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③ Dynamics: Stone's theorem and the spectral theorem

- **Def**: A spectral measure is a $*$-homomorphism $E: C_c^\infty(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$ s.t.
  - $E(\alpha f + g) = \alpha E(f) + E(g)$
  - $E(fg) = E(f)E(g)$
  - $E(f)^* = E(\bar{f})$
  - $\{E(f)\psi : f \in C_c^\infty(\mathbb{R}), \psi \in \mathcal{H}\}$ is dense in $\mathcal{H}$

Claim. A spectral measure has a unique extension from $C_c^\infty(\mathbb{R})$ to the set of Borel functions with the important property

$$E(f_n)\psi \to E(f)\psi$$

whenever $f_n \to f$ pointwise and $|f_n| \le g$

see functional analysis, essentially Riesz-Markov's theorem

We write, formally

$$E(f) = \int f(\lambda)\, dE(\lambda)$$

Note: $E(f)$ is densely defined unbounded

meaning:

$$\langle \psi, E(f)\psi \rangle = \int f(\lambda)\, d\mu_\psi(\lambda)$$

f is unbounded

a probability measure

Here, we set: $D(E(f)) = \{\psi \in \mathcal{H} : E(f)\psi \in \mathcal{H}\}$
$= \{\psi \in \mathcal{H} : \int |f(\lambda)|^2 d\mu_\psi(\lambda) < \infty\}$

- **Spectral theorem** For every spectral measure E, the operator: $A = E(id)$ i.e.

$$A = \int \lambda\, dE(\lambda) \qquad (\heartsuit)$$

is self-adjoint. Reciprocally, every self-adjoint operator has a spectral representation $(\heartsuit)$ where E is unique.

The proof of this theorem will use unitary groups.

- **Def**. A 1-parameter unitary group is a map $U: \mathbb{R} \to \mathcal{L}(\mathcal{H})$

s.t. * Unitarity $U(t)^{-1} = U(t)^*$
* $U(0) = \mathbb{1}$
* $U(t+s) = U(t)U(s)$
* $U(t)\psi \to \psi$ as $t \to 0$ for all $\psi \in \mathcal{H}$.

It immediately follows that

$$\lim_{t\to t_0} U(t)\psi = U(t_0)\psi$$

also written as $\operatorname{s-lim}_{t\to t_0} U(t) = U(t_0)$

as well as $U(-t) = U(t)^{-1}$

The generator of a unitary group is the operator A defined by:

$$D(A) = \{\psi \in \mathcal{H} : -i\lim_{t\to 0} t^{-1}(U(t)\psi - \psi) \text{ exists}\}$$

$$A\psi = -i\lim_{t\to 0} t^{-1}(U(t)\psi - \psi) \qquad \psi \in D(A).$$

Note that for all $\psi, \varphi \in D(A)$

$$0 = i\frac{d}{dt}\langle U(t)\psi, U(t)\varphi\rangle\Big|_{t=0}$$

$$= \langle A\psi, \varphi\rangle - \langle \psi, A\varphi\rangle$$

namely A is symmetric.

- Stone's theorem: The generator A of a 1-parameter unitary group is self-adjoint.
  Reciprocally every self-adjoint operator generates a 1-parameter unitary group, and $U(t)$ is uniquely defined by A.

- In quantum mechanics. The time evolution is a family of maps $V: t \mapsto V(t)$ s.t.
  * $D(V(t)) = \mathcal{H}$ for all $t \in \mathbb{R}$
  * $\|V(t)\psi\| = \|\psi\|$ "conservation of probability"
  * $V(0) = \mathbb{1}$
  * $V(t+s) = V(t)V(s)$
  * $V(t)\psi \to V(t_0)\psi$ as $t \to t_0$.

In other words: the quantum propagator $V(t)$

is a 1-parameter unitary group. It follows that there exist a unique self-adjoint operator H, the Hamiltonian, such that

$$-i\frac{d}{dt}U(t)\psi = -i\lim_{\varepsilon\to 0}\varepsilon^{-1}\left(U(t+\varepsilon)-U(t)\right)\psi$$

$$= -i\lim_{\varepsilon\to 0}\varepsilon^{-1}\left(U(\varepsilon)-\mathbb{1}\right)U(t)\psi = -iH\,U(t)\psi$$

In other, the state $\psi(t)=U(t)\psi$ solves Schrödinger equation

$$\begin{cases} -i\psi'(t) = H\psi(t) \\ \psi(0)=\psi_0 \end{cases}$$

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Hamiltonian is the generator of time translations.

Lemma. (i) Let E be a spectral measure. Then $A=E(id)$ is self-adjoint

(ii) Let $A=A^*$. Then A is the generator of a unique 1-parameter group U

(iii) Let U be a 1-parameter group. Then there is a unique spectral measure E s.t. $U(t)=E(f_t)$ where $f_t(\lambda)=e^{it\lambda}$

The three maps $E\mapsto A$, $A\mapsto U$, $U\mapsto E$ are injective

Proof of both theorems. With the lemma, it suffices to prove that the composition of the three maps in (i)(ii)(iii) is the identity. We start with $A=A^*$. By (ii, iii):

$$A\psi \overset{(ii)}{=} -i\lim_{t\to 0}t^{-1}\left(U(t)-\mathbb{1}\right)\psi \overset{(iii)}{=} -i\lim_{t\to 0}t^{-1}\left(E(e^{it\lambda})-\mathbb{1}\right)$$

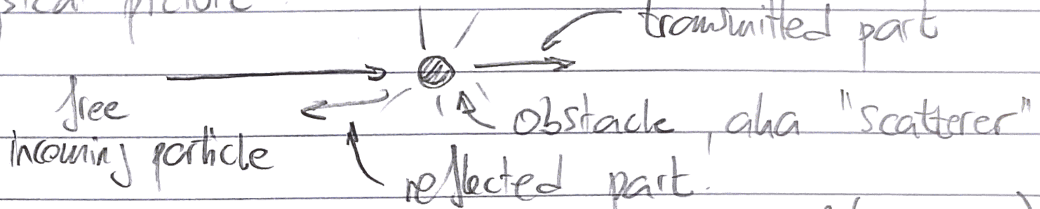
with $\psi\in D(A)$ iff the limit exists. We claim that $\mathbb{1}=E(1)$ (the constant function). Then by linearity

$$t^{-1}\left(E(e^{it\lambda})-\mathbb{1}\right) \overset{\mathbb{1}=E(1)}{=} E\left(t^{-1}(e^{it\lambda}-1)\right)$$

$$\left|\frac{e^{it\lambda}-1}{t}\right| \le |\lambda|$$

- A physical example of a unitary group

Physical picture:



Hilbert space $\mathcal{H} = \underset{\text{"left"}}{L^2(\mathbb{R})} \oplus \underset{\text{"right"}}{L^2(\mathbb{R})} \simeq L^2(\mathbb{R}; \mathbb{C}^2)$

In the absence of scatterer: $(U_0(t)\psi)(x) = \psi(x-t)$ (translation by t). U_0 is a unitary group.

With a scatterer:

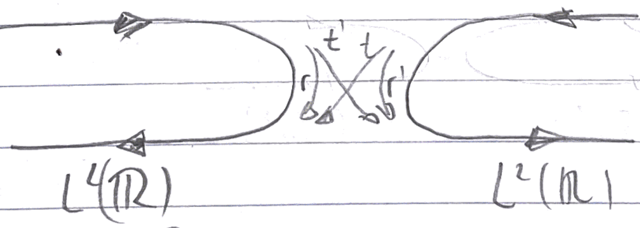
* for $t > 0$: the part of $\psi(x-t)$ that has crossed $x=0$ between times 0 and t is replaced by

$$S\psi(x-t) = \begin{pmatrix} r & t \\ t' & r' \end{pmatrix} \begin{pmatrix} \psi_{left}(x-t) \\ \psi_{right}(x-t) \end{pmatrix}$$

r, r' are reflection coefficients

t, t' are transmission coefficients

*
$$(U(t)\psi)(x) = \begin{cases} \psi(x-t) + \chi_{(0,t)}(x)(S-1)\psi(x-t) & (t>0) \\ \psi(x) & (t=0) \\ \psi(x-t) + \chi_{(-t,0)}(x)(S^*-1)\psi(x-t) & (t<0) \end{cases}$$



* Generators?

(i) of $U_0(t)$

$$\left(\frac{U(t)-1}{t}\psi\right)(x) = \frac{1}{t}(\psi(x-t) - \psi(x)) \to \psi'(x)$$

(in the sense of distributions)

Hence $(H_0\psi)(x) = \psi'(x)$

$\mathcal{D}(H_0) = \{\psi \in L^2(\mathbb{R}; \mathbb{C}^2) : \psi' \in L^2(\mathbb{R}; \mathbb{C}^2)\}$

is self-adjoint

(ii) of $U(t)$ see homework no "δ"-interaction

and by the property of the spectral measure $\lim_{t\to 0} t^{-1}(e^{it\lambda}-1) \stackrel{\circ}{=} i\lambda$ implies that
$$\lim_{t\to 0} E(t^{-1}(e^{it\lambda}-1))\psi = iE(id)\psi$$

Hence: $A \supset E(id)$. But $A = A^* \subset E(id)^* \stackrel{(i)}{=} E(id)$,
so we conclude that $A = E(id)$.
It remains to prove that $E(1) = \mathbb{1}$. This follows from $E(f)\psi = E(1)E(f)\psi$ by the properties of a spectral measure and so $E(1) \neq \mathbb{1}$ implies that $\{E(f)\psi : f \in C_c^\infty(\mathbb{R}), \psi \in \mathcal{H}\}$ is not dense $\blacksquare$

Proof of the lemma:

(i) Let $A = E(id)$. $A = A^*$ follows from $E(f)^* = E(\bar{f})$ for any f (the question of domain implied in $\supset$ must be treated in the extension of E to unbounded Borel functions)
Injectivity of $E \mapsto A$ {i.e. E uniquely determined by A. Since $(z-\lambda)(z-\lambda)^{-1} = 1$, we have that for $z : \mathrm{Im}(z) \neq 0$,
$$(z-A)\cdot E((z-\lambda)^{-1}) = E(1) = \mathbb{1}$$
[because $(z-\lambda)^{-1}$ is a bounded function. Similarly
ignore
$$E((z-\lambda)^{-1})(z-A) \subset \mathbb{1}$$
[again: properties of a spectral projection)
namely $E((z-\lambda)^{-1}) = (z-A)^{-1}$
In other words: A determines $E(f)$ for $f(\lambda) = (z-\lambda)^{-1}$
It follows, by linearity, that A determines $E(f)$ for all functions of the form
$$f(\lambda) = \sum_{j=1}^{N} a_j (z_j - \lambda)^{-n_j}$$
$(\mathrm{Im}(z_j) \neq 0,\ a_j \in \mathbb{C},\ n_j \in \mathbb{N})$
But these functions are dense in $C_\infty(\mathbb{R})$ (the continuous functions vanishing at ∞) w.r.t. to the

supremum norm (that is the Stone-Weierstrass theorem).
Finally: $C_\infty(\mathbb{R})$ is a subset of the Borel functions and $f_n(x) \to f(x)$ implies f is Borel. Since $E(f_n) \to E(f)$ we conclude that $E(f)$ is determined by A for all Borel functions f.

(ii) By definition, A is determined by U, namely $A \mapsto U$ is injective. We construct U as such

(a) Approximate A with bounded $A_n^\pm$

(b) Definition of $U(\pm t) = s\text{-}\lim_{n\to\infty} \exp(\pm i t A_n^\pm)$, $t \geq$

(c) Check: + $U(t)$ is a 1-parameter group
+ A is the generator of U

(a): Let

$$A_n^+ = inA(A+in)^{-1} = in + n^2(A+in)^{-1} \qquad (\lambda$$

(indeed: multiply by $(A+in)$: $inA = in(A+in) + n^2$ ✓)

It is bounded because the spectrum of a s.a operator is real.

Let $\psi \in D(A)$. Then $A_n^+\psi = in(A+in)^{-1}A\psi$.
We claim that $A_n^+\psi \to A\psi$, so it suffices to prove $in(A+in)^{-1}\varphi \to \varphi$ for all $\varphi \in \mathcal{H}$.
Since $\|in(A+in)^{-1}\| = n\|(A+in)^{-1}\| \leq n/n = 1$ uniformly in n, it suffices to prove this for $\varphi \in D(A)$

(indeed: $\varphi_j \to \varphi_0$, $\varphi_j \in D(A)$. Then

$$\|in(A+in)\varphi_0 - \varphi_0\| \leq \underbrace{\|in(A+in)(\varphi_0 - \varphi_j)\|}_{\leq \|\varphi_0 - \varphi_j\|} + \|in(A+in)\varphi_j - \varphi_j\| + \|\varphi_j - \varphi_0\|\;)$$

$$\varphi = (A+in)^{-1}(A+in)\varphi = in(A+in)^{-1}\varphi + (A+in)^{-1}A\varphi$$

and we conclude by noting that

$$\|(A+in)^{-1}A\varphi\| \leq \frac{1}{n}\|A\varphi\| \to 0 \quad \text{as } n \to \infty.$$

(b) Define:

$$U_n(t) = e^{itA_n^+} = \sum_{j=0}^{\infty} \frac{1}{j!}(itA_n^+)^j$$

is norm convergent, analytic and solves

$$\frac{d}{dt} U_n^+(t) = iA_n^+ U_n^+(t)$$

Now U_n^+ is a 1-parameter group, and since

$$U_n^+(t) = \exp(-nt)\exp(in^2(A+in)^{-1}t)$$

by (*), we have that $t \geq 0$.

$$\|U_n^+(t)\| \overset{\Delta \text{ ineq}}{\leq} e^{-nt} e^{t\underbrace{\|n^2(A+in)^{-1}\|}_{\leq n}} \leq 1$$

with this and

$$U_m^+(t) - U_n^+(t) = \int_0^t ds\, (U_n^+(t-s)U_m(s))'$$

$$= \int_0^t ds\, U_n^+(t-s)(A_m^+ - A_n^+)U_n(s)$$

we have:

$$\|(U_m^+(t) - U_n^+(t))\psi\| \leq t\,\|(A_m^+ - A_n^+)\psi\|$$

Hence: For $\psi \in D(A)$: $U_n^+(t)\psi$ is Cauchy so that it converges. We define

$$U(t)\psi = \lim_{n\to\infty} U_n^+(t)\psi$$

Since $U_n^+(t)$ is uniformly bounded, $U(t)$ can then be extended to all $\psi \in \mathcal{H}$.

Repeat with A_n^-, $U_n^-(t)$ defined with $i \to -i$

Finally: since $U_n^{\pm}$ are unitary groups and uniformly bounded, so is the limit U

(c) It remains to check that A is the generator of U. For all $\psi \in \mathcal{H}$:

$$U_n^+(t)\psi - \psi = i\int_0^t ds\, U_n^+(s)A_n^+\psi$$

If $\psi \in D(A)$, then the limit $n\to\infty$ yields:

$$U(t)\psi - \psi = i\int_0^t U(s)A\psi\, ds$$

by dominated convergence since

$$\|U_n^+(s)A_n^+\psi\| \leq \|A_n^+\psi\| = \|in(A+in)^{-1}A\psi\|$$
$$\leq \|A\psi\|, \text{ see above.}$$

It follows that $(U(t) - \mathbb{1})\psi$ is differentiable with

$$\lim_{t\to 0} t^{-1}(U(t)\psi - \psi) = iA\psi. \quad \text{indeed.}$$

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(iii) Here again $U(t) = E(e^{it\lambda})$ determines U from E, hence $U \mapsto E$ is injective. We construct $E(f)$ for $f \in C_c^\infty(\mathbb{R})$,

$$E(f) := \int dt\, \hat{f}(t)\, u(t) \qquad (\diamond)$$

where $\hat{f}(t) = (2\pi)^{-1} \int dx\, f(x)\, e^{-itx}$ is the Fourier transform

(think as $\int dt\, \hat{f}(t)\, e^{it\lambda}\, dE(\lambda) = \int f(\lambda)\, dE(\lambda) = E(f)$)

Note: This is well-defined since f compactly supported $\Rightarrow \hat{f}(t) \to 0$ as $|t| \to \infty$ faster than any inverse power.

Hence $E(f) \in \mathcal{L}(\mathcal{H})$

+ Linearity is immediate.

+ Since $\overline{e^{itx}}$

$$\hat{\bar{f}}(t) = (2\pi)^{-1} \int dx\, \overline{f(x)}\, e^{-itx} = \overline{\hat{f}(-t)}$$

$$E(\bar{f}) = \int dt\, \overline{\hat{f}(-t)}\, u(t) = \int dt\, \overline{\hat{f}(t)}\, u(-t)$$

$$= \int dt\, (\hat{f}(t) u(t))^* = (E(f))^*$$

+ Homomorphism.

Note: $f(x)g(x) = \int dt\,ds\, \hat{f}(t)\hat{g}(s)\, e^{i(t+s)x}$
$= \int dt\, e^{itx} \int ds\, \hat{f}(t-s)\, \hat{g}(s)$

so that
$$\widehat{fg}(t) = \int ds\, \hat{f}(t-s)\, \hat{g}(s)$$

Hence
$$E(fg) = \int dt \left(\int ds\, \hat{f}(t-s) g(s) \right) u(t)$$
$$= \int dt\, ds\, \hat{f}(t)\, \hat{g}(s)\, \underbrace{u(t+s)}_{= U(t)U(s)} = E(f)\, E(g)$$

+ Density of $\{E(f)\psi \quad f \in C_c^\infty(\mathbb{R}), \psi \in \mathcal{H}\}$.

Let φ: $\langle \varphi, E(f)\psi \rangle = 0 \quad \forall f, \psi$

In particular:
$$\langle \varphi, E(f)\varphi \rangle = 0 \qquad \forall f \in C_c^\infty(\mathbb{R})$$

namely

$$\int dt\, \hat{f}(t)\, \langle \varphi, U(t)\varphi \rangle \qquad \forall f \in C_c^\infty(\mathbb{R})$$

Since $t \mapsto \langle \varphi, U(t)\varphi \rangle$ is continuous, it follows that $\langle \varphi, U(t)\varphi \rangle = 0$ $\forall t$. At $t=0$: $\|\varphi\|^2 = 0$, hence $\varphi = 0$.

* It remains to prove that $(\Diamond)$ yields $U(t) = E(e^{it\lambda})$

With $e^{itx} f(x) = \int ds\, \hat{f}(s)\, e^{ix(t+s)} = \int ds\, \hat{f}(s-t) e^{ixs}$,

$$E(e^{itx}) E(f)\psi = E(e^{itx} f)\psi = \int ds\, \hat{f}(s-t) U(s)\psi$$
$$= U(t) \int ds\, \hat{f}(s) U(s)\psi = U(t) E(f)\psi$$

Hence $U(t) = E(e^{itx})$ since $\{E(f)\psi\}$ is dense and $\|U(t)\| \leq 1$. ■

• Example: the momentum operator

* On $L^2(\mathbb{R})$: Translation
$$(U(t)\psi)(x) = \psi(x-t)$$
is a 1-parameter group of unitaries. Generator
$$(P\psi)(x) = -i \lim_{t \to 0} t^{-1} \big(\psi(x-t) - \psi(x)\big) = i\psi'(x)$$

Namely $D(P) = \{\psi \in L^2(\mathbb{R}) : \psi'(x) \in L^2(\mathbb{R})\}$
$(P\psi)(x) = i\psi'(x)$.

* On $L^2([0,1])$. The analog of P above is $\tilde{P}$ which is not self-adjoint. This corresponds to the fact that $x \mapsto x-t$ does not preserve the interval $[0,1]$ and hence translation cannot be a unitary group. Hence the need to wrap $[0,1]$ into a circle, by defining

$$(U_\alpha(t)\psi)(x) = \alpha^{[x-t]}\psi(\{x-t\})$$

- We briefly consider two additional properties of self-adjoint operators.

<u>Theorem</u>: Let $T = T^*$ acting on $\mathcal{H}$. Then

(i) $\sigma(T) \subset \mathbb{R}$

(ii) $\|(z-T)^{-1}\| \leq \frac{1}{\mathrm{Im}(z)}$ $\quad (\mathrm{Im}(z) \neq 0)$.

<u>Proof</u>: First claim: $\mathrm{Ran}((z-T))$ is closed if $\mathrm{Im}(z) \neq 0$)

Let $(\varphi_n)_{n\in\mathbb{N}}$ be a sequence in the range which converges to a $\varphi \in \mathcal{H}$. There are $\psi_n \in \mathcal{D}(T)$ s.t. $T\psi_n - z\psi_n = \varphi_n$ and so

$$\underbrace{\langle \psi_n, T\psi_n \rangle}_{\in \mathbb{R} \text{ since } T \text{ is symmetric}} - z\langle \psi_n, \psi_n \rangle = \langle \psi_n, \varphi_n \rangle$$

$\Rightarrow |\mathrm{Im}(z)| \|\psi_n\|^2 \leq |\langle \psi_n, \varphi_n \rangle| \leq \|\psi_n\| \|\varphi_n\| \quad (*)$

Applying this to $\psi_n - \psi_m$ we conclude that

$$\|\psi_n - \psi_m\| \leq |\mathrm{Im}(z)|^{-1} \|\varphi_n - \varphi_m\|$$

so that $(\psi_n)_n$ is a Cauchy sequence and hence converges, say to ψ.

We have:

$$\lim_{n\to\infty} T\psi_n = \lim_{n\to\infty} (z\psi_n + \varphi_n) = z\psi + \varphi \quad (**)$$

so $(T\psi_n)_n$ converges, to ξ. Let $\zeta \in \mathcal{D}(T)$.

Then by symmetry $\langle T\psi_n, \zeta \rangle = \langle \psi_n, T\zeta \rangle$ and taking the limit:

$$\langle \xi, \zeta \rangle = \langle \psi, T\zeta \rangle$$

from which we conclude $\psi \in \mathcal{D}(T^*) = \mathcal{D}(T)$ and $T\psi = \xi$

Comparing with $(**)$: $\varphi \in \mathrm{Ran}(T - z)$ and so $\mathrm{Ran}(z-T)$ is closed.

Now: $\mathrm{Ran}(z-T) = \mathcal{H}$. Otherwise $\exists\, \eta \in \mathcal{H}$ s.t.

$$\langle \eta, (z-T)\varphi \rangle = 0 \quad \forall \varphi \in \mathcal{D}(T)$$

$$\Leftrightarrow \quad \langle \bar{z}\eta, \varphi \rangle = \langle \eta, T\varphi \rangle$$

and since T is self-adjoint, this means

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that $\eta \in \mathcal{D}(T^*) = \mathcal{D}(T)$ with $T\eta = \bar{z}\eta$.
But then $\langle \eta, T\eta \rangle = \bar{z}\langle \eta, \eta \rangle$ is not real, contradiction. Hence $z - T$ is surjective.
Finally, $z - T$ is injective. Otherwise $\exists \varphi \in \mathcal{D}(T)$ s.t.
$$(z-T)\varphi = 0 \quad , \varphi \neq 0,$$
But by $(*)$, this implies that
$$|\mathrm{Im}(z)|\,\|\varphi\| \leq 0 \quad , \text{contradiction.}$$
We conclude: $\mathrm{Im}(z) \neq 0 \Rightarrow (z-T)$ is bijective
and $(*)$ reads:
$$|\mathrm{Im}(z)|\,\|(z-T)^{-1}\varphi\| \leq \|\varphi\| \quad \text{namely}$$
$(z-T)^{-1}$ is bounded with $\|(z-T)^{-1}\| \leq |\mathrm{Im}(z)|^{-1}$. ∎

where $y = [y]_{\mathbb{Z}} + (y)$
integer part   fractional part

with this and with ψ continuous,
$(U_\alpha(t)\psi)(x)$ is continuous everywhere but at
$x = t$: (in fact $t = x + n$, $n \in \mathbb{Z}$)
$(U_\alpha(t)\psi)(t-) = \alpha^{-1}\psi(1)$
$(U_\alpha(t)\psi)(t+) = \psi(0)$

Hence $U_\alpha(t)\psi$ is continuous
iff $\psi \in \mathcal{D}(\tilde{P})$ and $\psi(1) = \alpha\psi(0)$
namely $\psi \in \mathcal{D}(P_\alpha)$
$\Rightarrow$ P_α is the generator of U_α.

- Recall that a Borel measure μ on $\mathbb{R}$ is
  - * Absolutely continuous if $\mu(\Omega) = 0$ for all Borel sets Ω with $|\Omega| = 0$ ($|\Omega|$ Lebesgue measure of Ω)
    Radon-Nikodym theorem: If $\mu(\mathbb{R}) < \infty$, there is a function $f \in L^1(\mathbb{R}; d\lambda)$ s.t.
    $$\mu(\Omega) = \int_\Omega f(\lambda)\, d\lambda$$
  - * Singular (w.r.t. Lebesgue) if $\exists\, \Omega$ with $|\Omega| = 0$
    $\mu(\mathbb{R} \setminus \Omega) = 0$
    $\hookrightarrow$ Any singular measure can be decomposed as
    $$\mu = \mu_{pp} + \mu_{sc}$$
    "pure point"   "singular continuous"

    $\lambda \mapsto \mu((-\infty, \lambda])$ is a step function $\rightsquigarrow$ a countable sum of point measures

    $\lambda \mapsto \mu((-\infty, \lambda])$ is continuous. $\rightsquigarrow$ e.g. the Cantor measure

- We consider a self-adjoint operator A, a vector $\psi \in \mathcal{H}$ and the corresponding measure given by
$$\mu_\psi^A((-\infty, \lambda]) = \langle \psi, E^A(\chi_{(-\infty,\lambda]})\psi \rangle$$

Def: $\mathcal{H}_{ac} = \{\psi \in \mathcal{H} : \mu_\psi \text{ is a.c.}\}$
$\mathcal{H}_{pp} = \{\psi \in \mathcal{H} : \mu_\psi \text{ is p.p.}\}$
$\mathcal{H}_{sc} = \{\psi \in \mathcal{H} : \mu_\psi \text{ is s.c.}\}$

Lemma: $\mathcal{H} = \mathcal{H}_{ac} \oplus \mathcal{H}_{pp} \oplus \mathcal{H}_{sc}$.

Hence we can define three orthogonal projectors

$$\mathcal{H}_\# = P_\# \mathcal{H}$$

Correspondingly: $\sigma_\#(A) = \sigma(P_\# A P_\#)$, in particular

Lemma: $\sigma_{pp}(A)$ is the closure of the set of closed eigenvalues of A.

- Let us now consider this from the point of view of the quantum dynamics. Let $U(t) = e^{itH}$, defined by Stone's theorem.

For any $\psi \in \mathcal{H}$:

$$\langle \psi, U(t)\psi \rangle = \int e^{it\lambda}\, d\mu_\psi(\lambda) = \hat{\mu}_\psi(t)$$

$d\mu_\psi(\lambda) = \mu_\psi((-\infty, \lambda])$; $\hat{\mu}_\psi(t)$ bounded continuous function

is the Fourier transform of the measure μ_ψ.

- If ψ is an eigenvector for the eigenvalue E (in particular $\psi \in \mathcal{H}_{pp}$) then for any $\varphi \in \mathcal{H}$:

$$|\langle \varphi, U(t)\psi \rangle| = |\langle \varphi, \psi \rangle|$$

- However let $\psi \in \mathcal{H}_{ac}$. Then

$$\hat{\mu}_\psi(t) = \int e^{it\lambda} f_\psi(\lambda)\, d\lambda = \hat{f}_\psi(t)$$

in the "usual" sense of Fourier transform.

The classical Riemann–Lebesgue lemma states that if $f \in L^1(\mathbb{R}, d\lambda)$, then $\hat{f}$ is continuous and vanishes at infinity;

Hence:

$$\lim_{t\to\infty} \hat{\mu}_\psi(t) = 0$$

Finally, for any $\varphi \in \mathcal{H}$ the complex measure

(*) $\mu^A_{\varphi,\psi}(\Omega) = \langle \varphi, E^A(\chi_\Omega)\psi \rangle$

is also ac whenever ψ is. Indeed if $\mu^A_\psi(\Omega) = 0$ then

$$|\mu^A_{\varphi,\psi}(\Omega)| \leq \| E^A(\chi_\Omega)\varphi\| \, \|E^A(\chi_\Omega)\psi\|$$
$$= \mu_\varphi(\Omega)\, \mu_\psi(\Omega) = 0$$

Altogether:

If $\psi \in \mathcal{H}_{ac}$, then

$$\lim_{t\to\infty} \langle \varphi, U(t)\psi \rangle = \lim_{t\to\infty} \hat{f}_{\varphi,\psi}(t) = 0 \qquad (**)$$

namely: The evolved state $U(t)\psi$ becomes orthogonal to any fixed vector φ.

We say: $U(t)P_{ac}$ converges weakly to zero.

(*) Note that $\mu^A_{\varphi,\psi}$ is related to $\mu^A_\varphi, \mu^A_\psi$ by the polarization identity:

$$\mu^A_{\psi,\varphi}(\Omega) = \frac{1}{4}\left(\mu^A_{\psi+\varphi}(\Omega) - \mu^A_{\psi-\varphi}(\Omega) + i\mu^A_{\psi-i\varphi}(\Omega) - i\mu^A_{\psi+i\varphi}(\Omega)\right)$$

In fact: more is true, although only in average sense:

Lemma: Let μ be a finite complex measure on $\mathbb{R}$ and let

$$\hat{\mu}(t) = \int \exp(-it\lambda)\, d\mu(\lambda)$$

Then

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T |\hat{\mu}(t)|^2 dt = \sum_{\lambda\in\mathbb{R}} |\mu_{pp}(\{\lambda\})|^2$$

Note that the sum is necessarily countable.

Consequence: If $\psi \in \mathcal{H}_{ac} \oplus \mathcal{H}_{sc}$ and for any $\varphi \in \mathcal{H}$

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \underbrace{|\langle \varphi, e^{-itH}\psi \rangle|}_{} dt = 0$$

$= \| P_\varphi U(t)\psi \|^2$

probability to find $\psi(t)$ in φ

An operator in $\mathcal{L}(\mathcal{H})$ is called <u>compact</u> if it is the norm limit of finite-rank operators.
An operator $K : D(K) \to \mathcal{H}$ is relatively compact with respect to the self-adjoint H if $D(H) \subset D(K)$
$$K(H-z)^{-1}$$
is compact for a $z \in \rho(H)$

<u>Example</u>: $H = -\Delta$ on $\mathcal{H} = L^2(\mathbb{R}^3)$
$K =$ multiplication by $\chi_\Omega(x)$, with Ω compact in $\mathbb{R}^3$

For this we need the following result:
<u>Lemma</u> Let $T : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ be such that
$$(T\psi)(x) = \int k(x,y)\psi(y)\,dy$$
with $k \in L^2(\mathbb{R}^6)$. Then T is compact.

<u>Proof</u>. Let $(\varphi_n)_{n\in\mathbb{N}}$ be any ON-basis of $L^2(\mathbb{R}^3)$. Then $(\varphi_i \overline{\varphi_j})_{i,j\in\mathbb{N}}$ is an ON-basis of $L^2(\mathbb{R}^6)$ and so
$$k(x,y) = \sum_{i,j} c_{ij}\varphi_i(x)\overline{\varphi_j(y)}$$
with $\sum |c_{ij}|^2 = \|k\|^2_{L^2(\mathbb{R}^6)} < \infty$. It follows that
$$(T\psi)(x) = \sum_{ij} c_{ij}\varphi_i(x)\langle\varphi_j,\psi\rangle$$
We note that T is bounded with $\underbrace{\|T\|^2}_{\text{op norm}} \leq \underbrace{\|K\|^2}_{L^2(\mathbb{R}^6)\text{ norm.}}$

in part: $\sum_j \|T\varphi_j\|^2 \leq \sum_{i,j} |c_{ij}|^2 < \infty$. (*)

Now $T\varphi_j = \sum c_{ij}\varphi_i$ so that $k = \sum_j \overline{\varphi_j}\, T\varphi_j$
The kernels
$$k_n(x,y) = \sum_{j=1}^{N} \overline{\varphi_j(y)}\, T\varphi_j(x)$$
define a sequence of finite rank operators
$$(T_n\psi)(x) = \int k_n(x,y)\psi(y)\,dy$$
and we claim that $T_n \to T$ in norm. Indeed, for any $\psi(x) = \sum_i \alpha_i\varphi_i(x)$:
$$|((T_n-T)\psi)(x)| \leq \sum_{j>n}|\alpha_j|\,\|T\varphi_j\| \overset{\text{C.-S.}}{\leq} \|\psi\|\underbrace{\Big(\sum_{j>n}\|T\varphi_j\|^2\Big)^{1/2}}_{\to 0\ (n\to\infty)\ \text{by (*)}}$$
$\boxtimes$

36)

Now: Since $\widehat{f'}(\xi) = \int e^{-i\xi x} f'(x)\,dx = i\xi \hat{f}(\xi)$, we see that $-\Delta$ acts in Fourier space as a multiplication operator by $|\xi|^2$, hence

$$\widehat{(-\Delta+1)^{-1}\psi}(\xi) = (\xi^2+1)^{-1}\hat{\psi}(\xi)$$

We conclude that

$$((-\Delta+1)^{-1}\psi)(x) = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} e^{i\xi x}\frac{\hat{\psi}(\xi)}{\xi^2+1}\,d\xi = \dots$$

$$= \frac{1}{4\pi}\int_{\mathbb{R}^3}\frac{e^{-|x-y|}}{|x-y|}\psi(y)\,dy$$

Hence, the operator $\chi_\Omega(-\Delta+1)^{-1}$ is given by an integral kernel:

$$(\chi_\Omega(-\Delta+1)^{-1}\psi)(x) = \frac{1}{4\pi}\int_{\mathbb{R}^3}\underbrace{\chi_\Omega(x)\frac{e^{-|x-y|}}{|x-y|}}_{K(x,y)}\psi(y)\,dy$$

and $K(x,y)$ is in $L^2(\mathbb{R}^6)$. We conclude that χ_Ω is $(-\Delta+1)$-relatively compact.

The next result shows that if $\psi \in \mathcal{H}_{ac}$ for $-\Delta$, then

$$\|\chi_\Omega e^{it\Delta}\psi\| \to 0 \qquad (t\to\infty)$$

namely: the probability that the particle is found in any compact set vanishes for large times.

It is actually easy to see that $\mathcal{H}_{ac} = \mathcal{H}$ here.

<u>Theorem</u>. Let $H = H^*$ and let K be relatively compact w.r.t. H. Then if $\psi \in \mathcal{H}_{ac}$ for H:

$$\lim_{t\to\infty}\|Ke^{-itH}\psi\| = 0$$

<u>Note</u>: if $\psi \in \mathcal{H}_{sc}$, the same holds in average sense.

<u>Proof</u>. Let $\psi \in \mathcal{H}_{ac}$. There is $\varphi \in \mathcal{H}_{ac}$ s.t.

$$\psi = (H-z)^{-1}\varphi \qquad \text{for a } z \in \rho(H)$$

Hence:

$$Ke^{-itH}\psi = \underbrace{K(H-z)^{-1}}_{\text{compact}}e^{-itH}\varphi$$

$$\mu^{\varphi}((-\infty,\lambda]) = \langle\varphi, E(\chi_{(-\infty,\lambda]})\varphi\rangle = \langle\psi, E((x-\bar{z})^{-1})E(\chi_{(-\infty,\lambda]}(x))E((x-z)^{-1})\psi\rangle$$
$$= \langle\psi, E(\tfrac{\chi}{(x)})\psi\rangle \text{ is a.c.}$$

so it suffices to prove the result for a compact K. We start with K of finite rank:

$$K\psi = \sum_j \alpha_j \langle \psi_j, \psi \rangle \varphi_j$$

for ON families $\{\psi_1, \dots, \psi_n\}$, $\{\varphi_1, \dots, \varphi_n\}$. Then

$$Ke^{-itH}\psi = \sum_j \alpha_j \langle \psi_j, e^{-itH}\psi \rangle \varphi_j$$

and each term vanishes as $t \to \infty$ by (4*).

For K compact, let $K_n \to K$, K_n finite rank. Then

$$\|Ke^{-itH}\psi\| \leq \|K - K_n\| + \|K_n e^{-itH}\psi\|$$

and the claim follows since K_n are uniformly bounded. ▨

- Note: A deep result known as RAGE theorem yields that the converse holds: the spectral subspace can be characterized by the long-time behaviour of $e^{-itH}\psi$.

- Our next goal is to study the well posedness of the dynamics generated by atomic Hamiltonians of the form

$$-\Delta + V$$

for V in a suitable class of functions.

- The graph of an operator A is the subspace $\Gamma(A) \subset \mathcal{H} \oplus \mathcal{H}$

$$\Gamma(A) = \{(\psi, A\psi) : \psi \in D(A)\}.$$

A is closed if $\Gamma(A)$ is a closed subspace of $\mathcal{H} \oplus \mathcal{H}$.

Namely: If $(\psi_n) \in D(A)$ is so that

$$\psi_n \to \psi \quad \text{and} \quad A\psi_n \to \varphi$$

then $\varphi \in D(A)$ & $\varphi = A\psi$.

Lemma: A^* is closed.

Proof: Let $(\psi_n) \in D(A^*)$ s.t. $\psi_n \to \psi$ and $A^*\psi_n \to \varphi$. By definition of $D(A^*)$

$$\langle A^*\psi_n, \xi \rangle = \langle \psi_n, A\xi \rangle \quad \forall \xi \in D(A)$$

and hence $\langle \varphi, \xi \rangle = \langle \psi, A\xi \rangle \quad \forall \xi \in D(A)$

by letting $n \to \infty$. It follows that $\psi \in D(A^*)$ and that $\varphi = A^*\psi$ (by def of A^*). $\square$

With this, we have the following criteria for self-adjointness:

- Theorem: Let $H : D(H) \to \mathcal{H}$ be symmetric and densely defined. T.f.a.e.

(i) H is self-adjoint

(ii) H is closed and $Ker(H^* \pm i) = \{0\}$

(iii) $Ran(H \pm i) = \mathcal{H}$.

We need the following

Lemma: For any densely defined op A:

+ $Ker(A^* \pm \bar{z}) = Ran(A \pm z)^{\perp}$

+ If A is closed and symmetric, then $Ran(A \pm i)$ are closed.

Proof: + $\psi \in Ran(A \pm z)^{\perp}$

$\iff \langle \psi, (A \pm z)\varphi \rangle = 0 \quad \forall \varphi \in D(A)$

$\iff \psi \in D(A^*)$ and $(A \pm z)^* \psi = 0$

(equiv. $(A^* \pm \bar{z})\psi = 0$)

$\iff \psi \in D(A^*)$ and $\psi \in Ker(A^* \pm \bar{z})$

* If A is symmetric: $\langle \psi, A\psi \rangle = \langle A\psi, \psi \rangle$

$\langle A\psi, \psi \rangle$

$\Rightarrow \langle \psi, A\psi \rangle \in \mathbb{R}$. Therefore for $\psi \in D(A)$:

$\|(A + i)\psi\|^2 = \|A\psi\|^2 + \|\psi\|^2 - \langle A\psi, \psi \rangle - \langle i\psi, A\psi \rangle$

but $-(\ldots) = -i\langle A\psi, \psi \rangle + i\langle \psi, A\psi \rangle = 0$

$\Rightarrow \|(A + i)\psi\|^2 = \|A\psi\|^2 + \|\psi\|^2 \geq \|\psi\|^2$

In particular: $Ker(A + i) = \{0\}$

and $(A + i)^{-1} : Ran(A + i) \to D(A)$ exists and is bounded. Let $\psi_n \in Ran(A + i)$ be s.t. $\psi_n \to \psi$ and let $\varphi_n = (A + i)^{-1}\psi_n$. Then φ_n converges. Since A is closed, $(\varphi_n, (A + i)\varphi_n) \to (\varphi, (A + i)\varphi)$ namely $\psi \in Ran(A + i)$ $\square$

Proof of theorem:

(i) $\Rightarrow$ (ii) $H = H^*$ is closed. If $\psi_{\pm} \in Ker(H^* \pm i)$, then $H\psi_{\pm} = \mp i\psi_{\pm}$ and hence ($\|\psi_{\pm}\| = 1$)

$\langle \psi_{\pm}, H\psi_{\pm} \rangle = \mp i$ which is a contradiction since this should be real. Hence $\psi_{\pm} = 0$

(ii) ⇒ (iii) By the lemma $\ker(H^* \pm i) = \{0\} = \mathrm{Ran}(H \mp i)^\perp$

Hence $\overline{\mathrm{Ran}(H \mp i)} = \mathcal{H}$, and by the lemma again $\mathrm{Ran}(H \pm i) = \mathcal{H}$.

(iii) ⇒ (i) H symmetric ⇒ $H \subset H^*$. We show $H^* \subset H$.
Let $\psi \in \mathcal{D}(H^*)$. Since $\mathrm{Ran}(H \pm i) = \mathcal{H}$, $\exists\, \varphi_\pm \in \mathcal{D}(H)$
s.t. $(H^* \pm i)\psi = (H \pm i)\varphi_\pm = (H^* \pm i)\varphi_\pm$
[since $H \subset H^*$]
namely $\varphi_\pm - \psi \in \ker(H^* \pm i) = \mathrm{Ran}(H \mp i)^\perp = \{0\}$
⇒ $\psi \in \mathcal{D}(H)$ since φ does. □

A, B densely defined s.t. $\mathcal{D}(A) \subset \mathcal{D}(B)$. B is called relatively bounded w.r.t. A if $\exists\, a, b \geq 0$ s.t.

$$\|B\psi\| \leq a\|A\psi\| + b\|\psi\| \qquad \psi \in \mathcal{D}(A)$$

infimum over all possible a is the A-bound of B.
(Note: if B is bounded, then the A-bound is 0)

Theorem [Kato-Rellich]. Let A be self-adjoint on $\mathcal{D}(A)$, and let B be symmetric on $\mathcal{D}(B)$. If B is relatively bounded with A-bound < 1, then $A+B$ is self-adjoint on $\mathcal{D}(A+B) = \mathcal{D}(A) \cap \mathcal{D}(B) = \mathcal{D}(A)$

Proof $A = A^*$ ⇒ $\mathrm{Ran}\,(A + \lambda \mathbb{1})^{-1}$ is bounded for any $\lambda \in \mathbb{C} \setminus \mathbb{R}$. and $\mathrm{Ran}(A+\lambda)^{-1} = \mathcal{D}(A)$

Hence: $\underbrace{(\mathbb{1} + B(A \pm \lambda)^{-1})}_{\text{makes sense}}(A \pm \lambda) = A + B \pm \lambda$ (*) on $\mathcal{D}(A)$

$A = A^*$ ⇒ $\mathrm{Ran}(A \pm \lambda) = \mathcal{H}$ so in order to prove that $\mathrm{Ran}\,(A + B \pm \lambda) = \mathcal{H}$ it suffices to show that $\mathrm{Ran}\left(\mathbb{1} + B(A \pm \lambda)^{-1}\right) = \mathcal{H}$

We claim that $\|B(A \pm \lambda)^{-1}\| < 1$, (for $\lambda = i\mu$, $\mu > 0$ large enough.) With this,

$$\sum_{n=0}^{\infty} \left(-B(A \pm \lambda)^{-1}\right)^n = \left(\mathbb{1} + B(A \pm \lambda)^{-1}\right)^{-1}$$

(norm-convergent Neuman series)
namely $\mathbb{1} + B(A \pm \lambda)^{-1}$ is invertible, in part. surjective

Let $\psi \in \mathcal{D}(A)$ and $\varphi_\pm$ s.t. $\psi = (A \pm \lambda)^{-1}\varphi_\pm$

We pick $\pm\lambda = \pm i\mu$, $\mu \in \mathbb{R}_+$. Hence

$\|(A \pm i\mu)\psi\|^2 = \|A\psi\|^2 + \mu^2\|\psi\|^2$

In terms of $\varphi_\pm$

$$\|\varphi_\pm\|^2 = \|A(A \pm i\mu)^{-1}\varphi_\pm\|^2 + \mu^2\|(A \pm i\mu)^{-1}\varphi_\pm\|^2$$

Hence & $\|A(A \pm i\mu)^{-1}\varphi_\pm\| \le \|\varphi_\pm\|$

& $\|(A \pm i\mu)^{-1}\varphi_\pm\| \le \frac{1}{\mu}\|\varphi_\pm\|$

We can use the A-bound to get:

$$\|B(A \pm i\mu)^{-1}\varphi_\pm\| \le a\|A(A \pm i\mu)^{-1}\varphi_\pm\| + b\|(A \pm i\mu)^{-1}\varphi_\pm\|$$
$$\le \underbrace{\left(a + \frac{b}{\mu}\right)}_{<1 \text{ for } \mu \text{ large enough}}\|\varphi_\pm\| \qquad (**)$$

□

Note that this yields a lower bound on $A+B$ provided $A \ge E_0\mathbb{1}$. Indeed $(A + E\mathbb{1})^{-1}$ is invertible for all $E \ge -E_0$ and the same procedure yields $\|B(A+E)^{-1}\| < 1$ if $-E < E_0 - \max\left\{\frac{b}{1-a}; aE_0\right\}$

We turn to $H = -\Delta + V$ on $L^2(\mathbb{R}^3)$

Recall:

$$\hat{f}(\xi) = \frac{1}{(2\pi)^{3/2}}\int e^{-i\xi \cdot x} f(x)\,dx \qquad (*)$$

is well-defined on $L^1(\mathbb{R}^3)$ with $\|\hat{f}\|_{L^\infty} \le (2\pi)^{-3/2}\|f\|_{L^1}$

Note that is not a priori well-defined on L^2, but

Theorem: (i) If $f \in L^1 \cap L^2$, then $\hat{f} \in L^2$, with

$\|\hat{f}\|_{L^2} = \|f\|_{L^2}$

(ii) The map $\mathcal{F}$: $\mathcal{F}(f) = \hat{f}$ extends to a bounded map on L^2.

(iii) $\langle \hat{f}, \hat{g} \rangle_{L^2} = \langle f, g \rangle_{L^2}$

Proof: $\hat{f} \in L^\infty$ implies that $\forall \varepsilon > 0$:

$$\int |\hat{f}(\xi)|^2 e^{-\varepsilon\xi^2}\,d\xi < \infty, \quad \text{and}$$

$$\int |\hat{f}(\xi)|^2 e^{-\varepsilon\xi^2}\,d\xi = \frac{1}{(2\pi)^3}\int \overline{f(x)} f(y)\, e^{i\xi(x-y)}\, e^{-\varepsilon\xi^2}\,d\xi\,dx\,dy$$

by Fubini. The Gaussian integral in ξ can be carried out by contour integration to get

$$\int e^{i\xi(x-y)-\varepsilon\xi^2} d\xi = \frac{1}{(4\varepsilon\pi)^{3/2}} e^{-(x-y)^2/4\varepsilon} = j_\varepsilon(x-y)$$

hence:

$$(\dots) = \langle f, f * j_\varepsilon \rangle_{L^2(\mathbb{R}^3; dx)}$$

Now:

$$f * j_\varepsilon \to f \quad \text{in } L^2 \quad \text{so that}$$

$$\langle f, f * j_\varepsilon \rangle \to \|f\|_2^2 \quad \text{in } L^2$$

In particular: $\hat{f}(\xi) e^{-\frac{\varepsilon}{2}\xi^2}$ is convergent in $L^2(\mathbb{R}^3; d\xi)$. Since $\hat{f}(\xi)\exp(-\frac{\varepsilon}{2}\xi^2) \to \hat{f}(\xi)$ pointwise we conclude that

$$\lim_{\varepsilon \to 0} \int |\hat{f}(\xi)| e^{-\varepsilon\xi^2} d\xi = \int |\hat{f}(\xi)| d\xi = \|\hat{f}\|_2^2$$

(ii, iii) follow immediately $\square$

Now: For $f \in L^2(\mathbb{R}^3; dx)$ (not necessarily in L^1), we define

$$\hat{f}(\xi) = \frac{1}{(2\pi)^{3/2}} \lim_{n \to \infty} \int f(x) e^{-i\xi x - \frac{x^2}{n}} dx$$

where lim is taken in L^2-sense.

and the Fourier transform is a unitary operator on $L^2(\mathbb{R}^3)$. Its inverse is

$$\check{f}(x) = \hat{f}(-x) = \lim_{n \to \infty} \frac{1}{(2\pi)^{3/2}} \int f(x) e^{i\xi x - \frac{x^2}{n}} dx.$$

- Def: $H^2(\mathbb{R}^3) := \{ f \in L^2(\mathbb{R}^3) : |\xi|^2 \hat{f}(\xi) \in L^2(\mathbb{R}^3) \}$

It is a Hilbert space with inner product

$$\langle f, g \rangle_{H^2} = \int \overline{\hat{f}(\xi)}\, \hat{g}(\xi) (1 + |\xi|^2)^2 d\xi$$

- If $f \in H^2(\mathbb{R}^3) \cap C^2(\mathbb{R}^3)$, then by int by parts:

$$-\widehat{\Delta f}(\xi) = \xi^2 \hat{f}(\xi)$$

⇝ Free Hamiltonian H_0 on $L^2(\mathbb{R})$

(i) Multiplication op. on $L^2(\mathbb{R}^3, d\xi)$: $\hat{\psi}(\xi) \to \xi^2 \hat{\psi}($
with domain: $\{\hat{\psi} \in L^2 : \xi^2 \hat{\psi}(\xi) \in L^2\}$
is self-adjoint.

(ii) It is unitarily equivalent to H_0 on $L^2(\mathbb{R}^3, d$

$$\mathcal{D}(H_0) = H^2(\mathbb{R}^3)$$

$$H_0 \psi = -\Delta \psi = \left(\xi^2 \hat{\psi}(\xi)\right)^\vee$$

<u>Lemma</u>. For any $a>0$, $\exists b>0$ s.t. for all $\psi \in H^2$

$$\|\psi\|_\infty \le a\|-\Delta\psi\|_2 + b\|\psi\|_2$$

(Hence: functions in the domain of H_0 are bounded)

<u>Proof</u>: first of all:

$$\int (1+\xi^2)|\hat{\psi}(\xi)|(1+\xi^2)^{-1}\, d\xi \le \|(1+\xi^2)\hat{\psi}\|_2 \underbrace{\|(1+\xi^2)^{-1}\|_2}_{=:C<\infty}$$

so that $\hat{\psi} \in L^1$, with

(*) $$\|\hat{\psi}\|_1 \le C\left(\|\xi^2\hat{\psi}\|_2 + \|\hat{\psi}\|_2\right) = C\left(\|-\Delta\psi\|_2 + \|\psi\|_2\right)$$

We introduce the scaling $\hat{\psi}_\lambda(\xi) = \lambda^3 \hat{\psi}(\lambda\xi)$ for which

* $\|\hat{\psi}_\lambda\|_1 = \|\hat{\psi}\|_1$
* $\|\hat{\psi}_\lambda\|_2 = \lambda^{3/2}\|\hat{\psi}\|_2$
* $\|\xi^2\hat{\psi}_\lambda\|_2 = \lambda^{-1/2}\|\xi^2\hat{\psi}\|_2$

Hence (*) for $\hat{\psi}_\lambda$ yields

$$\|\hat{\psi}\|_1 \le C\lambda^{3/2}\|\hat{\psi}\|_2 + C\lambda^{-1/2}\|\xi^2\hat{\psi}\|_2$$

and the claim follows from $\|\psi\|_\infty \le (2\pi)^{-3/2}\|\hat{\psi}\|_1$
(by inverse F.T.)

Theorem Let $V = V_1 + V_2$ with $V_1 \in L^2(\mathbb{R}^3_x)$
$V_2 \in L^\infty(\mathbb{R}^3_x)$

Then $H = -\Delta + V$ is self-adjoint on
$\mathcal{D}(H) = H^2(\mathbb{R}^3_x)$

Proof V is self-adjoint on
$$\mathcal{D}(V) = \{\psi \in L^2(\mathbb{R}^3_x) : V\psi \in L^2(\mathbb{R}^3_x)\}$$
Moreover: if $\psi \in \mathcal{D}(H_0)$, then $\psi \in L^2(\mathbb{R}^3_x) \cap L^\infty(\mathbb{R}^3_x)$
so that
$$\|V\psi\|_2 \leq \|V_1\psi\|_2 + \|V_2\psi\|_2 \leq$$
$$\leq \|V_1\|_2 \|\psi\|_\infty + \|V_2\|_\infty \|\psi\|_2$$
and so $\mathcal{D}(H_0) \subset \mathcal{D}(V)$
Furthermore, by the lemma
$$\|V\psi\|_2 \leq a\|V_1\|_2 \|-\Delta\psi\|_2 + (b + \|V_2\|_\infty)\|\psi\|_2$$
for any $a > 0$.
Hence: V is H_0-bounded with H_0-bound 0 and the theorem follows from Kato-Rellich. $\square$

Note: the Coulomb potential $V(x) = -\frac{\alpha}{|x|}$ which is relevant for the electrostatic and gravitational forces belongs to $L^2 + L^\infty$

$$V(x) = \underbrace{\chi_{\{|x| \leq 1\}}(x)\, V(x)}_{\in L^2} + \underbrace{\chi_{\{|x| > 1\}}(x)\, V(x)}_{\in L^\infty}$$

since $\frac{1}{|x|^2}$ is integrable at 0.

Corollary
$$H_N = \sum_{i=1}^{N} -\Delta_{x_i} - \sum_{i=1}^{N}\sum_{j=1}^{M} \frac{\alpha Z_j}{|x_i - R_j|} + \sum_{1 \leq i < j \leq N} \frac{\alpha^2}{|x_i - x_j|}$$
is self-adjoint on $H^2(\mathbb{R}^3)$

Remarks: (i) Well-defined quantum dynamics for atoms and molecules

(ii) Since $-\Delta \geq 0$, Kato-Rellich yields a lower bound on the atomic/molecular Hamiltonian

$\Rightarrow$ Stability of the first kind.

Note that the lower bound for H_N will depend on N (and M).