

3 Dynamics, Stone's theorem and the spectral theorem

3.1 Spectral measures

Definition. A spectral measure is a $*$ -homomorphism $E : C_c^\infty(\mathbb{R}; \mathbb{C}) \rightarrow \mathcal{L}(\mathcal{H})$, namely

- $E(\alpha f + g) = \alpha E(f) + E(g)$,
- $E(fg) = E(f)E(g)$,
- $E(f)^* = E(\bar{f})$,

which is such that $\{E(f)\psi : f \in C_c^\infty(\mathbb{R}; \mathbb{C}), \psi \in \mathcal{H}\}$ is dense in $\mathcal{H}$.

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

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

whenever $f_n \rightarrow f$ pointwise (see functional analysis; essentially Riesz–Markov's theorem). In particular, the constant function $g \equiv 1$ is a bounded Borel function and so $E(f)\psi = E(1)E(f)\psi$ by the properties of a spectral measure. Hence $E(1) \neq \mathbb{1}$ would imply that $\{E(f)\psi : f \in C_c^\infty(\mathbb{R}), \psi \in \mathcal{H}\}$ is not dense. Therefore

$$E(1) = \mathbb{1}.$$

We write, formally,

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

meaning that for any normalized $\psi \in \mathcal{H}$,

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

where μ_ψ is a probability measure since $\int d\mu_\psi(\lambda) = \langle \psi, \mathbb{1}\psi \rangle = 1$.

Just as the right hand side can be extended to the general class of (possibly unbounded) Borel functions, so does a spectral measure (we again leave that construction for a functional analysis course). For an unbounded $f \in \mathcal{B}(\mathbb{R}; \mathbb{C})$, the operator $E(f)$ is in general unbounded and densely defined with

$$D(E(f)) = \{\psi \in \mathcal{H} : E(f)\psi \in \mathcal{H}\} = \left\{ \psi \in \mathcal{H} : \int |f(\lambda)|^2 d\mu_\psi(\lambda) < \infty \right\}.$$

We denote by id the Borel function $x \mapsto x$.

Theorem 1 (Spectral theorem). *For every spectral measure E , the operator $A = E(\text{id})$, i.e.*

$$A = \int \lambda dE(\lambda), \tag{1}$$

is self-adjoint. Reciprocally, every self-adjoint operator has a spectral representation (1), where E is unique.

The proof of this theorem will use unitary groups.

3.2 Unitary groups and Stone's theorem

Definition. A *one-parameter unitary group* is a map $U : \mathbb{R} \rightarrow \mathcal{L}(\mathcal{H})$ such that

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

It immediately follows that

$$\lim_{t \rightarrow t_0} U(t)\psi = U(t_0)\psi \quad \left(\text{also written as } \text{s-lim}_{t \rightarrow t_0} U(t) = U(t_0) \right),$$

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

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

$$D(A) = \left\{ \psi \in \mathcal{H} : \lim_{t \rightarrow 0} t^{-1}(U(t)\psi - \psi) \text{ exists} \right\},$$

$$A\psi = i \lim_{t \rightarrow 0} t^{-1}(U(t)\psi - \psi), \quad \psi \in D(A),$$

so that (at least formally at this point) $U(t) = e^{-itA}$. Note that for all $\psi, \phi \in D(A)$,

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

namely A is symmetric. Much more is true:

Theorem 2 (Stone). *The generator A of a one-parameter unitary group is self-adjoint. Reciprocally, every self-adjoint operator generates a one-parameter unitary group, and $U(t)$ is uniquely defined by A .*

3.2.1 Quantum dynamics

In quantum mechanics, the time evolution is a family of maps $V : t \mapsto V(t)$ such that

- $D(V(t)) = \mathcal{H}$ for all $t \in \mathbb{R}$,
- $\|V(t)\psi\| = \|\psi\|$ (“conservation of probability”),
- $V(0) = \mathbb{1}$,
- $V(t+s) = V(t)V(s)$,
- $V(t)\psi \rightarrow V(t_0)\psi$ as $t \rightarrow t_0$.

In other words, the *quantum propagator* $V(t)$ is a one-parameter unitary group. By Stone's theorem, for any quantum dynamics $V(t)$, there exists a unique self-adjoint operator H , the *Hamiltonian*, such that

$$\begin{aligned} i \frac{d}{dt} V(t)\psi &= i \lim_{\varepsilon \rightarrow 0} \varepsilon^{-1} (V(t+\varepsilon) - V(t))\psi \\ &= i \lim_{\varepsilon \rightarrow 0} \varepsilon^{-1} (V(\varepsilon) - \mathbb{1})V(t)\psi = HV(t)\psi. \end{aligned}$$

In other words, the quantum state $\psi(t) = V(t)\psi$ solves *Schrödinger's equation*

$$i\psi'(t) = H\psi(t), \quad \psi(0) = \psi_0.$$

3.3 Proof of the two theorems

Lemma 3. (i) Let E be a spectral measure. Then $A = E(\text{id})$ is self-adjoint.

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

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

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) and (iii),

$$A\psi \stackrel{(ii)}{=} i \lim_{t \rightarrow 0} t^{-1} (U(t) - \mathbb{1})\psi \stackrel{(iii)}{=} i \lim_{t \rightarrow 0} t^{-1} (E(e^{-it\lambda}) - \mathbb{1})\psi,$$

with $\psi \in D(A)$ if and only if the limit exists. Linearity and the fact that $\mathbb{1} = E(1)$ now yield

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

and by the property of the spectral measure, $\lim_{t \rightarrow 0} t^{-1}(e^{-it\lambda} - 1) = -i\lambda$ implies that

$$\lim_{t \rightarrow 0} E(t^{-1}(e^{-it\lambda} - 1))\psi = -i E(\text{id})\psi.$$

Note that passing to the limit is justified¹ if $\psi \in D(E(\text{id}))$. Hence $A \supseteq E(\text{id})$. But $A = A^* \subseteq E(\text{id})^* \stackrel{(i)}{=} E(\text{id})$, so we conclude that $A = E(\text{id})$. $\square$

Proof of Lemma 3. (i) Let $A = E(\text{id})$. That $A = A^*$ follows from $E(f)^* = E(\overline{f})$ for any f (the question of domains implied in $\overline{}$ here is treated in the extension of E to unbounded Borel functions). *Injectivity of $E \mapsto A$.* Let $\lambda \in \mathbb{R}$. Since $(z - \lambda)(z - \lambda)^{-1} = 1$, we have that for z with $\text{Im}(z) \neq 0$,

$$(z - A) E((z - \lambda)^{-1}) = E(1) = \mathbb{1}$$

because $(z - \lambda)^{-1}$ is a bounded function. Similarly $E((z - \lambda)^{-1})(z - A) \subseteq \mathbb{1}$ (again by the properties of a spectral measure), 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

$$f(\lambda) = \sum_{j=1}^N \frac{a_j}{z_j - \lambda} \quad (\text{Im}(z_j) \neq 0, a_j \in \mathbb{C}).$$

But these functions are dense in $C_\infty(\mathbb{R})$ (the continuous functions vanishing at ∞) with respect to the supremum norm — this is the Stone–Weierstrass theorem. Finally, $C_\infty(\mathbb{R})$ is a subset of the Borel functions, and $f_n(x) \rightarrow f(x)$ implies f Borel; since $E(f_n) \rightarrow E(f)$, we conclude that $E(f)$ is determined by A for all Borel functions f .

(ii) By definition and the uniqueness of limits, A is determined by U , namely $A \mapsto U$ is injective. We construct U as follows:

¹This is really dominated convergence with $\left| \frac{e^{-it\lambda} - 1}{t} \right| \leq |\lambda|$.

- (a) approximate A with bounded $A_n^\pm$;
- (b) define $U(\pm t) = \text{s-lim}_{n \rightarrow \infty} \exp(\mp it A_n^\pm)$, $t \geq 0$;
- (c) check that $U(t)$ is a one-parameter group and that A is the generator of U .

(a) Let

$$A_n^\pm = \mp in A (A \mp in)^{-1} = \mp in + n^2 (A \mp in)^{-1} \quad (2)$$

(indeed, multiply by $(A \mp in)$: $\mp in A = \mp in (A \mp in) + n^2$). It is bounded because the spectrum of a self-adjoint operator is real.

Let $\psi \in D(A)$. Then $A_n^+ \psi = -in(A - in)^{-1} A \psi$. To prove that $A_n^+ \psi \rightarrow A \psi$, it suffices to prove that $-in(A - in)^{-1} \phi \rightarrow \phi$ for all $\phi \in \mathcal{H}$. Since $\| -in(A - in)^{-1} \| = n \| (A - in)^{-1} \| \leq n/n = 1$ uniformly in n , it suffices to prove this for $\phi \in D(A)$. Indeed, if $\phi_j \rightarrow \phi_0$ with $\phi_j \in D(A)$, then

$$\| -in(A - in)^{-1} \phi_0 - \phi_0 \| \leq \underbrace{\| -in(A - in)^{-1} (\phi_0 - \phi_j) \|}_{\leq \| \phi_0 - \phi_j \|} + \| -in(A - in)^{-1} \phi_j - \phi_j \| + \| \phi_j - \phi_0 \|.$$

Now

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

and we conclude by noting that $\| (A - in)^{-1} A \phi \| \leq \frac{1}{n} \| A \phi \| \rightarrow 0$ as $n \rightarrow \infty$.

(b) Define

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

which is norm convergent, analytic, and solves $\frac{d}{dt} U_n^+(t) = -iA_n^+ U_n^+(t)$. Now U_n^+ is a homomorphism $[0, \infty) \rightarrow \mathcal{B}(\mathcal{H})$, and since, by (2),

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

we have, for $t \geq 0$,

$$\| U_n^+(t) \| \leq e^{-nt} e^{t \| n^2(A - in)^{-1} \|} \leq 1, \quad \| n^2(A - in)^{-1} \| \leq n.$$

With this and

$$U_m^+(t) - U_n^+(t) = \int_0^t ds \frac{d}{ds} (U_n^+(t-s) U_m^+(s)) = -i \int_0^t ds U_n^+(t-s) (A_m^+ - A_n^+) U_m^+(s),$$

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

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

Since $U_n^+(t)$ is uniformly bounded, $U(t)$ can then be extended to all $\psi \in \mathcal{H}$. Repeat with A_n^- and $U_n^-(-t)$ defined for $t \geq 0$.

For $t > 0$, we have that

$$U_n^+(t) U_n^-(-t) - \mathbb{1} = i \int_0^t ds U_n^+(s) U_n^-(-s) (A_n^+ - A_n^-)$$

and so

$$\|U_n^+(t)U_n^-(-t)\psi - \psi\| \leq t\|(A_n^+ - A_n^-)\psi\| \rightarrow 0$$

as $n \rightarrow \infty$ for all $\psi \in D(A)$. This proves that $U(t)U(-t) = \mathbb{1}$ and a similar argument yields $U(-t)U(t) = \mathbb{1}$. With this, the group property holds not only for s, t of the same sign. Indeed, if $s \geq t \geq 0$, then $U(s) = U(s-t)U(t) = U(t)U(s-t)$ now implies that $U(s)U(-t) = U(s-t)$ and $U(-t)U(s) = U(s-t)$. Hence $U(t)$ is a one-parameter unitary group.

Finally, since the $U_n^\pm$ 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 $n \rightarrow \infty$ yields

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

by dominated convergence, since

$$\|U_n^+(s)A_n^+\psi\| \leq \|A_n^+\psi\| = \|n(A - in)^{-1}A\psi\| \leq \|A\psi\|$$

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

$$\lim_{t \rightarrow 0} t^{-1}(U(t)\psi - \psi) = -iA\psi.$$

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

$$E(f) = \int dt \widehat{f}(t)U(t), \quad (3)$$

where $\widehat{f}(t) = (2\pi)^{-1} \int dx f(x)e^{itx}$ is the Fourier transform, so that $f(x) = \int dt \widehat{f}(t)e^{-itx}$. (Think of (3) as $\int dt \widehat{f}(t)e^{-it\lambda} dE(\lambda) = \int f(\lambda) dE(\lambda) = E(f)$.) Note that this is well defined since the differentiability of f implies that $\widehat{f}(t) \rightarrow 0$ as $|t| \rightarrow \infty$ faster than any inverse power; hence $E(f) \in \mathcal{L}(\mathcal{H})$.

Linearity is immediate.

**-property.* Since $\widehat{\bar{f}}(t) = (2\pi)^{-1} \int dx \overline{f(x)}e^{-itx} = \overline{\widehat{f}(-t)}$,

$$E(\bar{f}) = \int dt \overline{\widehat{f}(-t)}U(t) = \int dt \overline{\widehat{f}(t)}U(-t) = \int dt (\widehat{f}(t)U(t))^* = E(f)^*.$$

Homomorphism. Note that

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

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

$$E(fg) = \int dt \left(\int ds \widehat{f}(t-s)\widehat{g}(s) \right) U(t) = \int dt ds \widehat{f}(t)\widehat{g}(s) \underbrace{U(t+s)}_{=U(t)U(s)} = E(f)E(g).$$

Density of $\{E(f)\psi : f \in C_c^\infty(\mathbb{R}), \psi \in \mathcal{H}\}$. Let ϕ satisfy $\langle \phi, E(f)\psi \rangle = 0$ for all f, ψ . In particular $\langle \phi, E(f)\phi \rangle = 0$ for all $f \in C_c^\infty(\mathbb{R})$, namely

$$\int dt \widehat{f}(t) \langle \phi, U(t)\phi \rangle = 0 \quad \forall f \in C_c^\infty(\mathbb{R}).$$

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

It remains to prove that (3) yields $U(t) = E(e^{-itx})$. With $e^{-itx}f(x) = \int ds \widehat{f}(s)e^{-ix(s+t)} = \int ds \widehat{f}(s-t)e^{-isx}$,

$$\begin{aligned} E(e^{-itx})E(f)\psi &= E(e^{-itx}f)\psi = \int ds \widehat{f}(s-t)U(s)\psi \\ &= U(t) \int ds \widehat{f}(s)U(s)\psi = U(t)E(f)\psi. \end{aligned}$$

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

Example: the momentum operator

On $L^2(\mathbb{R})$, the translations

$$(U(t)\psi)(x) = \psi(x-t)$$

form a one-parameter group of unitaries. Its generator is

$$(P\psi)(x) = i \lim_{t \rightarrow 0} t^{-1} (\psi(x-t) - \psi(x)) = -i\psi'(x),$$

namely

$$D(P) = \{ \psi \in L^2(\mathbb{R}; \mathbb{C}) : \psi' \in L^2(\mathbb{R}; \mathbb{C}) \}, \quad (P\psi)(x) = -i\psi'(x).$$

On $L^2([0, 1]; \mathbb{C})$, the analogue 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

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

where $y = [y] + (y)$ splits y into its integer part and its fractional part. With this, and with ψ continuous, $(U_\alpha(t)\psi)(x)$ is continuous everywhere but at $x = t$ (in fact at $t = x + n$, $n \in \mathbb{Z}$):

$$(U_\alpha(t)\psi)(t^-) = \alpha^{-1}\psi(1), \quad (U_\alpha(t)\psi)(t^+) = \psi(0).$$

Hence $U_\alpha(t)\psi \in D(\tilde{P})$ (it must be continuous) if and only if $\psi \in D(\tilde{P})$ and $\psi(1) = \alpha\psi(0)$, namely $\psi \in D(P_\alpha)$. So P_α is the generator of U_α .

3.4 Spectral subspaces

Recall that a Borel measure μ on $\mathbb{R}$ is

- *absolutely continuous* if $\mu(\Omega) = 0$ for all Borel sets Ω with $|\Omega| = 0$ ($|\Omega|$ the Lebesgue measure of Ω). Radon–Nikodym theorem: if μ is absolutely continuous with $\mu(\mathbb{R}) < \infty$, then there is a function $f \in L^1(\mathbb{R}, d\lambda)$ such that $\mu(\Omega) = \int_\Omega f(\lambda) d\lambda$;
- *singular* (with respect to Lebesgue) if there is Ω with $|\Omega| = 0$ and $\mu(\mathbb{R} \setminus \Omega) = 0$.

Any singular measure can be decomposed as $\mu = \mu_{\text{pp}} + \mu_{\text{sc}}$, “pure point” and “singular continuous”: $\lambda \mapsto \mu((-\infty, \lambda])$ is a step function in the first case (a countable sum of point measures), and continuous in the second (e.g. the Cantor measure).

We consider a self-adjoint operator A , a vector $\psi \in \mathcal{H}$, and the corresponding measure given by

$$\mu_\psi^A((-\infty, \lambda]) = \langle \psi, E^A(\chi_{(-\infty, \lambda]}) \psi \rangle.$$

Definition.

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

Lemma 4. $\mathcal{H} = \mathcal{H}_{\text{ac}} \oplus \mathcal{H}_{\text{pp}} \oplus \mathcal{H}_{\text{sc}}$.

Hence we can define three orthogonal projectors, $\mathcal{H}_\# = P_\# \mathcal{H}$. Correspondingly,

$$\sigma_\#(A) = \sigma(P_\# A P_\#).$$

Lemma 5. $\mathcal{H}_{\text{pp}}$ is the closed span of the eigenvectors of A and $\sigma_{\text{pp}}(A)$ is the closure of the set of eigenvalues of A .

3.4.1 The dynamical point of view

Let $U(t) = e^{-itH}$, defined by Stone’s theorem. For any $\psi \in \mathcal{H}$,

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

is the Fourier transform of the measure μ_ψ .

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

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

is constant.

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

$$\widehat{\mu_\psi}(t) = \int e^{-it\lambda} f(\lambda) d\lambda = \widehat{f}(t)$$

in the “usual” sense of Fourier transform. The classical Riemann–Lebesgue lemma states that if $f \in L^1(\mathbb{R}, d\lambda)$, then $\widehat{f}$ is continuous and vanishes at infinity. Hence

$$\lim_{t \rightarrow \infty} \widehat{\mu_\psi}(t) = 0.$$

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

$$\mu_{\phi, \psi}^A(\Omega) = \langle \phi, E^A(\chi_\Omega) \psi \rangle$$

is also absolutely continuous whenever μ_ψ is. Indeed, if $\mu_\psi(\Omega) = 0$, then

$$|\mu_{\phi, \psi}^A(\Omega)| \leq \|E^A(\chi_\Omega)\phi\| \|E^A(\chi_\Omega)\psi\| = \mu_\phi(\Omega)^{1/2} \mu_\psi(\Omega)^{1/2} = 0.$$

Altogether: if $\psi \in \mathcal{H}_{\text{ac}}$, then

$$\lim_{t \rightarrow \infty} \langle \phi, U(t)\psi \rangle = \lim_{t \rightarrow \infty} \widehat{\mu_{\phi, \psi}^A}(t) = 0, \tag{4}$$

namely: the evolved state $\psi(t) = U(t)\psi$ becomes orthogonal to any fixed vector ϕ . We say that $U(t)P_{\text{ac}}$ converges weakly to zero.

Remark. $\mu_{\phi,\psi}^A$ is related to μ_ϕ^A and μ_ψ^A by the polarization identity:

$$\mu_{\phi,\psi}^A(\Omega) = \frac{1}{4} \left(\mu_{\phi+\psi}^A(\Omega) - \mu_{\phi-\psi}^A(\Omega) + i \mu_{\phi-i\psi}^A(\Omega) - i \mu_{\phi+i\psi}^A(\Omega) \right).$$

In fact more is true, although only in an average sense. The ergodic average concentrates in the long-time limit on the stationary points of the dynamics, namely the vectors corresponding to the pure point spectrum.

Proposition 6 (Wiener). *Let μ be a finite complex measure on $\mathbb{R}$ and let $\widehat{\mu}(t) = \int \exp(-it\lambda) d\mu(\lambda)$. Then*

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

Note that the sum is necessarily countable.

Proof. For $T > 0$ and $t \in \mathbb{R}$, we let

$$L_T(t) = \frac{1}{T} \int_0^T e^{i\lambda t} d\lambda = \begin{cases} \frac{e^{iTt} - 1}{iTt} = e^{iTt/2} \frac{\sin(Tt/2)}{Tt/2}, & t \neq 0, \\ 1, & t = 0. \end{cases}$$

Then $|L_T(t)| \leq 1$, and

$$\lim_{T \rightarrow \infty} L_T(t) = \begin{cases} 1, & t = 0, \\ 0, & t \neq 0. \end{cases}$$

Indeed, $L_T(0) = 1$ for all T , so that the limit at $t = 0$ is 1. For $t \neq 0$, we have $|e^{iTt} - 1| \leq 2$, so $|L_T(t)| \leq \frac{2}{T|t|} \rightarrow 0$ as $T \rightarrow \infty$. By Fubini's theorem,

$$|\widehat{\mu}(t)|^2 = \widehat{\mu}(t) \overline{\widehat{\mu}(t)} = \int_{\mathbb{R}} e^{-it\lambda} d\mu(\lambda) \int_{\mathbb{R}} e^{it\xi} d\bar{\mu}(\xi) = \iint_{\mathbb{R} \times \mathbb{R}} e^{it(\xi-\lambda)} d(\mu \times \bar{\mu})(\lambda, \xi).$$

The integrand $(t, \lambda, \xi) \mapsto e^{it(\xi-\lambda)}$ is continuous and bounded by 1. Moreover, Lebesgue measure on $[0, T]$ times $|\mu| \times |\mu|$ is finite. So we may average over $t \in [0, T]$ and interchange the integrals again to obtain

$$\frac{1}{T} \int_0^T |\widehat{\mu}(t)|^2 dt = \iint_{\mathbb{R} \times \mathbb{R}} L_T(\xi - \lambda) d(\mu \times \bar{\mu})(\lambda, \xi).$$

By the initial remark, $L_T(\xi - \lambda)$ is bounded by 1 and converges pointwise to $\mathbf{1}_\Delta(\lambda, \xi)$, where $\Delta = \{(x, x) : x \in \mathbb{R}\}$ is the diagonal. The diagonal is closed, hence Borel. Since $|\mu| \times |\mu|$ is finite, dominated convergence yields

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T |\widehat{\mu}(t)|^2 dt = (\mu \times \bar{\mu})(\Delta).$$

By Fubini again,

$$(\mu \times \bar{\mu})(\Delta) = \int_{\mathbb{R}} \left(\int_{\mathbb{R}} \mathbf{1}_{\{\xi\}}(\lambda) d\mu(\lambda) \right) d\bar{\mu}(\xi) = \int_{\mathbb{R}} f(\xi) d\bar{\mu}(\xi), \quad \text{where } f(\xi) = \mu(\{\xi\}).$$

The function f vanishes off the countable set $\Lambda = \{\lambda_1, \lambda_2, \dots\}$ of atoms of μ (namely those $x \in \mathbb{R}$ such that $\mu(\{x\}) \neq 0$). In particular, f is Borel and $|f| \leq \|\mu\|$. Dominated convergence finally yields

$$\int_{\mathbb{R}} f d\bar{\mu} = \int_{\Lambda} f d\bar{\mu} = \sum_k \mu(\{\lambda_k\}) \bar{\mu}(\{\lambda_k\}) = \sum_k |\mu(\{\lambda_k\})|^2 = \sum_{\lambda \in \mathbb{R}} |\mu_{\text{pp}}(\{\lambda\})|^2,$$

concluding the proof. $\square$

Consequence. If $\psi \in \mathcal{H}_{\text{ac}} \oplus \mathcal{H}_{\text{sc}}$, then for any $\phi \in \mathcal{H}$ with $\|\phi\| = 1$,

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \underbrace{|\langle \phi, e^{-itH} \psi \rangle|^2}_{= \|P_\phi U(t) \psi\|^2} dt = 0,$$

the integrand being the probability to find $\psi(t)$ in ϕ . (Indeed $\|E^A(\chi_{\{\lambda\}})\psi\|^2 = \mu_\psi(\{\lambda\}) = 0$ for every λ , so $E^A(\chi_{\{\lambda\}})\psi = 0$ and $\mu_{\phi, \psi}$ has no pure point part either.)

3.4.2 Compact operators and local decay

An operator in $\mathcal{L}(\mathcal{H})$ is called *compact* if it is the norm limit of finite-rank operators. An operator $K : D(K) \rightarrow \mathcal{H}$ is *relatively compact* with respect to the self-adjoint H if $D(H) \subset D(K)$ and

$$K(H - z)^{-1}$$

is compact for a $z \in \rho(H)$.

Example. $H = -\Delta$ on $\mathcal{H} = L^2(\mathbb{R}^3)$, and K the multiplication by $\chi_\Omega(x)$ with Ω compact in $\mathbb{R}^3$. For this we need the following result.

Lemma 7. Let $T : L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3)$ 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.

Proof. Let $(\phi_n)_{n \in \mathbb{N}}$ be any orthonormal basis of $L^2(\mathbb{R}^3)$. Then $(\phi_i \otimes \phi_j)_{i, j \in \mathbb{N}}$ is an orthonormal basis of $L^2(\mathbb{R}^6)$ and so

$$K(x, y) = \sum_{i, j} c_{ij} \phi_i(x) \overline{\phi_j(y)}, \quad \sum_{i, j} |c_{ij}|^2 = \|K\|_{L^2(\mathbb{R}^6)}^2 < \infty.$$

It follows that

$$(T\psi)(x) = \sum_{i, j} c_{ij} \phi_i(x) \langle \phi_j, \psi \rangle,$$

and we note that T is bounded, with $\|T\|^2 \leq \|K\|^2$ (operator norm on the left, $L^2(\mathbb{R}^6)$ norm on the right).

Now $T\phi_j = \sum_i c_{ij} \phi_i$, so that $K = \sum_j \overline{\phi_j} T\phi_j$. The kernels

$$K_n(x, y) = \sum_{j=1}^n \overline{\phi_j(y)} (T\phi_j)(x)$$

define a sequence of finite-rank operators $(T_n\psi)(x) = \int K_n(x, y)\psi(y) dy$, and we claim that $T_n \rightarrow T$ in norm. Indeed, for any $\psi = \sum_j \alpha_j \phi_j$,

$$\|(T_n - T)\psi\| \leq \sum_{j>n} |\alpha_j| \|T\phi_j\| \stackrel{\text{C-S}}{\leq} \|\psi\| \left(\sum_{j>n} \|T\phi_j\|^2 \right)^{1/2} \longrightarrow 0 \quad (n \rightarrow \infty).$$

□

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

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

We conclude that

$$((-\Delta + 1)^{-1}\psi)(x) = \frac{1}{(2\pi)^{3/2}} \int e^{i\xi x} \frac{\widehat{\psi}(\xi)}{\xi^2 + 1} d\xi = \cdots = \frac{1}{4\pi} \int \frac{e^{-|x-y|}}{|x-y|} \psi(y) dy.$$

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

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

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

The next result shows that if $\psi \in \mathcal{H}_{ac}$ for $-\Delta$, then $\|\chi_\Omega e^{it\Delta}\psi\| \rightarrow 0$ as $t \rightarrow \infty$; 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.)

Theorem 8. *Let $H = H^*$ and let K be relatively compact with respect to H . Then if $\psi \in \mathcal{H}_{ac}$ for H ,*

$$\lim_{t \rightarrow \infty} \|K e^{-itH} \psi\| = 0.$$

Note. If $\psi \in \mathcal{H}_{sc}$, the same holds in an average sense.

Proof. Assume first $\psi \in D(H) \cap \mathcal{H}_{ac}$, and set $\phi = (H - z)\psi$, so that $\psi = (H - z)^{-1}\phi$; here $\phi \in \mathcal{H}_{ac}$ because $\mathcal{H}_{ac}$ is invariant under functions of H . (The general case $\psi \in \mathcal{H}_{ac}$ then follows by density, $D(H) \cap \mathcal{H}_{ac}$ being dense in $\mathcal{H}_{ac}$ and $K(H - z)^{-1}$ bounded.) Hence

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

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

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

for orthonormal families $\{\psi_1, \dots, \psi_n\}$, $\{\phi_1, \dots, \phi_n\}$. Then

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

and each term vanishes as $t \rightarrow \infty$ by (4). For K compact, let $K_n \rightarrow K$ with K_n of finite rank. Then

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

and the claim follows since the K_n are uniformly bounded. $\square$

Remark. *The decomposition into pure point and continuous spectrum therefore has a profound quantum mechanical meaning. For atomic and molecular Hamiltonians, the pure point spectrum corresponds to bound states of the electrons, while the continuous spectrum is made up of scattering states, namely states where the electrons are not bound and scatter off to infinity as $t \rightarrow \pm\infty$.*

3.5 A criterion for self-adjointness

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.

Recall that 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 such that $\psi_n \rightarrow \psi$ and $A\psi_n \rightarrow \phi$, then $\psi \in D(A)$ and $\phi = A\psi$.

Lemma 9. A^* is closed.

Proof. Let $(\psi_n) \in D(A^*)$ be such that $\psi_n \rightarrow \psi$ and $A^*\psi_n \rightarrow \phi$. 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 $\langle \phi, \xi \rangle = \langle \psi, A\xi \rangle$ for all $\xi \in D(A)$ by letting $n \rightarrow \infty$. It follows that $\psi \in D(A^*)$ and that $\phi = A^*\psi$ (by definition of A^*). $\square$

With this, we have the following criterion for self-adjointness.

Theorem 10. Let $H : D(H) \rightarrow \mathcal{H}$ be symmetric and densely defined. The following are equivalent:

- (i) H is self-adjoint;
- (ii) H is closed and $\text{Ker}(H^* \pm i) = \{0\}$;
- (iii) $R(H \pm i) = \mathcal{H}$.

We need the following.

Lemma 11. For any densely defined A :

- $\text{Ker}(A^* \pm \bar{z}) = R(A \pm z)^\perp$;
- if A is closed and symmetric, then $R(A \pm i)$ are closed.

Proof. $\psi \in R(A \pm z)^\perp \iff \langle \psi, (A \pm z)\phi \rangle = 0$ for all $\phi \in D(A) \iff \psi \in D(A^*)$ and $(A^* \pm \bar{z})\psi = 0 \iff \psi \in \text{Ker}(A^* \pm \bar{z})$.

If A is symmetric, then $\langle \psi, A\psi \rangle = \langle A\psi, \psi \rangle = \overline{\langle \psi, A\psi \rangle}$, so $\langle \psi, A\psi \rangle \in \mathbb{R}$. Therefore, for $\psi \in D(A)$,

$$\|(A \pm i)\psi\|^2 = \|A\psi\|^2 + \|\psi\|^2 \underbrace{\mp i\langle A\psi, \psi \rangle \pm i\langle \psi, A\psi \rangle}_{=0} \geq \|\psi\|^2.$$

In particular $\text{Ker}(A \pm i) = \{0\}$, and $(A \pm i)^{-1} : R(A \pm i) \rightarrow D(A)$ exists and is bounded. Let $\psi_n \in R(A + i)$ be such that $\psi_n \rightarrow \psi$, and let $\phi_n = (A + i)^{-1}\psi_n$. Then ϕ_n converges. Since A is closed, $(\phi_n, (A + i)\phi_n) \rightarrow (\psi, (A + i)\psi)$, namely $\psi \in R(A + i)$. $\square$

Proof of Theorem 10. (i) $\Rightarrow$ (ii). $H = H^*$ is closed. If $\psi_\pm \in \text{Ker}(H^* \mp i)$ with $\|\psi_\pm\| = 1$, then $H\psi_\pm = \pm i\psi_\pm$ and hence $\langle \psi_\pm, H\psi_\pm \rangle = \pm i$, which is a contradiction since this should be real. Hence $\psi_\pm = 0$.

(ii) $\Rightarrow$ (iii). By Lemma 11, $\text{Ker}(H^* \mp i) = \{0\} = \overline{R(H \pm i)}^\perp$. Hence $\overline{R(H \pm i)} = \mathcal{H}$, and by the lemma again (closed range) $R(H \pm i) = \mathcal{H}$.

(iii) $\Rightarrow$ (i). H symmetric implies $H \subset H^*$. We show $H^* \subset H$. Let $\psi \in D(H^*)$. Since $R(H \mp i) = \mathcal{H}$, there is $\phi_{\pm} \in D(H)$ such that

$$(H^* \pm i)\psi = (H \pm i)\phi_{\pm} = (H^* \pm i)\phi_{\pm}$$

(the last step since $H \subset H^*$), namely

$$\phi_{\pm} - \psi \in \text{Ker}(H^* \pm i) = R(H \mp i)^{\perp} = \{0\}.$$

Hence $\psi \in D(H)$, since $\phi_{\pm}$ does. $\square$

Let A, B be densely defined with $D(A) \subset D(B)$. B is called *relatively bounded* with respect to A if there are $a, b \geq 0$ such that

$$\|B\psi\| \leq a\|A\psi\| + b\|\psi\|, \quad \psi \in D(A).$$

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

Theorem 12 (Kato–Rellich). *Let A be self-adjoint on $D(A)$ and let B be symmetric on $D(B)$. If B is relatively bounded with A -bound < 1 , then $A + B$ is self-adjoint on $D(A + B) = D(A) \cap D(B) = D(A)$.*

Proof. On $D(A)$ the operator $A + B$ is symmetric, being the sum of a self-adjoint and a symmetric operator; we verify criterion (iii) of Theorem 10, which holds equally with $\pm i$ replaced by $\pm i\mu$ for any $\mu > 0$ (the proof is unchanged).

$A = A^*$ implies that $(A + \lambda\mathbb{1})^{-1}$ is bounded for any $\lambda \in \mathbb{C} \setminus \mathbb{R}$, with $R((A + \lambda)^{-1}) = D(A)$. Hence

$$(\mathbb{1} + B(A \pm \lambda)^{-1})(A \pm \lambda) = A + B \pm \lambda \quad \text{on } D(A). \quad (*)$$

Since $A = A^*$ gives $R(A \pm \lambda) = \mathcal{H}$, in order to prove $R(A + B \pm \lambda) = \mathcal{H}$ it suffices to show that $R(\mathbb{1} + B(A \pm \lambda)^{-1}) = \mathcal{H}$.

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

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

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

Let $\phi_{\pm} \in D(A)$ and $\psi = (A \pm \lambda)^{-1}\phi_{\pm}$. 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 $\phi_{\pm}$:

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

Hence

$$\|A(A \pm i\mu)^{-1}\phi_{\pm}\| \leq \|\phi_{\pm}\|, \quad \|(A \pm i\mu)^{-1}\phi_{\pm}\| \leq \frac{1}{\mu}\|\phi_{\pm}\|.$$

We can now use the A -bound to get

$$\|B(A \pm i\mu)^{-1}\phi_{\pm}\| \leq a\|A(A \pm i\mu)^{-1}\phi_{\pm}\| + b\|(A \pm i\mu)^{-1}\phi_{\pm}\| \leq \left(a + \frac{b}{\mu}\right)\|\phi_{\pm}\|,$$

which is < 1 for μ large enough. $\square$

3.6 The Fourier transform and $H^2(\mathbb{R}^3)$

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

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

is well defined on $L^1(\mathbb{R}^3)$, with $\|\widehat{f}\|_\infty \leq (2\pi)^{-3/2} \|f\|_1$. Note that it is not a priori well defined on L^2 , but:

Theorem 13 (Plancherel). *(i) If $f \in L^1 \cap L^2$, then $\widehat{f} \in L^2$, with $\|\widehat{f}\|_2 = \|f\|_2$.*

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

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

Proof. $\widehat{f} \in L^\infty$ implies that for all $\varepsilon > 0$, $\int |\widehat{f}(\xi)|^2 e^{-\varepsilon \xi^2} \, d\xi < \infty$, and

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

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

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

Hence the above equals $\langle f, f * j_\varepsilon \rangle_{L^2(\mathbb{R}^3, dx)}$. Now $f * j_\varepsilon \rightarrow f$ in L^2 , so that $\langle f, f * j_\varepsilon \rangle \rightarrow \|f\|_2^2$. In particular $\widehat{f}(\xi) e^{-\varepsilon \xi^2/2}$ is convergent in $L^2(\mathbb{R}^3, d\xi)$; since $\widehat{f}(\xi) \exp(-\varepsilon \xi^2/2) \rightarrow \widehat{f}(\xi)$ pointwise, we conclude that

$$\lim_{\varepsilon \rightarrow 0} \int |\widehat{f}(\xi)|^2 e^{-\varepsilon \xi^2} \, d\xi = \int |\widehat{f}(\xi)|^2 \, d\xi = \|\widehat{f}\|_2^2.$$

(ii) and (iii) follow immediately. □

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

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

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

$$\check{f}(x) = \widehat{f}(-x) = \frac{1}{(2\pi)^{3/2}} \lim_{n \rightarrow \infty} \int f(\xi) e^{i\xi x - \xi^2/n} \, d\xi.$$

Definition.

$$H^2(\mathbb{R}^3) := \{ f \in L^2(\mathbb{R}^3) : |\xi|^2 \widehat{f}(\xi) \in L^2(\mathbb{R}^3) \}.$$

It is a Hilbert space with inner product

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

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

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

3.6.1 The free quantum particle

The free Hamiltonian H_0 on $L^2(\mathbb{R}^3)$:

- (i) multiplication on $L^2(\mathbb{R}^3, d\xi)$, $\widehat{\psi}(\xi) \mapsto |\xi|^2 \widehat{\psi}(\xi)$, with domain $\{\widehat{\psi} \in L^2 : \xi^2 \widehat{\psi}(\xi) \in L^2\}$, is self-adjoint;
- (ii) it is unitarily equivalent to H_0 on $L^2(\mathbb{R}^3, dx)$, with $D(H_0) = H^2(\mathbb{R}^3)$ and

$$H_0 \psi = -\Delta \psi = (\xi^2 \widehat{\psi}(\xi))^\vee.$$

Lemma 14. *For any $a > 0$ there is $b > 0$ such that, for all $\psi \in H^2$,*

$$\|\psi\|_\infty \leq a \|\Delta \psi\|_2 + b \|\psi\|_2.$$

Hence functions in the domain of H_0 are bounded.

Proof. First of all,

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

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

$$\|\widehat{\psi}\|_1 \leq C(\|\xi^2 \widehat{\psi}\|_2 + \|\widehat{\psi}\|_2) = C(\|-\Delta \psi\|_2 + \|\psi\|_2). \quad (5)$$

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

$$\|\widehat{\psi}_\lambda\|_1 = \|\widehat{\psi}\|_1, \quad \|\widehat{\psi}_\lambda\|_2 = \lambda^{3/2} \|\widehat{\psi}\|_2, \quad \|\xi^2 \widehat{\psi}_\lambda\|_2 = \lambda^{-1/2} \|\xi^2 \widehat{\psi}\|_2.$$

Hence (5) expressed for ψ_λ yields

$$\|\widehat{\psi}\|_1 \leq C \lambda^{3/2} \|\widehat{\psi}\|_2 + C \lambda^{-1/2} \|\xi^2 \widehat{\psi}\|_2,$$

and the claim follows from $\|\psi\|_\infty \leq (2\pi)^{-3/2} \|\widehat{\psi}\|_1$, choosing λ large enough. $\square$

3.6.2 Atomic and molecular Hamiltonians

Theorem 15. *Let $V = V_1 + V_2$ with $V_1 \in L^2(\mathbb{R}^3)$ and $V_2 \in L^\infty(\mathbb{R}^3)$. Then $H = -\Delta + V$ is self-adjoint on $D(H) = H^2(\mathbb{R}^3)$.*

Proof. V is real valued, hence self-adjoint on $D(V) = \{\psi \in L^2(\mathbb{R}^3) : V\psi \in L^2(\mathbb{R}^3)\}$. Moreover, if $\psi \in D(H_0)$, then $\psi \in L^2(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, so that

$$\|V\psi\|_2 \leq \|V_1\psi\|_2 + \|V_2\psi\|_2 \leq \|V_1\|_2 \|\psi\|_\infty + \|V_2\|_\infty \|\psi\|_2,$$

and so $D(H_0) \subset D(V)$. Furthermore, by Lemma 14,

$$\|V\psi\|_2 \leq a \|V_1\|_2 \|\Delta \psi\|_2 + (b \|V_1\|_2 + \|V_2\|_\infty) \|\psi\|_2$$

for any $a > 0$. Hence V is H_0 -bounded with H_0 -bound 0, and the theorem follows from Kato–Rellich. $\square$

Remark. 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 16.

$$H_N = -\sum_{i=1}^N \Delta_{x_i} - \sum_{i=1}^N \sum_{j=1}^M \frac{\alpha z_j}{|x_i - R_j|} + \sum_{1 \leq i < k \leq N} \frac{\alpha}{|x_i - x_k|}$$

is self-adjoint on $H^2(\mathbb{R}^{3N})$.

Remarks. (i) The corollary does not follow from the theorem applied verbatim in $\mathbb{R}^{3N}$: the proof of Lemma 14 uses $\|(1 + \xi^2)^{-1}\|_{L^2(\mathbb{R}^d)} < \infty$, and $\int (1 + r^2)^{-2} r^{d-1} dr$ converges only for $d < 4$, so the argument breaks already for $N = 2$. One argues instead one interaction term at a time: each summand of V depends on only three of the $3N$ coordinates, so Lemma 14 applies in those three variables with the remaining ones as parameters.

(ii) This proves that atoms and molecules have a well-defined global dynamics.

(iii) Since $-\Delta \geq 0$, Kato–Rellich yields a lower bound on the atomic/molecular Hamiltonian, and therefore *stability of the first kind*. Note that the lower bound obtained this way will depend on N (and M).