remark: Stone's theorem shows that the best we can do to understand the original Schrödinger equation $i\frac{d}{dt}\psi(t) = S\psi(t)$ on page 3 is to find a dense subspace of $\mathcal{H}$ for which the right hand side makes sense, and then look for self-adjoint extensions of S. As we will see later, even if S is symmetric, any of the following can happen:

1) $\bar{S}$ is the unique self-adjoint extension (S.A.E.)
2) There are (infinitely) many S.A.E.
3) There are no S.A.E.

* If 1) happens, we should just be happy.
* 2) means that we forgot to "put in all the physics" in the Schrödinger equation. Typical examples are boundary conditions.
* 3) means that the (physical) system is not closed, and we are either forced to "leak" or "inject probability". (roughly speaking)

5.16. Examples: Three standard ways of defining operators on $\mathcal{H} = L^2(\Omega)$ when $\Omega \subset \mathbb{R}^d$, open subset: multiplication, integral, and differential operators.

1) Multiplication operators (potentials)

Let $V : \Omega \to \mathbb{C}$ be Lebesgue measable. The corresponding multiplication operator M_V (also denoted $\hat{V}$ or simply V) is a mapping $D(M_V) \to \mathcal{H}$ defined by

$$(M_V \psi)(x) = V(x)\psi(x), \quad x \in \Omega$$

on

$$D(M_V) := \{\psi \in \mathcal{H} \mid V\psi \in L^2(\Omega)\}.$$

M_V has the following properties: (Ex. 5.2.)

a) M_V is a closed, densely defined operator.

b) $(M_V)^* = M_{V^*}$

c) M_V self-adjoint $\Leftrightarrow$ $V(x) \in \mathbb{R}$ a.e. $x \in \Omega$.

* Thus every $V : \Omega \to \mathbb{R}$, which is Lebesgue measurable, generates a strongly cont. USG. With $U_t = e^{-itM_V} = M_{(e^{-itV})}$.