

Mathematical Methods of Quantum Mechanics

Niels Benedikter

Dipartimento di Matematica, Università degli Studi di Milano

Anno accademico 2026/2027

Contents

0	Basic functional analysis [Teschl, Sections 0.2–0.6]	2
1	Spectrum and resolvent [Teschl, Section 2.4]	4
2	Symmetric and self-adjoint operators [Teschl, Section 2.2]	7
3	Self-adjoint Extensions [Teschl, Section 2.6]	13
4	Schrödinger Operators [Teschl, Section 7.1 and 7.2]	14
5	Existence of Solutions to the Schrödinger equation. Strongly Continuous Unitary Groups [Teschl, Section 5.1]	19
6	Scattering Theory [Teschl, Chapter 12 & Reed–Simon Vol. 3]	26

Quantum mechanics [Teschl, Section 2.1]

A quantum theory consists of a complex Hilbert space $(\mathcal{H}, \langle \cdot, \cdot \rangle)$ and self-adjoint operators $A_1, A_2, \dots, H$.

- Vectors $\psi \in \mathcal{H}$ describe states of the system.
- $A_1, A_2, \dots$ correspond to observables, e.g., position and momentum.
- H corresponds to the observable “total energy”.
- States evolve according to the Schrödinger initial-value problem

$$i \frac{d}{dt} \psi(t) = H \psi(t), \quad \psi(0) = \psi_0 \in \mathcal{H}.$$

- In experiments we obtain averages $\langle \psi, A_i \psi \rangle \in \mathbb{R}$.

Example. $\mathcal{H} = L^2(\mathbb{R}^3)$, $H = -\Delta$ (kinetic energy), or $H = -\Delta + V$ (Schrödinger operator). The observables include $p = -i\nabla$ (momentum), x (position), and angular momentum. Interpretation of the wave function $\psi \in L^2(\mathbb{R}^3)$: Given a measurable set $\Omega \subset \mathbb{R}^3$,

$$\int_{\Omega} |\psi(x)|^2 dx = \text{probability of finding a particle in } \Omega.$$

States are therefore typically normalized: $\|\psi\|_2^2 = \int_{\mathbb{R}^3} |\psi(x)|^2 dx = 1$.

0 Basic functional analysis [Teschl, Sections 0.2–0.6]

Definition. A *Banach space* is a complex vector space with norm $\|\cdot\|$ that is complete: every Cauchy sequence converges. A sequence (x_n) is Cauchy if

$$\forall \varepsilon > 0 \exists N \in \mathbb{N} \forall k, \ell \geq N : \|x_k - x_\ell\| < \varepsilon.$$

Example (L^p spaces). For $1 \leq p < \infty$,

$$L^p(\mathbb{R}^d) := \{[f] : f : \mathbb{R}^d \rightarrow \mathbb{C} \text{ measurable and } \int |f|^p dx < \infty\}, \quad \|[f]\|_p := \left(\int |f|^p dx \right)^{1/p}.$$

Here $[f]$ denotes the equivalence class of functions equal to f almost everywhere (outside a set of measure zero). Also,

$$L^\infty(\mathbb{R}^d) := \{[f] : f : \mathbb{R}^d \rightarrow \mathbb{C} \text{ measurable and } \operatorname{ess\,sup}_{x \in \mathbb{R}^d} |f(x)| < \infty\},$$

$$\|[f]\|_\infty = \inf_{g \in [f]} \sup_{x \in \mathbb{R}^d} |g(x)|.$$

These are Banach spaces. In the following we write f rather than $[f]$.

Definition. Let X, Y be normed vector spaces. An *operator* is a linear map $A : X \rightarrow Y$:

$$A(x + x') = Ax + Ax', \quad A(\lambda x) = \lambda Ax \quad \forall x, x' \in X, \lambda \in \mathbb{C}.$$

It is *bounded* if its *operator norm*

$$\|A\| := \sup_{x \in X, \|x\|=1} \|Ax\|$$

is finite.

Lemma 0.1. *An operator is continuous if and only if it is bounded.*

Proof. If A is continuous, it is continuous at zero. Thus there is $\delta > 0$ such that $\|x\| < \delta$ implies $\|Ax\| < 1$. For $x \neq 0$,

$$\|Ax\| = \left\| A \left(\frac{x}{\|x\|} \frac{\delta}{2} \right) \right\| \cdot \frac{2}{\delta} \|x\| \leq \frac{2}{\delta} \|x\|.$$

Thus A is bounded. Conversely, if $C = \sup_{\|x\|=1} \|Ax\| < \infty$, then for $x \neq y$,

$$\|A(x - y)\| = \left\| A \frac{x - y}{\|x - y\|} \|x - y\| \right\| \leq C \|x - y\|.$$

Hence A is continuous (in fact even Lipschitz continuous). $\square$

Definition. $\mathcal{L}(X, Y)$ is the space of bounded operators $X \rightarrow Y$; $\mathcal{L}(X) := \mathcal{L}(X, X)$; and $X^* := \mathcal{L}(X, \mathbb{C})$ is the *dual space* of X .

Remark. • $\mathcal{L}(X, Y)$ is a vector space with $(A + B)x = Ax + Bx$ and $(\lambda A)x = \lambda(Ax)$.

- If Y is a Banach space, then $\mathcal{L}(X, Y)$ with the operator norm is a Banach space.
- We have $\|Ax\| \leq \|A\| \|x\|$. Therefore, if $A \in \mathcal{L}(X, Y)$ and $B \in \mathcal{L}(Y, Z)$, then $\|BA\| \leq \|B\| \|A\|$.

Definition. A *Hilbert space* is a complex vector space $\mathcal{H}$ with an inner product $\langle \cdot, \cdot \rangle : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{C}$ satisfying

$$\begin{aligned} \langle x, y + z \rangle &= \langle x, y \rangle + \langle x, z \rangle, & \langle x, \lambda y \rangle &= \lambda \langle x, y \rangle, \\ \langle x, y \rangle &= \overline{\langle y, x \rangle}, & \langle x, x \rangle &> 0 \quad \forall x \neq 0, \end{aligned}$$

which is complete for the induced norm $\|x\| := \sqrt{\langle x, x \rangle}$.

We use the physicists' convention: the inner product is antilinear in the first variable and linear in the second. Mathematicians often use the opposite convention.

Lemma 0.2 (Cauchy–Schwarz inequality). *We have $|\langle x, y \rangle| \leq \|x\| \|y\|$ for all $x, y \in \mathcal{H}$.*

Example. $L^2(\mathbb{R}^d)$ with $\langle f, g \rangle = \int \overline{f(x)} g(x) dx$ is a Hilbert space.

Theorem 0.3 (Fréchet–Riesz). *For every $f \in \mathcal{H}^*$ there is a unique $x \in \mathcal{H}$ such that $f(y) = \langle x, y \rangle$ for all $y \in \mathcal{H}$. In Dirac bra-ket notation, $f = \langle x, \cdot \rangle = \langle x|$.*

Theorem 0.4 (Bounded inverse theorem). *If X, Y are Banach spaces and $A : X \rightarrow Y$ is bounded and bijective, then $A^{-1} : Y \rightarrow X$ is bounded.*

Definition. For vector spaces X, Y , the cartesian product $X \times Y$ equipped with the vector space operations

$$(x_1, y_1) + (x_2, y_2) := (x_1 + x_2, y_1 + y_2), \quad \lambda(x, y) := (\lambda x, \lambda y)$$

is called the *direct sum* $X \oplus Y$. If X, Y are normed, set $\|(x, y)\|^2 = \|x\|^2 + \|y\|^2$. The *graph* of a linear map $A : X \rightarrow Y$ is

$$\Gamma_A = \{(x, y) \in X \oplus Y : y = Ax\}.$$

The operator is called *closed* if its graph is closed, i. e., every convergent sequence in Γ_A has its limit in Γ_A .

Theorem 0.5 (Closed graph theorem). *Let X, Y be Banach spaces and $A : X \rightarrow Y$ linear (defined on all of X !). Then A is bounded if and only if A is closed.*

Proof. If A is continuous and $(x_n, y_n) \in \Gamma_A$ converges to $(x, y) \in X \oplus Y$, then $y = \lim y_n = \lim Ax_n = Ax$. Thus $(x, y) \in \Gamma_A$. So Γ_A is closed.

Conversely, if Γ_A is closed, it is itself a Banach space. The map

$$P : \Gamma_A \rightarrow X, \quad (x, y) \mapsto x$$

is linear, bijective and continuous. By the bounded inverse theorem, $P^{-1} : X \rightarrow \Gamma_A$ is bounded. Hence

$$\|Ax\| \leq \sqrt{\|x\|^2 + \|Ax\|^2} = \|(x, Ax)\| = \|P^{-1}x\| \leq \|P^{-1}\|\|x\|.$$

So A is continuous. □

In physics we encounter unbounded but closed operators. This is possible because they are not defined on all of X , but only on a dense subspace. A bounded operator defined on a dense subspace can always be extended by continuity to the whole space.

1 Spectrum and resolvent [Teschl, Section 2.4]

Definition. Let X be a Banach space and $D \subset X$ a linear subspace. A *linear operator in X with domain D* is a linear map $A : D \rightarrow X$:

$$A(\lambda_1 x_1 + \lambda_2 x_2) = \lambda_1 Ax_1 + \lambda_2 Ax_2.$$

Its range is $\text{ran } A := \{Ax : x \in D\}$. It is *densely defined* if $\overline{D} = X$, and *closed* if $\Gamma_A = \{(x, Ax) : x \in D\}$ is closed in $X \oplus X$. An operator B is an *extension* of A , written $A \subset B$, if $D(A) \subset D(B)$ and $Ax = Bx$ for every $x \in D(A)$.

Remark. An operator consists of both a mapping prescription and a domain! $A = B$ means equality of domains and actions.

Adding unbounded operators requires care with their domains: the intersection of the domains may be only $\{0\}$.

We often write $A - \lambda$ for $A - \lambda \mathbf{1}$. Since $\mathbf{1}$ is defined everywhere, $A - \lambda$ is naturally defined on $D(A)$.

End of Lecture 1

Definition. The *resolvent set*, *resolvent*, *spectrum* and *point spectrum* are

$$\begin{aligned} \rho(A) &:= \{\lambda \in \mathbb{C} : A - \lambda : D(A) \rightarrow X \text{ is bijective and } (A - \lambda)^{-1} \text{ is bounded}\}, \\ R_\lambda(A) &:= (A - \lambda)^{-1}, \quad \lambda \in \rho(A), \\ \sigma(A) &:= \text{spec}(A) = \mathbb{C} \setminus \rho(A), \\ \sigma_p(A) &:= \{\lambda \in \mathbb{C} : \lambda \text{ is an eigenvalue of } A\}. \end{aligned}$$

Reminder: boundedness of the inverse means $\|(A - \lambda)^{-1}\| = \sup_{\|x\|=1} \|(A - \lambda)^{-1}x\| < \infty$.

Remark. $\sigma_p(A) \subset \sigma(A)$, but in general they are not equal.

Example. 1. If $X = \mathbb{C}^n$ and $A \in \mathcal{L}(X)$, then $\sigma(A) = \sigma_p(A)$ is the set of eigenvalues of the matrix A .

2. On $X = L^2(\mathbb{R})$, let $D := \{f \in L^2(\mathbb{R}) : \int |xf(x)|^2 dx < \infty\}$ and $(Af)(x) := xf(x)$ (position operator). Then $\sigma(A) = \mathbb{R}$, $\sigma_p(A) = \emptyset$, and $\rho(A) = \mathbb{C} \setminus \mathbb{R}$.
3. Let $X = C([0, 1])$ with $\|f\| := \sup_{x \in [0, 1]} |f(x)|$ and $A_k : D_k \subset X \rightarrow X$, $(A_k f)(x) := f'(x)$, $k = 1, 2, 3, 4$, where

$$\begin{aligned} D_1 &:= C^1([0, 1]), \\ D_2 &:= \{f \in D_1 : f(0) = 0\}, \\ D_3 &:= \{f \in D_1 : f(0) = f(1)\} && \text{(periodic boundary conditions),} \\ D_4 &:= \{f \in D_1 : f(0) = 0 = f(1)\} && \text{(Dirichlet boundary conditions).} \end{aligned}$$

All A_k are closed, and

	$\sigma(A_k)$	$\sigma_p(A_k)$
A_1	$\mathbb{C}$	$\mathbb{C}$
A_2	$\emptyset$	$\emptyset$
A_3	$2\pi i\mathbb{Z}$	$2\pi i\mathbb{Z}$
A_4	$\mathbb{C}$	$\emptyset$

Proof. For closedness, consider a sequence $\varphi_n \in D_1$, $\varphi_n \rightarrow \varphi$ and $A_1 \varphi_n = \varphi'_n \rightarrow \psi$ in X . According to the chosen norm on X , both convergences are uniform convergence. Therefore $\varphi \in C^1([0, 1])$ and $\varphi' = \psi$. Thus A_1 is closed. If $\varphi_n \in D_k$, $k = 2, 3, 4$, then the same argument applies, and additionally the limit satisfies the same boundary conditions, so these operators are also closed.

To show $\sigma(A_1) = \sigma_p(A_1) = \mathbb{C}$: For every $\lambda \in \mathbb{C}$, the function $x \mapsto e^{\lambda x}$ belongs to D_1 and is an eigenfunction of A_1 with eigenvalue λ .

To show $\sigma(A_2) = \emptyset$, we construct its resolvent explicitly. Solving $(A_2 - \lambda)f = g$ for f means finding $f \in C^1([0, 1])$ with $f(0) = 0$ and $f' - \lambda f = g$. The unique solution of this ordinary differential equation is

$$f(x) = \int_0^x e^{\lambda(x-t)} g(t) dt =: (Sg)(x).$$

The operator S is bounded, $SX \subset D_2$, and $(A_2 - \lambda)Sg = g$. To complete the proof that $S = (A_2 - \lambda)^{-1}$, it remains to show $S(A_2 - \lambda)g = g$. In fact, for $g \in D_2$,

$$S(A_2 - \lambda)g(x) = \int_0^x e^{\lambda(x-t)} (g'(t) - \lambda g(t)) dt = g(x).$$

Thus $S = R_\lambda(A_2)$. The spectra of A_3, A_4 are left as an exercise. □

Proposition 1.1. *Let $A : D \subset X \rightarrow X$ be a linear operator and $\lambda, \mu \in \rho(A)$. Then*

- (i) $R_\lambda(A) - R_\mu(A) = (\lambda - \mu)R_\lambda(A)R_\mu(A)$;
- (ii) $R_\lambda(A)R_\mu(A) = R_\mu(A)R_\lambda(A)$;
- (iii) $R_\lambda(A)A \subset AR_\lambda(A)$;
- (iv) $AR_\lambda(A) = \mathbf{1} + \lambda R_\lambda(A)$.

Proof. For (i),

$$\begin{aligned} (A - \lambda)^{-1} - (A - \mu)^{-1} &= (A - \lambda)^{-1}[(A - \mu) - (A - \lambda)](A - \mu)^{-1} \\ &= (\lambda - \mu)(A - \lambda)^{-1}(A - \mu)^{-1}. \end{aligned}$$

Part (ii) follows by applying (i) twice. For (iii) and (iv): if $x \in D$, then

$$R_\lambda(A)Ax = R_\lambda(A)(A - \lambda)x + \lambda R_\lambda(A)x = x + \lambda R_\lambda(A)x.$$

For every $x \in X$,

$$AR_\lambda(A)x = (A - \lambda)R_\lambda(A)x + \lambda R_\lambda(A)x = x + \lambda R_\lambda(A)x.$$

□

Definition. Let $U \subset \mathbb{C}$ be open. A function $L : U \rightarrow \mathcal{L}(X)$, $z \mapsto L(z)$, is called *analytic* if $z \mapsto f(L(z)x)$ is analytic for every $x \in X$ and $f \in X^*$.

Recall that a complex-valued function is analytic if every point has a neighbourhood where f is equal to its Taylor series in that point. Equivalently a complex-valued function is analytic if it is complex differentiable (holomorphic).

The following lemma is fundamental for what comes next. For now, it is our main method for constructing inverse operators and hence resolvents.

Lemma 1.2 (Neumann series, simplified). *Let X be Banach and $T \in \mathcal{L}(X)$ with $\|T\| < 1$. Then $\mathbf{1} - T$ is bijective, the inverse is also bounded, and*

$$(\mathbf{1} - T)^{-1} = \sum_{n=0}^{\infty} T^n.$$

Note that this is just the geometric series generalized to operators. In fact, the proof is the same as for the geometric series in complex numbers.

Proof. Set $S_k := \sum_{n=0}^k T^n$. For $\ell > k$,

$$\|S_\ell - S_k\| = \left\| \sum_{n=k+1}^{\ell} T^n \right\| \leq \sum_{n=k+1}^{\ell} \|T\|^n \leq \sum_{n=k+1}^{\infty} \|T\|^n \rightarrow 0.$$

Thus (S_k) is Cauchy in the Banach space $\mathcal{L}(X)$, and therefore converges to some S . We still have to prove that S is actually the inverse:

$$(\mathbf{1} - T)S_k = \sum_{n=0}^k T^n - \sum_{n=0}^k T^{n+1} = \mathbf{1} - T^{k+1} \rightarrow \mathbf{1},$$

since $\|T^{k+1}\| \leq \|T\|^{k+1} \rightarrow 0$. Since T is bounded, it is also continuous, so $(\mathbf{1} - T)S = \lim_{k \rightarrow \infty} (\mathbf{1} - T)S_k = \mathbf{1}$. By the same method we can show that $S(\mathbf{1} - T) = \mathbf{1}$. □

Theorem 1.3. *Let $A : D \subset X \rightarrow X$ be a linear operator. Then:*

(i) $\rho(A)$ is open, $\sigma(A)$ is closed, and $z \mapsto R_z(A)$ is analytic on $\rho(A)$. For $z_0 \in \rho(A)$,

$$B_{\|R_{z_0}(A)\|^{-1}}(z_0) \subset \rho(A).$$

Moreover, for all z in this ball we have

$$R_z(A) = \sum_{n=0}^{\infty} R_{z_0}(A)^{n+1} (z - z_0)^n.$$

(Here $B_r(z_0)$ denotes the open ball of radius r about z_0 .)

(ii) For all $z_0 \in \rho(A)$ we have $\|R_{z_0}(A)\| \geq \frac{1}{\text{dist}(z_0, \sigma(A))}$.

Proof. For $z_0 \in \rho(A)$ and $z \in \mathbb{C}$,

$$A - z = A - z_0 - (z - z_0) = [\mathbf{1} - (z - z_0)R_{z_0}(A)](A - z_0).$$

The second factor has a bounded inverse. If $|z - z_0|\|R_{z_0}(A)\| < 1$, the Neumann series inverts the first factor:

$$[\mathbf{1} - (z - z_0)R_{z_0}(A)]^{-1} = \sum_{n=0}^{\infty} R_{z_0}(A)^n (z - z_0)^n.$$

Consequently $z \in \rho(A)$ and the asserted expansion follows. In particular, the resolvent is analytic. This proves (i).

If $z \in \sigma(A)$, the same argument shows that $|z - z_0|\|R_{z_0}(A)\| \geq 1$ (otherwise we'd have a contradiction). Taking the infimum over $z \in \sigma(A)$ proves (ii), where we use the convention $\text{dist}(z_0, \emptyset) = \infty$. $\square$

Theorem 1.4 (Liouville). *If a function is analytic on all of $\mathbb{C}$ and bounded, then it is constant.*

Proof reference. For complex-valued functions, see for example Rudin, *Real and Complex Analysis*. For operator-valued functions, use the result for complex-valued functions and the definition of analyticity above. $\square$

Corollary 1.5. *If $A \in \mathcal{L}(X)$ and $X \neq \{0\}$, then*

$$\sigma(A) \subset \{z \in \mathbb{C} : |z| \leq \|A\|\}, \quad \sigma(A) \neq \emptyset.$$

End of Lecture 2

Proof. For $|z| > \|A\|$, write $z - A = z(\mathbf{1} - z^{-1}A)$. Both factors have bounded inverses, the second by the Neumann series. Thus $z \in \rho(A)$, and

$$(z - A)^{-1} = \sum_{n=0}^{\infty} (z^{-1}A)^n z^{-1} = -R_z(A).$$

Suppose now that $\sigma(A) = \emptyset$. The map $z \mapsto (z - A)^{-1}$ is analytic on all of $\mathbb{C}$, and

$$\|(z - A)^{-1}\| \leq \frac{1}{|z|} \sum_{n=0}^{\infty} \|z^{-1}A\|^n = \frac{1}{|z| - \|A\|} \rightarrow 0 \quad (|z| \rightarrow \infty).$$

Being continuous and converging to zero at infinity, the function is bounded. So Liouville implies that it is constant. The only constant value compatible with convergence to zero at infinity is zero. This contradicts $(A - z)R_z(A) = \mathbf{1}$. $\square$

2 Symmetric and self-adjoint operators [Teschl, Section 2.2]

Throughout the chapter, $\mathcal{H}$ is a Hilbert space.

Definition. Let $A : D(A) \subset \mathcal{H} \rightarrow \mathcal{H}$ be linear and densely defined. Its *adjoint* operator $A^* : D(A^*) \subset \mathcal{H} \rightarrow \mathcal{H}$ is defined as follows: $\varphi \in D(A^*)$ if there exists $\varphi^* \in \mathcal{H}$ such that

$$\langle \varphi, A\psi \rangle = \langle \varphi^*, \psi \rangle \quad \text{for all } \psi \in D(A).$$

Set $A^*\varphi := \varphi^*$.

Check that φ^* is unique and that $\varphi \mapsto \varphi^*$ is linear.

Remark. • $A \subset B$ implies $A^* \supset B^*$.

- It can happen that $D(A^*) = \{0\}$.

From now on, $A : D \subset \mathcal{H} \rightarrow \mathcal{H}$ always means a linear densely defined operator, unless explicitly stated otherwise.

Proposition 2.1. *The adjoint A^* is always closed.*

Proof. Consider a convergent sequence in Γ_{A^*} , that is, let $\varphi_n \in D(A^*)$, $\varphi_n \rightarrow \varphi$, and $A^*\varphi_n \rightarrow \psi \in \mathcal{H}$. We have to show that the limit point (φ, ψ) is in Γ_{A^*} , i. e., that $\psi = A^*\varphi$.

For every $\eta \in D(A)$, continuity of the inner product gives

$$\langle \varphi, A\eta \rangle = \lim_{n \rightarrow \infty} \langle \varphi_n, A\eta \rangle = \lim_{n \rightarrow \infty} \langle A^*\varphi_n, \eta \rangle = \langle \psi, \eta \rangle.$$

Thus $\varphi \in D(A^*)$ and $A^*\varphi = \psi$, proving closedness. $\square$

Definition. Vectors $x, y \in \mathcal{H}$ are *orthogonal*, written $x \perp y$, if $\langle x, y \rangle = 0$. For $M \subset \mathcal{H}$, its *orthogonal complement* is $M^\perp = \{x \in \mathcal{H} : x \perp y \text{ for all } y \in M\}$.

Remark. $M^\perp$ is a closed subspace; $M \subset (M^\perp)^\perp$; if M is a subspace, $(M^\perp)^\perp = \overline{M}$; and $(\overline{M})^\perp = M^\perp$.

Definition. The *kernel* of A is $\ker A := \{\varphi \in D(A) : A\varphi = 0\}$.

Proposition 2.2. *For densely defined A , $\ker A^* = (\text{ran } A)^\perp$. In particular, $(\text{ran } A)^\perp \subset D(A^*)$. Moreover, $\ker A^* = \{0\}$ implies $\overline{\text{ran } A} = \mathcal{H}$.*

Proof. $\ker A^* = (\text{ran } A)^\perp$: By density of $D(A)$,

$$\begin{aligned} \varphi \in \ker A^* &\iff \langle A^*\varphi, \psi \rangle = 0 \ (\forall \psi \in D(A)) \\ &\iff \langle \varphi, A\psi \rangle = 0 \ (\forall \psi \in D(A)) \iff \varphi \in (\text{ran } A)^\perp. \end{aligned}$$

Reading this in the reverse direction, $\varphi \in (\text{ran } A)^\perp$ implies $\varphi \in D(A^*)$, with $A^*\varphi = 0$. $(\text{ran } A)^\perp \subset D(A^*)$: Follows from the first part and $\ker A^* \subset D(A^*)$.

$\ker A^* = \{0\}$ implies $\overline{\text{ran } A} = \mathcal{H}$:

$$\mathcal{H} = \{0\}^\perp = (\ker A^*)^\perp = ((\text{ran } A)^\perp)^\perp = \overline{\text{ran } A}.$$

This concludes the proof. $\square$

Definition. A densely defined operator A is called *symmetric* if $A \subset A^*$, or equivalently if $\langle A\varphi, \psi \rangle = \langle \varphi, A\psi \rangle$ for all $\varphi, \psi \in D(A)$.

It is called *self-adjoint* if $A = A^*$, i. e., it is symmetric and $D(A) = D(A^*)$.

Remark. For bounded operators, symmetric, self-adjoint and Hermitian mean the same thing.

Theorem 2.3 (Hellinger–Toeplitz). *Let $A : \mathcal{H} \rightarrow \mathcal{H}$ be linear and symmetric, defined on all of $\mathcal{H}$. Then A is bounded.*

Proof. We show that Γ_A is closed, then boundedness follows from the closed graph theorem.

Let $x_n \rightarrow x$ and $Ax_n \rightarrow y$ for some $y \in \mathcal{H}$. For all $z \in \mathcal{H}$, we have

$$\langle z, y \rangle = \lim_{n \rightarrow \infty} \langle z, Ax_n \rangle = \lim_{n \rightarrow \infty} \langle Az, x_n \rangle = \langle Az, x \rangle = \langle z, Ax \rangle.$$

Thus $y = Ax$ and therefore the tuple (x, y) is in Γ_A . $\square$

In quantum mechanics we typically encounter symmetric unbounded operators, e.g., the position operator. Hellinger–Toeplitz shows that we inevitably have to study operators defined only on a dense subspace.

Definition. $C^\infty(\mathbb{R}^n)$ denotes the complex-valued arbitrarily many times differentiable (smooth) functions. For a multi-index $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}^n$, set

$$\partial^\alpha f := \frac{\partial^{|\alpha|} f}{\partial x_1^{\alpha_1} \cdots \partial x_n^{\alpha_n}}, \quad x^\alpha := x_1^{\alpha_1} \cdots x_n^{\alpha_n}, \quad |\alpha| := \alpha_1 + \cdots + \alpha_n.$$

The *Schwartz space* is

$$\mathcal{S}(\mathbb{R}^n) := \{f \in C^\infty(\mathbb{R}^n) : \sup_x |x^\alpha \partial^\beta f(x)| < \infty \text{ for all } \alpha, \beta \in \mathbb{N}^n\}.$$

Remark. Without proof we state the following facts:

1. $\mathcal{S}(\mathbb{R}^n)$ is dense in $L^2(\mathbb{R}^n)$, because $C_0^\infty(\mathbb{R}^n) \subset \mathcal{S}(\mathbb{R}^n)$ and $C_0^\infty(\mathbb{R}^n)$ is dense in $L^2(\mathbb{R}^n)$. Here C_0^∞ , also denoted C_c^∞ , consists of smooth functions with compact support.
2. The Fourier transform $\mathcal{F} : \mathcal{S}(\mathbb{R}^n) \rightarrow \mathcal{S}(\mathbb{R}^n)$ is bijective.

Example (Momentum operator). Let $\mathcal{H} = L^2(\mathbb{R})$, $D(A) = \mathcal{S}(\mathbb{R})$ and $Af = -if'$. Then A is symmetric, but not self-adjoint.

Proof of symmetry. For $f, g \in \mathcal{S}(\mathbb{R})$, integration by parts gives

$$\langle f, Ag \rangle = -i \int \overline{f(x)} g'(x) dx = \int \overline{-if'(x)} g(x) dx = \langle Af, g \rangle.$$

There are no boundary terms because Schwartz functions and their derivatives tend to zero as $x \rightarrow \pm\infty$. Thus $A \subset A^*$. $\square$

Proposition 2.4 (Generalized bounded inverse theorem). *Let X, Y be Banach spaces and $A : D \subset X \rightarrow Y$ linear, bijective and closed. Then $A^{-1} : Y \rightarrow X$ is bounded.*

This proposition is useful because almost all operators we encounter are closed. Recall that the definition of the resolvent set requires us to check that the resolvent is bounded. According to the present theorem, the boundedness comes for free and does not have to be checked for closed operators. The most common operators in quantum mechanics are self-adjoint, therefore we know that they are closed.

Proof of Proposition 2.4. Since $AD = Y$,

$$\begin{aligned} \Gamma_{A^{-1}} &= \{(y, A^{-1}y) : y \in Y\} \\ &= \{(Ax, A^{-1}Ax) : x \in D\} = \{(Ax, x) : x \in D\} = I\Gamma_A, \end{aligned}$$

where $I : X \oplus Y \rightarrow Y \oplus X$, $I(x, y) = (y, x)$, is a bijective isometry (that means, leaves the norm invariant). Thus $\Gamma_{A^{-1}}$ is closed if and only if Γ_A is closed. But Γ_A is closed by assumption. Now apply the closed graph theorem to A^{-1} . $\square$

Lemma 2.5. *Let A be symmetric and $\lambda, \mu \in \mathbb{R}$. For every $\varphi \in D(A)$,*

$$\|(A - \lambda - i\mu)\varphi\|^2 = \|(A - \lambda)\varphi\|^2 + \mu^2\|\varphi\|^2.$$

Proof. Expanding the squared norm and recalling that the inner product is antilinear in the first argument but linear in the second gives

$$\begin{aligned}\|(A - \lambda - i\mu)\varphi\|^2 &= \langle (A - \lambda)\varphi, (A - \lambda)\varphi \rangle \\ &\quad - i\mu \langle (A - \lambda)\varphi, \varphi \rangle + i\mu \langle \varphi, (A - \lambda)\varphi \rangle + \mu^2 \|\varphi\|^2.\end{aligned}$$

The mixed terms cancel by symmetry of the operator A . $\square$

End of Lecture 3

Set $\mathbb{C}_+ := \{z \in \mathbb{C} : \operatorname{Im} z > 0\}$ and $\mathbb{C}_- := \{z \in \mathbb{C} : \operatorname{Im} z < 0\}$.

Proposition 2.6. *Let A be symmetric. If there exists $z \in \mathbb{C}_+$ such that $\operatorname{ran}(A - z) = \mathcal{H}$, then $\mathbb{C}_+ \subset \rho(A)$. The analogous assertion holds for $\mathbb{C}_-$.*

Proof. Let $z \in \mathbb{C}_+$ with

$$\operatorname{ran}(A - z) = \mathcal{H}. \quad (1)$$

Lemma 2.5 gives

$$\|(A - z)\varphi\| \geq |\operatorname{Im} z| \|\varphi\|. \quad (2)$$

Since $|\operatorname{Im} z| > 0$, $A - z$ is injective; by (1) it is also surjective, and thus bijective. So the inverse exists, we just have to show that the inverse is bounded. Taking $\varphi = (A - z)^{-1}\psi$ in (2), for arbitrary normalized $\psi \in \mathcal{H}$, yields

$$\|(A - z)^{-1}\| \leq \frac{1}{|\operatorname{Im} z|}.$$

Thus $z \in \rho(A)$. It remains to show that actually the whole half-plane is in resolvent set. Theorem 1.3 gives

$$B_{|\operatorname{Im} z|}(z) \subset \rho(A).$$

Now we iterate this reasoning, as sketched in Figure 1: choose z_1 in the ball $B_{|\operatorname{Im} z|}(z)$ and above z , obtain a larger ball around z_1 , and repeat to cover the whole upper half-plane. The same argument applies to the lower half-plane. $\square$

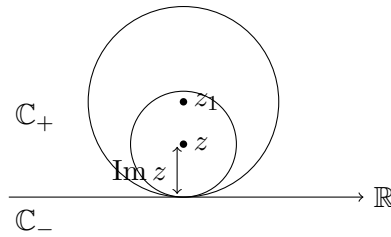


Figure 1: Iteration used in the proof of Proposition 2.6.

Theorem 2.7 (Basic criterion for self-adjointness). *Let A be symmetric. Then the following are equivalent:*

- (i) $A = A^*$;
- (ii) $\sigma(A) \subset \mathbb{R}$;
- (iii) $\operatorname{ran}(A - z_+) = \mathcal{H}$ and $\operatorname{ran}(A - z_-) = \mathcal{H}$ for some $z_+ \in \mathbb{C}_+$ and some $z_- \in \mathbb{C}_-$;
- (iv) A is closed and $\ker(A^* - z_+) = \{0\} = \ker(A^* - z_-)$ for some $z_+ \in \mathbb{C}_+$ and $z_- \in \mathbb{C}_-$.

Remark. Without the symmetry assumption on A , $\sigma(A) \subset \mathbb{R}$ does not imply $A = A^*$, already for matrices.

In quantum mechanics, $\sigma(A)$ is the set of possible measurement values of the observable A , so there is good reason to demand a real spectrum.

Proof. (i) $\Rightarrow$ (iv). Since A^* is closed, so is $A = A^*$. By Lemma 2.5, $\|(A - z_\pm)\varphi\| \geq |\operatorname{Im} z_\pm| \|\varphi\|$. Since $|\operatorname{Im} z_\pm| > 0$:

$$(A - z_\pm)\varphi = 0 \quad \Rightarrow \quad \varphi = 0,$$

and this implies $\ker(A - z_\pm) = \{0\}$. Since $A = A^*$, then also $\ker(A^* - z_\pm) = \{0\}$, as claimed.

(iv) $\Rightarrow$ (iii). Proposition 2.2 implies

$$(\operatorname{ran}(A - \overline{z_\pm}))^\perp = \ker(A^* - z_\pm) = \{0\},$$

and therefore

$$\overline{\operatorname{ran}(A - \overline{z_\pm})} = (\operatorname{ran}(A - \overline{z_\pm}))^\perp^\perp = \{0\}^\perp = \mathcal{H}.$$

For arbitrary $\psi \in \mathcal{H}$, we have to show $\psi \in \operatorname{ran}(A - \overline{z_\pm})$. We use that A is closed! By density of $\operatorname{ran}(A - \overline{z_\pm})$, there exists a sequence $\varphi_n \in D(A)$ with $(A - \overline{z_\pm})\varphi_n \rightarrow \psi$. Then $(A - \overline{z_\pm})\varphi_n$ is a Cauchy sequence. By

$$\|(A - \overline{z_\pm})(\varphi_n - \varphi_m)\| \geq |\operatorname{Im} z_\pm| \|\varphi_n - \varphi_m\|,$$

also (φ_n) is a Cauchy sequence. By completeness its limit φ exists. Since $A - \overline{z_\pm}$ is closed, $\varphi \in D(A)$ and $(A - \overline{z_\pm})\varphi = \psi$. So ψ is in the range. Since ψ was arbitrary, this concludes the proof.

(iii) $\Rightarrow$ (ii). Apply Proposition 2.6.

(ii) $\Rightarrow$ (i). By assumption $A \subset A^*$; it remains to prove $D(A^*) \subset D(A)$. Let $\varphi \in D(A^*)$. Since $\sigma(A) \subset \mathbb{R}$, we know that $A + i$ is surjective. So there exists $\eta \in D(A)$ such that

$$(A + i)\eta = (A^* + i)\varphi.$$

As $A \subset A^*$, the left hand side equals $(A^* + i)\eta$. This then implies $(A^* + i)(\eta - \varphi) = 0$. Recall

$$\ker(A^* + i) = (\operatorname{ran}(A - i))^\perp = \mathcal{H}^\perp = \{0\}.$$

Hence $\varphi = \eta$, and we know that $\eta \in D(A)$. □

The next result shows that adding a sufficiently small perturbation to a self-adjoint operator preserves self-adjointness. This will be useful for Hamiltonians of the form $H = -\Delta + V$.

Theorem 2.8 (Kato–Rellich). *Let $A = A^*$, $B \subset B^*$ and $D(B) \supset D(A)$. If there exist $0 \leq a < 1$ and $b \geq 0$ such that*

$$\|B\varphi\| \leq a\|A\varphi\| + b\|\varphi\| \quad \forall \varphi \in D(A),$$

then $A + B$, with domain $D(A)$, is self-adjoint.

Remark. The inclusion $D(B) \supset D(A)$ ensures that $(A + B)\varphi = A\varphi + B\varphi$ is well-defined on $D(A)$. The theorem answers whether this operator is self-adjoint on domain $D(A)$. If, for example, the two domains intersected in $\{0\}$, the problem would be much more serious.

Proof. It is easy to see that the operator $A + B$ with domain $D(A)$ is symmetric. For self-adjointness, we use Theorem 2.7(iii); in fact, we show not only surjectivity but even invertibility. As before, for all $\psi \in D(A)$ and real $\mu \neq 0$,

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

Taking $\psi = (A - i\mu)^{-1}\varphi$ gives

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

and hence

$$\|A(A - i\mu)^{-1}\varphi\| \leq \|\varphi\|, \quad \|(A - i\mu)^{-1}\varphi\| \leq \frac{1}{|\mu|}\|\varphi\| \quad \forall \varphi \in \mathcal{H}. \quad (3)$$

Obviously we have

$$A + B - i\mu = [\mathbf{1} + B(A - i\mu)^{-1}](A - i\mu). \quad (4)$$

The second factor is invertible because A is self-adjoint, see (ii) of Theorem 2.7. By (3),

$$\begin{aligned} \|B(A - i\mu)^{-1}\varphi\| &\leq a\|A(A - i\mu)^{-1}\varphi\| + b\|(A - i\mu)^{-1}\varphi\| \\ &\leq \left(a + \frac{b}{|\mu|}\right)\|\varphi\|. \end{aligned}$$

For sufficiently large $|\mu|$, we conclude $\|B(A - i\mu)^{-1}\| < 1$, so the first factor in (15) is invertible by the Neumann series. Thus $A + B - i\mu$ is also invertible, and in particular surjective. $\square$

The Schrödinger equation. Recall: a state of a quantum system is represented by $\psi \in \mathcal{H}$ with $\|\psi\| = 1$. The time evolution is described by the initial value problem

$$i\frac{d}{dt}\varphi(t) = H\varphi(t), \quad \varphi(0) = u, \quad (\text{SE})$$

where H is typically unbounded. A solution on an interval I containing zero is a function $\varphi : I \rightarrow \mathcal{H}$ such that

- $\varphi(t) \in D(H)$ for all $t \in I$;
- $\varphi(0) = u$;
- $\lim_{h \rightarrow 0} \frac{\varphi(t+h) - \varphi(t)}{h} = -iH\varphi(t)$.

The limit of the differential quotient is intended in the norm of the Hilbert space.

Proposition 2.9. *If for every $u \in D(H)$ equation (SE) has a solution with $\|\varphi(t)\| = \|u\|$ for every $t \in I$, then $H \subset H^*$. Conversely, if $H \subset H^*$, the norm of every solution is constant, and solutions with the same initial datum are unique.*

Proof. If the norm is constant, then

$$0 = \frac{d}{dt} \langle \varphi(t), \varphi(t) \rangle \Big|_{t=0} = i(\langle Hu, u \rangle - \langle u, Hu \rangle).$$

Thus $\langle Hu, u \rangle = \langle u, Hu \rangle$ for every $u \in D(H)$, which is equivalent to symmetry (check this, using the polarization identity!). Conversely, symmetry makes the same derivative vanish at every time.

Finally, if φ, ϕ are two solutions with the same initial datum, their difference is also a solution and

$$\|\varphi(t) - \phi(t)\| = \|\varphi(0) - \phi(0)\| = \|u - u\| = 0.$$

This concludes the proof of uniqueness. $\square$

Proposition 2.10. *Let $H : D \subset \mathcal{H} \rightarrow \mathcal{H}$ be symmetric and closed. If, for every $u \in D$, equation (SE) has a global solution $\varphi : \mathbb{R} \rightarrow \mathcal{H}$, then $H = H^*$.*

End of Lecture 4

Proof. It suffices to show $\ker(H^* \pm i) = \{0\}$. Suppose

$$(H^* + i)\omega = 0. \quad (5)$$

For $u \in D$, let φ be the solution with $\varphi(0) = u$. Then

$$\begin{aligned} \frac{d}{dt} \langle \omega, \varphi(t) \rangle &= \langle \omega, -iH\varphi(t) \rangle = \langle H^*\omega, -i\varphi(t) \rangle \\ &= \langle -i\omega, -i\varphi(t) \rangle = \langle \omega, \varphi(t) \rangle, \end{aligned}$$

where we used (5) to get to the second line. Solving this $\mathbb{C}$ -valued ODE gives $\langle \omega, \varphi(t) \rangle = \langle \omega, u \rangle e^t$. On the other hand,

$$|\langle \omega, \varphi(t) \rangle| \leq \|\omega\| \|\varphi(t)\| = \|\omega\| \|u\| e^t.$$

How can this agree with the exponential solution? The only possibility is $\langle \omega, u \rangle = 0$ for all $u \in D$. Density of D implies $\omega = 0$. For $H^* - i$, the same argument applies. $\square$

If H is bounded, the solution of (SE) is given by

$$\varphi(t) = e^{-iHt}u := \sum_{n=0}^{\infty} \frac{(-iHt)^n}{n!} u.$$

For an unbounded operator, already H^2 need not be well-defined, so this series cannot be used without further justification. Later we will give meaning to e^{-iHt} .

3 Self-adjoint Extensions [Teschl, Section 2.6]

Remark. A self-adjoint operator is maximal among symmetric operators: if $A = A^*$ and B is symmetric with $B \supset A$, then $B = A$. Indeed,

$$A \subset B \subset B^* \subset A^* = A.$$

Starting with a very small domain makes an operator easy to define, but typically gives only a symmetric operator. One then tries to enlarge its domain until it becomes self-adjoint.

Typical workflow.

1. Start with a formal expression for the Hamiltonian H , based on physical ideas.
2. Find a good domain of nicely behaved functions on which $H \subset H^*$.
3. Find a self-adjoint extension.
4. Study the physical problems: the spectrum, scattering theory, eigenfunctions, and so on.

There may be no self-adjoint extension, or there may be many. Their classification uses von Neumann's deficiency indices. Different extensions often correspond to different boundary conditions; physical input is needed to choose the relevant one. For the examples on $L^2(\mathbb{R}^3)$ considered here, the only reasonable boundary condition is effectively that of decay to zero at infinity, and so over $\mathbb{R}^3$ the self-adjoint extension is usually unique.

A particularly convenient situation is essential self-adjointness.

Definition. An operator $A : D \subset X \rightarrow X$ is *closable* if it has a closed extension $B \supset A$. Its smallest closed extension is called its *closure*, denoted $\overline{A}$.

Remark. A symmetric operator A is always closable because $A \subset A^*$ and A^* is closed.

Definition. A symmetric operator A is called *essentially self-adjoint* if $\overline{A}$ is self-adjoint.

Theorem 3.1 (Kato–Rellich for essential self-adjointness). *Let A be essentially self-adjoint, B symmetric and $D(B) \supset D(A)$. Assume that*

$$\|B\varphi\| \leq a\|A\varphi\| + b\|\varphi\| \quad \forall \varphi \in D(A)$$

with $0 \leq a < 1$ and $b \geq 0$. Then $A + B$ with domain $D(A)$ is essentially self-adjoint and

$$D(\overline{A + B}) = D(\overline{A}), \quad \overline{A + B} = \overline{A} + \overline{B}.$$

We skip the proof of this version of the Kato–Rellich theorem.

Remark. Sometimes $D(\overline{A})$ is not explicitly known, but a convenient domain $D(A)$ is available on which A is essentially self-adjoint. In applications, one can often do calculations on this smaller domain and extend to the domain of self-adjointness later.

Proposition 3.2. *Let $H : D \subset \mathcal{H} \rightarrow \mathcal{H}$ be symmetric (without assuming closedness). If for every $u \in D$ the initial value problem*

$$i \frac{d}{dt} \varphi(t) = H\varphi(t), \quad \varphi(0) = u$$

has a global solution $\varphi : \mathbb{R} \rightarrow \mathcal{H}$, then H is essentially self-adjoint.

We skip the proof of this proposition as well.

4 Schrödinger Operators [Teschl, Section 7.1 and 7.2]

Goal: define $H = -\Delta + V$. The idea is to define $-\Delta$ using the Fourier transform and then add a multiplication operator V as a perturbation using Kato–Rellich.

Recall that an operator $U : \mathcal{H}_1 \rightarrow \mathcal{H}_2$ is *unitary* if $U^* = U^{-1}$. In that case,

$$\langle Uf, Ug \rangle = \langle f, U^*Ug \rangle = \langle f, U^{-1}Ug \rangle = \langle f, g \rangle,$$

so $\|Uf\| = \|f\|$ and $\|U\| = 1$.

Theorem 4.1 (Fourier transform). *There is a unique unitary operator $\mathcal{F} : L^2(\mathbb{R}^n) \rightarrow L^2(\mathbb{R}^n)$ such that*

$$(\mathcal{F}f)(p) = \lim_{R \rightarrow \infty} \frac{1}{(2\pi)^{n/2}} \int_{|x| \leq R} e^{-ip \cdot x} f(x) dx,$$

where the limit is taken with respect to the L^2 -norm.

Remark. • The cutoff at R is needed because a general L^2 function need not be integrable.

- Notation: $\mathcal{F}f = \hat{f}$ and $\mathcal{F}^{-1}f = \mathcal{F}^*f = \check{f}$.
- Key property of the Fourier transform (easy to verify for Schwartz functions):

$$\mathcal{F}\left(-i \frac{\partial}{\partial x_j} f\right)(p) = p_j \hat{f}(p).$$

- Generalized derivatives are defined by Fourier multipliers: for $\alpha \in \mathbb{N}$ we define

$$\left(-i \frac{\partial}{\partial x_j}\right)^\alpha f := \mathcal{F}^{-1}(p_j^\alpha \mathcal{F}f).$$

The natural domain of this operator is functions f such that $p_j^\alpha \mathcal{F}f$ has finite L^2 -norm.

Sketch of proof of Theorem 4.1. • Using the derivative identity, show that $\mathcal{FS}(\mathbb{R}^n) \subset \mathcal{S}(\mathbb{R}^n)$, where $\mathcal{S}(\mathbb{R}^n)$ is Schwartz space.

- Use Fourier inversion and the fact that $\widehat{g} = g$ for $g(x) = e^{-|x|^2/2}$ to show bijectivity on Schwartz space:

$$\begin{aligned} (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{ip \cdot x} \widehat{f}(p) \, dp &= \lim_{\varepsilon \downarrow 0} (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{ip \cdot x} e^{-\varepsilon |p|^2/2} \widehat{f}(p) \, dp \\ &= f(x). \end{aligned}$$

- The Plancherel identity shows that $\langle \mathcal{F}f, \mathcal{F}g \rangle = \langle f, g \rangle$ for $f, g \in \mathcal{S}(\mathbb{R}^n)$; in particular $\|\mathcal{F}\| = 1$.
- Now we can extend from $\mathcal{S}(\mathbb{R}^n)$ to $L^2(\mathbb{R}^n)$ by continuity.

□

Definition (Sobolev spaces). For $s \geq 0$,

$$\begin{aligned} H^s(\mathbb{R}^n) &:= \left\{ u \in L^2(\mathbb{R}^n) : \int_{\mathbb{R}^n} |\widehat{u}(p)|^2 (1 + |p|^2)^s \, dp < \infty \right\}, \\ \langle u, v \rangle_{H^s} &:= \int_{\mathbb{R}^n} \overline{\widehat{u}(p)} \widehat{v}(p) (1 + |p|^2)^s \, dp. \end{aligned} \tag{6}$$

Remark. $H^0(\mathbb{R}^n) = L^2(\mathbb{R}^n)$, and $H^s(\mathbb{R}^n) \subset H^{s'}(\mathbb{R}^n)$ for $s > s' \geq 0$.

Definition. For measurable $f : \mathbb{R}^n \rightarrow \mathbb{C}$, the *multiplication operator* T_f is

$$T_f : D(T_f) \subset L^2(\mathbb{R}^n) \rightarrow L^2(\mathbb{R}^n), \quad D(T_f) := \{\varphi \in L^2(\mathbb{R}^n) : f\varphi \in L^2(\mathbb{R}^n)\},$$

with

$$(T_f \varphi)(x) := f(x) \varphi(x) \quad \text{almost everywhere.}$$

Remark. This is the largest natural domain. Anything larger is clearly impossible.

A multiplication operator is analogous to a diagonal matrix.

If $f \in L^\infty(\mathbb{R}^n)$, then $D(T_f) = L^2(\mathbb{R}^n)$ and $\|T_f\| \leq \|f\|_\infty$.

Definition. Let X be a Banach space, $A : D \subset X \rightarrow X$ an operator and $\lambda \in \mathbb{C}$. A sequence $(x_n) \subset D$ with $\|x_n\| = 1$ and $\|(A - \lambda)x_n\| \rightarrow 0$ is called a *Weyl sequence* for λ .

Lemma 4.2 (Weyl criterion). *If a Weyl sequence for λ exists, then $\lambda \in \sigma(A)$. Conversely, if $\lambda \in \sigma(A) \cap \partial \rho(A)$, a Weyl sequence for λ exists.*

Proof. The first implication is assigned as an exercise. To prove the second implication, consider a sequence $z_n \in \rho(A)$ with $z_n \rightarrow \lambda \in \sigma(A)$. Recall that

$$\|R_{z_n}(A)\| \geq \frac{1}{\text{dist}(z_n, \sigma(A))} \rightarrow \infty.$$

By definition of the operator norm there exist nonzero $\varphi_n \in X$ such that

$$\|R_{z_n}(A)\varphi_n\| \geq \frac{1}{2 \text{dist}(z_n, \sigma(A))} \|\varphi_n\|. \tag{7}$$

Define

$$\tilde{\varphi}_n = \frac{\varphi_n}{\|R_{z_n}(A)\varphi_n\|}, \quad \tilde{\psi}_n = R_{z_n}(A)\tilde{\varphi}_n.$$

Clearly we have $\|\tilde{\psi}_n\| = 1$. By (7) we obtain $\|\tilde{\varphi}_n\| \rightarrow 0$. Moreover,

$$\begin{aligned} \|(A - \lambda)\tilde{\psi}_n\| &= \|(A - z_n)\tilde{\psi}_n + (z_n - \lambda)\tilde{\psi}_n\| \\ &= \|\tilde{\varphi}_n + (z_n - \lambda)\tilde{\psi}_n\| \\ &\leq \|\tilde{\varphi}_n\| + |z_n - \lambda| \rightarrow 0. \end{aligned}$$

Thus $(\tilde{\psi}_n)$ is a Weyl sequence. □

Proposition 4.3. *For measurable $f : \mathbb{R}^n \rightarrow \mathbb{C}$, we have*

$$\sigma(T_f) = W_f, \quad \text{where } W_f := \{z \in \mathbb{C} : m(f^{-1}(B_\varepsilon(z))) > 0 \text{ for every } \varepsilon > 0\},$$

where m is the Lebesgue measure. If f is continuous, W_f is the closure of the image of f .

Proof. Let $z \in W_f$. For $k \geq 1$ let

$$E_k := f^{-1}(B_{1/k}(z)) \quad \text{and} \quad \varphi_k := \frac{\chi_{E_k}}{\sqrt{m(E_k)}}.$$

Here χ_{E_k} is the characteristic function, equal to one on E_k and zero outside. (If $m(E_k) = \infty$, replace E_k by a measurable subset with $0 < m(E_k) < \infty$.) Check that $\varphi_k \in D(T_f)$ and $\|\varphi_k\| = 1$. Moreover we find

$$\|(T_f - z)\varphi_k\| = \left(\int_{E_k} \frac{|f(x) - z|^2}{m(E_k)} dx \right)^{1/2} \leq \frac{1}{k} \|\varphi_k\| \rightarrow 0.$$

So (φ_k) is a Weyl sequence and $z \in \sigma(T_f)$.

Conversely, let $z \notin W_f$. We prove that $z \notin \sigma(T_f)$ by constructing the resolvent explicitly. By definition of W_f , there is $\varepsilon > 0$ such that $m(f^{-1}(B_\varepsilon(z))) = 0$. Our candidate for the resolvent is T_g , where we define

$$g(x) := \begin{cases} (f(x) - z)^{-1}, & \text{for } f(x) \notin B_\varepsilon(z), \\ 0, & \text{for } f(x) \in B_\varepsilon(z). \end{cases}$$

The second case concerns a null set, so can be expected to be irrelevant in L^2 . By construction $g \in L^\infty$, so T_g is bounded. For $\varphi \in D(T_f)$,

$$T_g(T_f - z)\varphi = g(f - z)\varphi = \varphi \quad \text{a.e.}$$

Also $fg \in L^\infty$, so $T_g L^2 \subset D(T_f)$ and, for every $\varphi \in L^2$,

$$(T_f - z)T_g\varphi = (f - z)g\varphi = \varphi \quad \text{a.e.}$$

Hence $T_g = R_z(T_f)$ and $z \in \rho(T_f)$. □

Lemma 4.4. *If f is real-valued, T_f is self-adjoint.*

Proof. T_f is symmetric. Proposition 4.3 gives $\sigma(T_f) \subset \mathbb{R}$, so the basic criterion implies self-adjointness. □

Proposition 4.5 (Unitary equivalence). *If $A : D(A) \subset \mathcal{H} \rightarrow \mathcal{H}$ is self-adjoint and $U \in \mathcal{L}(\mathcal{H})$ is unitary, then*

$$B = UAU^{-1} : UD(A) \subset \mathcal{H} \rightarrow \mathcal{H}$$

is self-adjoint and $\sigma(A) = \sigma(B)$.

Proof. It is easy to see that B is symmetric. We show $\sigma(A) = \sigma(B)$, then the basic criterion will imply that B is self-adjoint. For $z \in \rho(A)$, the bounded operator $U(A - z)^{-1}U^{-1}$ is the resolvent of B at z , so $z \in \rho(B)$. Conversely, for $z \in \rho(B)$, $U^{-1}(B - z)^{-1}U$ is the resolvent of A at z . Thus $\rho(A) = \rho(B)$, hence $\sigma(A) = \sigma(B) \subset \mathbb{R}$. $\square$

Example. • The momentum operator on $L^2(\mathbb{R})$ is

$$-i \frac{d}{dx} : H^1(\mathbb{R}) \subset L^2(\mathbb{R}) \rightarrow L^2(\mathbb{R}), \quad -i \frac{d}{dx} := \mathcal{F}^{-1} T_f \mathcal{F}, \quad f(p) := p.$$

It is self-adjoint and $\sigma(-i d/dx) = \mathbb{R}$.

• The Laplace operator (kinetic energy) is

$$-\Delta : H^2(\mathbb{R}^n) \subset L^2(\mathbb{R}^n) \rightarrow L^2(\mathbb{R}^n), \quad -\Delta := \mathcal{F}^{-1} T_f \mathcal{F}, \quad f(p) := |p|^2 = \sum_{j=1}^n p_j^2.$$

It is self-adjoint on $D(\mathcal{F}^{-1} T_f \mathcal{F}) = H^2(\mathbb{R}^n)$ and $\sigma(-\Delta) = [0, \infty)$. Its restriction to $\mathcal{S}(\mathbb{R}^n)$ is essentially self-adjoint.

End of Lecture 5

Interpretation. For $m > 0$, $H = -\Delta/(2m)$ describes the energy of a free particle of mass m (we chose units of energy such that the Planck constant has value $\hbar = 1$). In three dimensions, momentum is represented by the triple of three operators

$$-i\nabla = \begin{pmatrix} -i\partial/\partial x_1 \\ -i\partial/\partial x_2 \\ -i\partial/\partial x_3 \end{pmatrix}, \quad -\frac{\Delta}{2m} = \frac{1}{2m}(-i\nabla)^2.$$

Compare the classical Hamiltonian of a free particle $H(p, q) = |p|^2/(2m)$, with momentum $p \in \mathbb{R}^n$ and position $q \in \mathbb{R}^n$. A classical charged particle attracted by a fixed charge placed in the origin has Hamiltonian

$$H(p, q) = \frac{|p|^2}{2m} - \frac{1}{|q|},$$

where $-1/|q|$ is the Coulomb potential. The next goal is to define a self-adjoint Hamiltonian operator for the quantum analogue of this system, as an example of a Schrödinger operator.

Definition. *Schrödinger operators* are operators of the form

$$-\Delta + V : D \subset L^2(\mathbb{R}^n) \rightarrow L^2(\mathbb{R}^n),$$

where $V = T_V$ is a multiplication operator.

Remark. It is a common abuse of notation to denote T_V by V or $V(x)$.

Sobolev inequalities are a wide class of inequalities which permit us to reduce the exponent of Lebesgue norms at the expense of introducing higher derivatives of the functional.

These are extremely useful both in operator theory as in nonlinear partial differential equations. See [Lieb & Loss, Chapter 8] for a detailed introduction. We only cite some variations of Sobolev inequalities which will be used in the study of Schrödinger operators.

Theorem 4.6 (Some Sobolev inequalities). *(i) Let $n \geq 3$ and $1 < p < n$. There exists a constant $C_{n,p} > 0$ such that, for $q := p \frac{n}{n-p}$, we have*

$$\|\nabla f\|_{L^p} \geq C_{n,p} \|f\|_{L^q} \quad \forall f \in C_0^\infty(\mathbb{R}^n). \quad (8)$$

(ii) Let $f \in H^s(\mathbb{R}^n)$ (as defined in (6)) and $k \in \mathbb{N}$ with $k + \frac{n}{2} < s$. Then

$$C_{n,s,k} \|f\|_{H^s} \geq \sup_{|\alpha| \leq k} \|\partial^\alpha f\|_{L^\infty},$$

where the supremum is over multi-indices $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}^n$ with $|\alpha| := \alpha_1 + \alpha_2 + \dots + \alpha_n \leq m$, and $\partial^\alpha := \partial_{x_1}^{\alpha_1} \partial_{x_2}^{\alpha_2} \dots \partial_{x_n}^{\alpha_n}$ in terms of partial weak derivatives defined through multiplication by the corresponding coordinate in Fourier space.

Often, inequalities like (8) are stated without specifying carefully the function space, relying on the convention that the norms are considered to be $+\infty$ when not well-defined. However, at least some decay at infinity still has to be imposed, otherwise any non-vanishing constant function would constitute a counterexample.

It is useful to remember these two Sobolev inequalities also by reading them from the right to the left for some common values of q , for example $q = 4, 6$, in three space dimensions $n = 3$.

Theorem 4.7. *Let $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, i. e., there exist $V_2 \in L^2(\mathbb{R}^3)$ and $V_\infty \in L^\infty(\mathbb{R}^3)$ such that $V(x) = V_2(x) + V_\infty(x)$ almost everywhere. Assume moreover that V is real-valued. Then*

$$-\Delta + V : D \subset L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3)$$

is self-adjoint for $D = H^2(\mathbb{R}^3)$, and its restriction to $\mathcal{S}(\mathbb{R}^3)$ is essentially self-adjoint.

Proof. By the Kato–Rellich theorem it suffices to show that there exist $a < 1$ and $b \geq 0$ such that

$$\|V\varphi\|_2 \leq a \|\Delta\varphi\|_2 + b \|\varphi\|_2 \quad \forall \varphi \in H^2(\mathbb{R}^3).$$

Without loss of generality we can assume the part V_2 to be arbitrarily small: in fact, for every $\varepsilon > 0$ there is a decomposition

$$V = V_2^\varepsilon + V_\infty^\varepsilon, \quad \|V_2^\varepsilon\|_2 < \varepsilon, \quad V_\infty^\varepsilon \in L^\infty(\mathbb{R}^3).$$

(See the next assignment for the construction of this decomposition.) By Hölder's inequality,

$$\begin{aligned} \|V\varphi\|_2 &\leq \|V_2^\varepsilon\varphi\|_2 + \|V_\infty^\varepsilon\varphi\|_2 \leq \|V_2^\varepsilon\|_2 \|\varphi\|_\infty + \|V_\infty^\varepsilon\|_\infty \|\varphi\|_2 \\ &\leq \varepsilon \|\varphi\|_\infty + \|V_\infty^\varepsilon\|_\infty \|\varphi\|_2. \end{aligned} \quad (9)$$

By the Sobolev inequality from Theorem 4.6(ii) and the definition of the H^2 norm give

$$\|\varphi\|_\infty \leq C \|\varphi\|_{H^2} \leq C\sqrt{2} (\|\Delta\varphi\|_2 + \|\varphi\|_2).$$

Using this in (9) we obtain

$$\|V\varphi\|_2 \leq \varepsilon C\sqrt{2} \|\Delta\varphi\|_2 + (\varepsilon C\sqrt{2} + \|V_\infty^\varepsilon\|_\infty) \|\varphi\|_2.$$

Choosing ε sufficiently small makes $\varepsilon C\sqrt{2} < 1$. Both versions of the Kato–Rellich theorem now apply. $\square$

Example (Coulomb potential). The potential

$$V(x) := \begin{cases} \pm \frac{1}{|x|}, & x \in \mathbb{R}^3 \setminus \{0\}, \\ 0, & x = 0, \end{cases}$$

is in $L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. (See the next assignment.)

Remark. For $x_1, \dots, x_N \in \mathbb{R}^3$, introduce multiplication operators by

$$\begin{aligned} (V_{ik}\varphi)(x_1, \dots, x_N) &:= V_{ik}(x_i - x_k)\varphi(x_1, \dots, x_N), \\ ((V_{\text{ext}})_k\varphi)(x_1, \dots, x_N) &:= V_{\text{ext}}(x_k)\varphi(x_1, \dots, x_N). \end{aligned}$$

If we take

$$\begin{aligned} V_{\text{ext}}(x) &= -\frac{1}{|x|} && \text{(attraction to an atomic nucleus),} \\ V_{ik}(x) &= \frac{1}{|x|} && \text{(repulsion between electrons)} \end{aligned}$$

we obtain a model for molecules (with fixed nuclei, i. e., in the Born–Oppenheimer approximation). The N -electron operator

$$H_N := \sum_{k=1}^N (-\Delta_k) + \sum_{k=1}^N (V_{\text{ext}})_k + \sum_{i=1}^N \sum_{k=i+1}^N V_{ik}$$

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

5 Existence of Solutions to the Schrödinger equation. Strongly Continuous Unitary Groups [Teschl, Section 5.1]

(The explicit construction of strongly continuous unitary groups is not in Teschl’s book.)

Definition. Let X, Y be Banach spaces. A sequence of bounded operators $A_n \in \mathcal{L}(X, Y)$ converges strongly to $A \in \mathcal{L}(X, Y)$ if

$$A_n x \longrightarrow Ax \quad (n \rightarrow \infty) \quad \forall x \in X.$$

We write $A = \text{s-lim}_{n \rightarrow \infty} A_n$. (This is just pointwise convergence in the case of operators.)

Remark. Norm convergence $\|A_n - A\| \rightarrow 0$ is stronger than strong convergence: it implies strong convergence, but the converse does not hold in general.

Lemma 5.1. Let X, Y, Z be Banach spaces.

(i) If $A = \text{s-lim}_{n \rightarrow \infty} A_n$ in $\mathcal{L}(X, Y)$ and $B = \text{s-lim}_{n \rightarrow \infty} B_n$ in $\mathcal{L}(Y, Z)$, then

$$\text{s-lim}_{n \rightarrow \infty} B_n A_n = BA.$$

(ii) If (A_n) is a bounded sequence in $\mathcal{L}(X, Y)$, i. e., $\sup_n \|A_n\| < \infty$, and $(A_n x)$ converges for every x in a dense subset $D \subset X$, then $\text{s-lim}_{n \rightarrow \infty} A_n$ exists in $\mathcal{L}(X, Y)$.

Proof sketch. Part (i) follows using the uniform boundedness principle. Part (ii) follows from an $\varepsilon/3$ -argument and the uniform bound on (A_n) . (Potential future exercise) $\square$

Definition. Let $\mathcal{H}$ be a Hilbert space. A *strongly continuous unitary group* (SCUG) is a map $U : \mathbb{R} \rightarrow \mathcal{L}(\mathcal{H})$ such that

- (i) $U(t)$ is unitary and $U(t+s) = U(t)U(s)$ for all $s, t \in \mathbb{R}$;
- (ii) $U(t)\varphi \rightarrow \varphi$ as $t \rightarrow 0$ for every $\varphi \in \mathcal{H}$.

Remark. $U(0) = U(0+0) = U(0)U(0)$ implies $U(0) = \mathbf{1}$. Condition (i) means that U is a group homomorphism from $(\mathbb{R}, +)$ to unitary operators. Compare the definition and the following results also to the theory of Lie groups.

Example (Translations). The map $U : \mathbb{R} \rightarrow \mathcal{L}(\mathcal{H})$ need not be continuous in the operator norm; only $t \mapsto U(t)\varphi$ is required to be continuous for each φ . To see the distinction, let

$$\mathcal{H} := L^2(\mathbb{R}), \quad (U(t)\varphi)(x) := \varphi(x-t) \quad \text{for } \varphi \in \mathcal{H}.$$

We verify that U is a SCUG. Properties (i) (unitarity and homomorphism property) are easy to see. Concerning property (ii) (strong continuity in zero), by Lemma 5.1(ii), strong continuity need only be checked on a dense set. For $\varphi \in C_0^\infty(\mathbb{R})$,

$$\|U(t)\varphi - \varphi\|_2^2 = \int_{\mathbb{R}} |\varphi(x-t) - \varphi(x)|^2 dx \rightarrow 0 \quad (t \rightarrow 0)$$

by dominated convergence.

Note however that U is not norm-continuous. In fact, for $\varepsilon > 0$, choose a “bump function” $\varphi_\varepsilon \in C_0^\infty(\mathbb{R})$ with $\|\varphi_\varepsilon\|_2 = 1$ and $\text{supp } \varphi_\varepsilon \subset B_{\varepsilon/2}(0)$. Then $U(\varepsilon)\varphi_\varepsilon \perp \varphi_\varepsilon$, since their supports do not overlap. Hence

$$\|(U(\varepsilon) - \mathbf{1})\varphi_\varepsilon\|_2^2 = \langle U(\varepsilon)\varphi_\varepsilon, U(\varepsilon)\varphi_\varepsilon \rangle + \langle \varphi_\varepsilon, \varphi_\varepsilon \rangle = 2.$$

Therefore $\|U(\varepsilon) - \mathbf{1}\| \geq \sqrt{2}$, which does not tend to zero.

Definition. Let $U : \mathbb{R} \rightarrow \mathcal{L}(\mathcal{H})$ be a SCUG. Its *generator* is the operator $A : D(A) \subset \mathcal{H} \rightarrow \mathcal{H}$ defined by

$$D(A) := \left\{ \varphi \in \mathcal{H} : \lim_{t \rightarrow 0} \frac{U(t)\varphi - \varphi}{t} \right\},$$

and

$$A\varphi := i \lim_{t \rightarrow 0} \frac{U(t)\varphi - \varphi}{t} = i \frac{d}{dt} U(t)\varphi \Big|_{t=0}.$$

Note that the limit of the difference quotient in both formulas is with respect to the Hilbert space norm. Thus $D(A)$ is the set of vectors for which the strong derivative at zero exists.

Theorem 5.2 (Stone, 1932). *Let A be the generator of a SCUG $U : \mathbb{R} \rightarrow \mathcal{L}(\mathcal{H})$. Then:*

- (i) A is densely defined and $A = A^*$.
- (ii) $U(t)D(A) \subset D(A)$, and for every $\varphi \in D(A)$ and $t \in \mathbb{R}$,

$$i \frac{d}{dt} U(t)\varphi = AU(t)\varphi = U(t)A\varphi. \tag{10}$$

(iii) U is uniquely determined by its generator A .

(iv) For all $z \in \mathbb{C}_\pm$ and all $\varphi \in \mathcal{H}$, we have the two integral representations

$$(A - z)^{-1}\varphi = i \int_0^{\pm\infty} e^{izt} U(t)\varphi dt. \tag{11}$$

Remark. The integral is a vector-valued Riemann integral, defined as a limit of Riemann sums followed by a limit of one of the ends of the integration interval to $\pm\infty$. It satisfies the usual rules of Riemann integrals. For example, for a continuous vector-valued function φ on a compact interval $[a, b]$, we have the triangle inequality

$$\left\| \int_a^b \varphi(t) dt \right\| \leq \int_a^b \|\varphi(t)\| dt.$$

If B is a bounded operator, then

$$B \int_a^b \varphi(t) dt = \int_a^b B\varphi(t) dt.$$

End of Lecture 6

Proof of Theorem 5.2. (ii). We first prove $U(t)D(A) \subset D(A)$. For $\varphi \in D(A)$,

$$\begin{aligned} \frac{i}{\varepsilon}(U(\varepsilon) - \mathbf{1})U(t)\varphi &= \frac{i}{\varepsilon}(U(t + \varepsilon) - U(t))\varphi \\ &= U(t)\frac{i}{\varepsilon}(U(\varepsilon) - \mathbf{1})\varphi \longrightarrow U(t)A\varphi \quad (\varepsilon \rightarrow 0). \end{aligned}$$

where in the last step we used that $U(t)$ is bounded, so it commutes with the limit $\varepsilon \rightarrow 0$. Existence of the limit means that $U(t)\varphi \in D(A)$ and $AU(t)\varphi = U(t)A\varphi$. The computation also shows validity of (10).

(i), *We show density of $D(A)$.* Let $\varphi \in \mathcal{H}$ and $\varepsilon > 0$. For any $\delta > 0$, define

$$\varphi_\delta := \frac{1}{\delta} \int_0^\delta U(s)\varphi ds.$$

We claim that $\varphi_\delta \rightarrow \varphi$ as $\delta \downarrow 0$. Indeed, given $\varepsilon > 0$, there exists δ so small that $\|U(s)\varphi - \varphi\| < \varepsilon$ for all $s \in [0, \delta]$. Then

$$\begin{aligned} \|\varphi_\delta - \varphi\| &= \left\| \frac{1}{\delta} \int_0^\delta U(s)\varphi ds - \frac{1}{\delta} \int_0^\delta \varphi ds \right\| \\ &\leq \frac{1}{\delta} \int_0^\delta \|U(s)\varphi - \varphi\| ds < \frac{1}{\delta} \int_0^\delta \varepsilon ds = \varepsilon. \end{aligned} \tag{12}$$

It remains to show $\varphi_\delta \in D(A)$. Using that $U(t)$ is bounded to pull it inside the integral, we have

$$U(t)\varphi_\delta = \frac{1}{\delta} \int_0^\delta U(t+s)\varphi ds = \frac{1}{\delta} \int_t^{t+\delta} U(r)\varphi dr.$$

Since the integrand is continuous, this is differentiable with respect to t at zero. By definition of the domain, this means $\varphi_\delta \in D(A)$.

(i), *We show $A \subset A^*$.* Let $\varphi, \psi \in D(A)$. Unitarity gives $\langle \varphi, \psi \rangle = \langle U(t)\varphi, U(t)\psi \rangle$, and hence

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

Thus A is symmetric.

(i), We show $A^* \subset A$. Let $\varphi \in D(A^*)$. For every $\eta \in D(A)$ and $t \neq 0$, using the fundamental theorem of calculus, we have

$$\begin{aligned}
\langle \eta, \frac{i}{t}(U(t) - \mathbf{1})\varphi \rangle &= \langle \frac{i}{-t}(U(-t) - \mathbf{1})\eta, \varphi \rangle \\
&= \frac{1}{-t} \int_0^{-t} \frac{d}{ds} \langle iU(s)\eta, \varphi \rangle ds \\
&\stackrel{(ii)}{=} \frac{1}{-t} \int_0^{-t} \langle AU(s)\eta, \varphi \rangle ds \quad (\text{using that } \eta \in D(A) \text{ by assumption}) \\
&= \frac{1}{-t} \int_0^{-t} \langle \eta, U(-s)A^*\varphi \rangle ds \quad (\text{using that } \varphi \in D(A^*) \text{ by assumption}) \\
&= \langle \eta, \frac{1}{t} \int_0^t U(s)A^*\varphi ds \rangle.
\end{aligned}$$

Since vectors $\eta \in D(A)$ are dense, it follows that

$$i \frac{U(t)\varphi - \varphi}{t} = \frac{1}{t} \int_0^t U(s)A^*\varphi ds \longrightarrow U(0)A^*\varphi = A^*\varphi \quad (t \rightarrow 0).$$

The limit of the integral is proven as in (12) above. By definition, the existence of this limit for $t \rightarrow 0$ means that $\varphi \in D(A)$, and $A\varphi = A^*\varphi$.

(iii). Let U, V be SCUGs with generator A . By (ii) and Lemma 5.1(i), the function $U(t)V(-t)\varphi$ is differentiable for $\varphi \in D(A)$, and

$$i \frac{d}{dt} U(t)V(-t)\varphi = U(t)AV(-t)\varphi - U(t)AV(-t)\varphi = 0.$$

Thus $U(t)V(-t)\varphi = \varphi$ for every $\varphi \in D(A)$. Since $D(A)$ is dense, this implies $U(t) = V(t)$.

(iv). Let $\varphi \in D(A)$ and $z \in \mathbb{C}_+$. Differentiating gives

$$i \frac{d}{dt} (e^{izt}U(t)\varphi) = (A - z)e^{izt}U(t)\varphi.$$

Consequently,

$$\begin{aligned}
\int_0^R e^{izt}U(t)\varphi dt &= \int_0^R (A - z)^{-1} i \frac{d}{dt} (e^{izt}U(t)\varphi) dt \\
&= (A - z)^{-1} i \underbrace{(e^{izR}U(R)\varphi - \varphi)}_{\rightarrow 0 \text{ (} R \rightarrow \infty)} \longrightarrow -i(A - z)^{-1}\varphi \quad (R \rightarrow \infty).
\end{aligned}$$

Here the resolvent could be taken outside the integral because it is a bounded operator. The convergence to zero on the second line was obtained because

$$\|e^{izR}U(R)\varphi\| = e^{-\text{Im } z R} \|\varphi\| \longrightarrow 0.$$

For arbitrary $\varphi \in \mathcal{H}$, choose $\varphi_n \in D(A)$ with $\varphi_n \rightarrow \varphi$. The resolvent is bounded, we can take the limit on the right hand side of the claimed identity. Also on the left hand side we can take the limit, because

$$\begin{aligned}
&\left\| \int_0^\infty e^{izt}U(t)\varphi_n dt - \int_0^\infty e^{izt}U(t)\varphi dt \right\| \\
&\leq \int_0^\infty e^{-\text{Im } z t} \|\varphi_n - \varphi\| dt = \frac{1}{\text{Im } z} \|\varphi_n - \varphi\| \longrightarrow 0.
\end{aligned}$$

This extends the identity to all of $\mathcal{H}$. For $z \in \mathbb{C}_-$, integrate over $(-\infty, 0]$ instead of $[0, +\infty)$. $\square$

Theorem 5.3 (Nelson). *Let $U : \mathbb{R} \rightarrow \mathcal{L}(\mathcal{H})$ be a SCUG with generator A . If $X \subset D(A)$ is a dense subspace of $\mathcal{H}$ invariant under $U(t)$, i. e., $U(t)X \subset X$ for every $t \in \mathbb{R}$, then*

$$A = \overline{A|_X}.$$

Thus a suitable dense subspace is sufficient for computing the generator.

Proof. For $\eta \in X$, consider the Schrödinger equation

$$i \frac{d}{dt} \varphi(t) = (A|_X) \varphi(t), \quad \varphi(0) = \eta.$$

It is solved by $\varphi(t) = U(t)\eta$. The criterion for essential self-adjointness from global solutions (Proposition 3.2) shows that $A|_X$ is essentially self-adjoint. Its closure is therefore self-adjoint and contained in A , so the two operators coincide. $\square$

Translation group and momentum operator. Let

$$\mathcal{H} := L^2(\mathbb{R}), \quad [U(t)\varphi](x) := \varphi(x-t), \quad X := C_0^\infty(\mathbb{R}).$$

Clearly $\overline{X} = \mathcal{H}$ and $U(t)X \subset X$. For $\varphi \in X$,

$$i \frac{d}{dt} [U(t)\varphi](x) \Big|_{t=0} = i \frac{d}{dt} \varphi(x-t) \Big|_{t=0} = -i\varphi'(x) \quad \text{for almost every } x. \quad (13)$$

This suggests that the restriction of the generator is $B := -i d/dx$ on X . We still have to show that the derivative exists in the L^2 norm (instead of almost everywhere pointwise as in (13)), as required by the definition of the generator. For $\varphi \in X$,

$$\left\| \frac{i}{t} (U(t)\varphi - \varphi) - B\varphi \right\|_2^2 = \int_{\mathbb{R}} \left| \frac{i}{t} (\varphi(x-t) - \varphi(x)) + i\varphi'(x) \right|^2 dx.$$

The integrand tends to zero pointwise as $t \rightarrow 0$. Choose R large enough that $\text{supp } \varphi \subset B_{R-1}(0)$. Without loss of generality we can assume $|t| < 1$. Then

$$\left| \frac{i}{t} (\varphi(x-t) - \varphi(x)) \right| \leq \|\varphi'\|_\infty \chi_{B_R(0)}(x), \quad |\varphi'(x)| \leq \|\varphi'\|_\infty \chi_{B_R(0)}(x).$$

The square of the sum of these bounds is integrable. Lebesgue's dominated convergence theorem therefore gives

$$\left\| \frac{i}{t} (U(t)\varphi - \varphi) - B\varphi \right\|_2 \longrightarrow 0 \quad (t \rightarrow 0).$$

Thus $X \subset D(A)$ and $A|_X = B$. By Nelson's theorem,

$$p := \overline{A|_X} = \overline{-i \frac{d}{dx} \Big|_{C_0^\infty(\mathbb{R})}} \quad (14)$$

generates U , and $p = p^*$. The operator (14) agrees with the definition of the momentum operator through the Fourier transform. Hence the self-adjoint momentum operator defined earlier is the generator of translations.

Rotations and angular momentum. Let $\mathcal{H} := L^2(\mathbb{R}^3)$. Every rotation $R \in \text{SO}(3)$ defines a unitary operator by

$$[U(R)\varphi](x) := \varphi(R^{-1}x).$$

We have $U(R_1)U(R_2) = U(R_1R_2)$, so this is a group representation. Choose a unit vector $e \in \mathbb{R}^3$ as rotation axis, and let R_t be the rotation through angle t about this axis. Check that

$$\left. \frac{d}{dt} R_t x \right|_{t=0} = e \wedge x,$$

where $\wedge$ denotes the vector product. Set $U(t) := U(R_t)$ and $X := C_0^\infty(\mathbb{R}^3)$. Then X is dense in $\mathcal{H}$ and invariant under $U(t)$. For $\varphi \in X$,

$$\begin{aligned} i \frac{d}{dt} [U(t)\varphi](x) \Big|_{t=0} &= i \frac{d}{dt} \varphi(R_{-t}x) \Big|_{t=0} = -i \nabla \varphi(x) \cdot (e \wedge x) \\ &= e \cdot (x \wedge (-i \nabla \varphi(x))) = (e \cdot L) \varphi(x), \end{aligned}$$

where $\cdot$ is the Euclidean inner product and

$$L := x \wedge p = \begin{pmatrix} L_1 \\ L_2 \\ L_3 \end{pmatrix}$$

is the triple of angular momentum operators. As in the previous example, check that this derivative also exists in the L^2 norm, not just pointwise almost everywhere. The operators L_1 , L_2 , and L_3 are essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$. The closure of $e \cdot L$ generates rotations about the e -axis.

We have seen that every SCUG has a self-adjoint generator. We now prove the converse: every self-adjoint operator generates a SCUG. In particular, if $H = H^*$ and $\psi \in D(H)$, then

$$i \frac{d}{dt} \psi(t) = H \psi(t), \quad \psi(0) = \psi,$$

has a global solution $\psi(t) = U(t)\psi$, where U is generated by H . Since $U(t)$ is unitary, this extends to initial data $\psi \notin D(H)$.

End of Lecture 7

Theorem 5.4. *Every self-adjoint operator A is the generator of a unique SCUG.*

This SCUG is denoted by

$$U(t) =: e^{-iAt}.$$

Sketch of proof of Theorem 5.4. Step 1: approximate A by bounded operators. For $m \in \mathbb{Z} \setminus \{0\}$, set

$$B_m := im(A + im)^{-1}.$$

For $\varphi \in D(A)$, the resolvent identities give

$$\begin{aligned} B_m \varphi &= (im + A - A)(A + im)^{-1} \varphi \\ &= \varphi - (A + im)^{-1} A \varphi \longrightarrow \varphi \quad \text{as } |m| \rightarrow \infty, \end{aligned}$$

since $\|(A + im)^{-1} A \varphi\| \leq |m|^{-1} \|A \varphi\|$. Moreover $\|B_m\| \leq 1$, so density and Lemma 5.1(ii) imply

$$\text{s-lim}_{|m| \rightarrow \infty} B_m = \mathbf{1}.$$

Define

$$A_m := B_m A B_{-m}.$$

This regularization has the following (very nice) properties:

- $A_m\varphi \rightarrow A\varphi$ for every $\varphi \in D(A)$.
- A_m is bounded and defined everywhere: B_{-m} maps $\mathcal{H}$ into $D(A)$, and AB_{-m} is an everywhere-defined closed operator, hence bounded by the closed graph theorem. Multiplication by the bounded B_m preserves boundedness.
- Since $B_m^* = B_{-m}$, we have $A_m^* = A_m$.

Since A_m is bounded, we can use the ordinary exponential series and then try to pass to the limit $m \rightarrow \infty$.

Step 2: construct the unitary group. Define

$$U_m(t) := e^{-iA_mt} := \sum_{k=0}^{\infty} \frac{(-itA_m)^k}{k!}.$$

This is well-defined because A_m is bounded. Each U_m is a SCUG, and the strong limit

$$U(t) := \text{s-lim}_{m \rightarrow \infty} U_m(t)$$

exists. See Assignment 2 for existence of this limit and for verification that the limit U is a SCUG generated by A . Uniqueness follows from Stone's theorem. $\square$

Definition. A possibly unbounded operator $B : D \subset \mathcal{H} \rightarrow \mathcal{H}$ and a bounded operator $C \in \mathcal{L}(\mathcal{H})$ *commute* if $CD \subset D$ and $CB\varphi = BC\varphi$ for every $\varphi \in D$. This is written as $CB \subset BC$.

How should we define commutation when both operators are unbounded? The general idea is to use their SCUGs or resolvents, which are natural ways of passing from unbounded operators to bounded operators. The two choices turn out to be equivalent (at least for self-adjoint operators).

Definition. Two self-adjoint operators B, C *commute* if one of the following conditions is satisfied:

- (i) $e^{-iCs}e^{-iBt} = e^{-iBt}e^{-iCs}$ for all $s, t \in \mathbb{R}$;
- (ii) $e^{-iCs}B \subset Be^{-iCs}$ for all $s \in \mathbb{R}$;
- (iii) $e^{-iCs}R_\mu(B) = R_\mu(B)e^{-iCs}$ for all $\mu \in \mathbb{C} \setminus \mathbb{R}$, $s \in \mathbb{R}$;
- (iv) $CR_\mu(B) \supset R_\mu(B)C$ for all $\mu \in \mathbb{C} \setminus \mathbb{R}$;
- (v) $R_\lambda(C)R_\mu(B) = R_\mu(B)R_\lambda(C)$ for all $\lambda, \mu \in \mathbb{C} \setminus \mathbb{R}$.

Proposition 5.5. *All the conditions (i)–(v) above are equivalent.*

Proof sketch. Pass from e^{-iBt} to B by differentiating on $D(B)$. Pass from the unitary group to the resolvent using (11). $\square$

Remark. Formal commutators “ $[B, C] = BC - CB$ ” can sometimes lead to wrong results for unbounded operators, although they are often a useful nonrigorous first attempt.

Definition. Consider the Schrödinger equation with $H = H^*$ and initial state ψ , and write $\psi(t) = e^{-iHt}\psi$.

- A self-adjoint operator A is called a *conserved quantity* if its expectation value does not change in time, that is

$$e^{-iHt}D(A) \subset D(A), \quad \langle \psi(t), A\psi(t) \rangle = \langle \psi, A\psi \rangle \quad \forall t \in \mathbb{R}, \psi \in D(A).$$

- A self-adjoint operator A generates a symmetry if

$$e^{-iAs}H \subset He^{-iAs} \quad \forall s \in \mathbb{R}.$$

The Noether theorem in classical mechanics shows that conserved quantities generate symmetries, and symmetries imply the existence of conserved quantities. The following is its quantum analogue. For example, translation invariance implies momentum conservation by the Noether theorem.

Theorem 5.6 (Quantum Noether theorem). *The following are equivalent:*

- (i) A is a conserved quantity;
- (ii) $e^{-iHt}A \subset Ae^{-iHt}$ for every $t \in \mathbb{R}$;
- (iii) A generates a symmetry.

Proof. The equivalence of (i) and (ii) follows from polarization of the expectation-value identity and unitarity. The equivalence with (iii) follows from Proposition 5.5. $\square$

Example. 1. Let $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ be real-valued and radial, i.e., $V(x) = f(|x|)$ for some function f . Then $H = -\Delta + V$ is *rotationally symmetric*: for $[U(R)\psi](x) = \psi(R^{-1}x)$ we have

$$U(R)H \subset HU(R).$$

The angular momentum operators L_1 , L_2 , and L_3 are therefore conserved quantities.

- 2. For $H = -\Delta$, the momentum operators $p_j = -i\partial/\partial x_j$, $j = 1, 2, 3$, are conserved. Check one of the equivalent conditions. In Fourier space this is easy, since the Fourier transform simultaneously diagonalizes $-\Delta$ and p_j .
- 3. For any $H = H^*$, the *total energy* H is a conserved quantity.

6 Scattering Theory [Teschl, Chapter 12 & Reed–Simon Vol. 3]

Scattering theory concerns the asymptotic dynamics of particles as $t \rightarrow \pm\infty$. It is a form of perturbation theory: a small perturbation leaves the qualitative behaviour unchanged.

In a typical scattering process, an incoming free particle encounters a potential, is deflected, and then moves freely towards infinity.

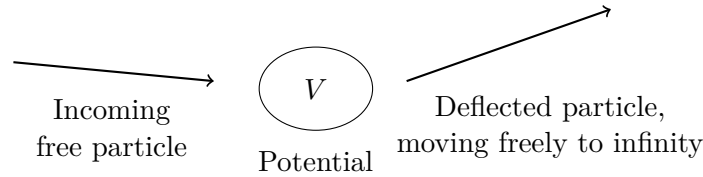


Figure 2: A particle comes in from infinity, scatters off the potential V , and flies away to infinity again.

Question. What is the relation between the incoming state and the outgoing state? We start by studying the free evolution (the behavior a long time before the particle reaches the potential, and a long time after the particles scattered). Later we will add the effect of the scattering.

Free evolution. Let

$$H_0 := -\frac{\Delta}{2} = \mathcal{F}^{-1} T_f \mathcal{F}, \quad f(p) := \frac{|p|^2}{2}.$$

Then

$$e^{-iH_0 t} = \mathcal{F}^{-1} e^{-iT_f t} \mathcal{F} = \mathcal{F}^{-1} T_{e^{-ift}} \mathcal{F}.$$

To check this, compute the generator on $D(H_0)$:

$$\begin{aligned} i \frac{d}{dt} \mathcal{F}^{-1} T_{e^{-ift}} \mathcal{F} \varphi \Big|_{t=0} &= \mathcal{F}^{-1} \left(i \frac{d}{dt} e^{-ift} \widehat{\varphi} \Big|_{t=0} \right) \\ &= \mathcal{F}^{-1} (f \widehat{\varphi}) = H_0 \varphi. \end{aligned}$$

We are going to calculate an explicit formula for $e^{-iH_0 t}$. For $\psi \in \mathcal{S}(\mathbb{R}^n)$,

$$\psi_t(x) := (e^{-iH_0 t} \psi)(x) = (\mathcal{F}^{-1}(e^{-ift} \widehat{\psi}))(x) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{ip \cdot x} e^{-i|p|^2 t/2} \widehat{\psi}(p) \, dp.$$

Theorem 6.1. For $\psi \in L^1(\mathbb{R}^n) \cap L^2(\mathbb{R}^n)$ and $t \neq 0$,

$$(e^{-iH_0 t} \psi)(x) = \frac{e^{-i\frac{\pi}{4} n \operatorname{sgn}(t)}}{(2\pi|t|)^{n/2}} \int_{\mathbb{R}^n} e^{i|x-y|^2/(2t)} \psi(y) \, dy.$$

Proof. First let $\psi \in \mathcal{S}(\mathbb{R}^n)$. Introducing a Gaussian regularization to obtain an integrable Fourier multiplier, by the convolution theorem we obtain

$$\begin{aligned} \psi_t(x) &= \lim_{\varepsilon \downarrow 0} \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{ip \cdot x} e^{-\frac{|p|^2}{2}(\varepsilon + it)} \widehat{\psi}(p) \, dp \\ &= \lim_{\varepsilon \downarrow 0} \mathcal{F}^{-1}(G_\varepsilon \widehat{\psi})(x) = \lim_{\varepsilon \downarrow 0} \frac{1}{(2\pi)^{n/2}} (\check{G}_\varepsilon * \psi)(x), \end{aligned}$$

where

$$G_\varepsilon(p) := e^{-\frac{|p|^2}{2}(\varepsilon + it)}, \quad \check{G}_\varepsilon(x) = \left(\frac{1}{\sqrt{\varepsilon + it}} \right)^n e^{-\frac{|x|^2}{2(\varepsilon + it)}}.$$

The last identity follows by completing the square in the exponent and then computing explicitly the integral along a trajectory in the complex plane. The complex square root is defined using the principal branch of the logarithm. In particular,

$$\sqrt{\varepsilon + it} \longrightarrow \sqrt{|t|} e^{i\frac{\pi}{4} \operatorname{sgn}(t)} \quad (\varepsilon \downarrow 0).$$

add details

For general $\psi \in L^1 \cap L^2$, approximate ψ by a sequence $\psi_k \in \mathcal{S}(\mathbb{R}^n)$. □

Corollary 6.2 (Dispersivity of the free evolution). Let $\psi_t = e^{-iH_0 t} \psi$.

(i) If $\psi \in L^1(\mathbb{R}^n) \cap L^2(\mathbb{R}^n)$, then

$$|\psi_t(x)| \leq \frac{1}{(2\pi|t|)^{n/2}} \|\psi\|_{L^1} \quad (t \neq 0).$$

(ii) For every $\psi \in L^2(\mathbb{R}^n)$, we have the weak convergence

$$\psi_t \rightharpoonup 0 \quad (t \rightarrow \pm\infty),$$

or equivalently, $\langle \varphi, \psi_t \rangle \rightarrow 0$ for every $\varphi \in L^2(\mathbb{R}^n)$.

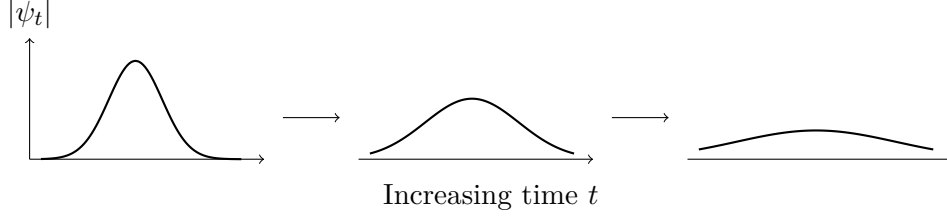


Figure 3: Sketch of $|\psi_t|$ according to the free Schrödinger evolution, from left to right at increasing time. The L^∞ norm tends to zero, whereas the L^2 norm is conserved by unitarity.

Proof. (i) Taking absolute values in Theorem 6.1 gives

$$|\psi_t(x)| \leq \frac{1}{(2\pi|t|)^{n/2}} \int_{\mathbb{R}^n} |\psi(y)| dy.$$

(ii) For $\varphi, \psi \in L^1 \cap L^2$ this follows immediately from (i). For general $\varphi, \psi \in L^2$, set

$$\varphi_N := \chi_{B_N(0)} \varphi, \quad \psi_N := \chi_{B_N(0)} \psi.$$

By rescaling, we may assume $\|\varphi\|_2, \|\psi\|_2 \leq 1$. We use an $\varepsilon/3$ argument: Let $\varepsilon > 0$. Choose N so large that $\|\varphi - \varphi_N\|_2 < \varepsilon/3$ and $\|\psi - \psi_N\|_2 < \varepsilon/3$. Since $\varphi_N, \psi_N \in L^1 \cap L^2$, there exists $T > 0$ such that $|t| > T$ implies $|\langle \varphi_N, \psi_{N,t} \rangle| < \varepsilon/3$. Hence

$$\begin{aligned} |\langle \varphi, \psi_t \rangle| &\leq |\langle \varphi - \varphi_N, \psi_t \rangle| + |\langle \varphi_N, \psi_t - \psi_{N,t} \rangle| + |\langle \varphi_N, \psi_{N,t} \rangle| \\ &\leq \|\varphi - \varphi_N\|_2 \|\psi\|_2 + \|\varphi_N\|_2 \|\psi - \psi_N\|_2 + |\langle \varphi_N, \psi_{N,t} \rangle| < \varepsilon. \end{aligned}$$

This completes the proof. $\square$

Definition. Let $H = H^*$ on $\mathcal{H} = L^2(\mathbb{R}^n)$, for example $H = H_0 + V$. A vector $\psi^+ \in \mathcal{H}$ is an *outgoing scattering state* if there exists $\psi \in \mathcal{H}$ such that

$$\|e^{-iHt}\psi^+ - e^{-iH_0t}\psi\| \longrightarrow 0 \quad (t \rightarrow +\infty).$$

We call ψ^+ *asymptotically free* and $e^{-iH_0t}\psi$ its *asymptotic state*. Equivalently,

$$\psi^+ = \lim_{t \rightarrow +\infty} e^{iHt} e^{-iH_0t} \psi.$$

Similarly, an *incoming scattering state* is a vector of the form

$$\psi^- = \lim_{t \rightarrow -\infty} e^{iHt} e^{-iH_0t} \psi.$$

Warning: The notation is inconsistent through the literature, for example Reed & Simon use ψ^+ for the limit $t \rightarrow -\infty$.

End of Lecture 8

Definition. A measurable function V belongs to $L^2_{\text{loc}}(\mathbb{R}^n)$ if $\chi_K V \in L^2(\mathbb{R}^n)$ for every compact set $K \subset \mathbb{R}^n$. Here χ_K is the indicator function of the set K .

Remark. The advantage of L^2_{loc} is that, while L^2 also imposes decay at infinity, L^2_{loc} only rules out excessively strong local singularities.

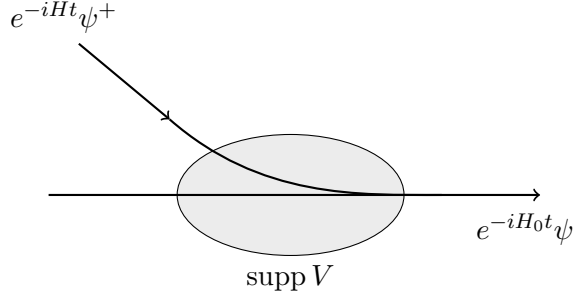


Figure 4: An asymptotically free state and its asymptotic state, represented by classical trajectories, in the case of a compactly supported potential.

Proposition 6.3. *Let $H = H_0 + V$ acting in the Hilbert space $L^2(\mathbb{R}^3)$, where $V \in L^2_{\text{loc}}(\mathbb{R}^3)$ is real-valued. Assume that there are $R > 0$, $\varepsilon > 0$, and $C > 0$ such that*

$$|V(x)| \leq \frac{C}{|x|^{1+\varepsilon}} \quad \text{for all } |x| > R.$$

Then the wave operators

$$\Omega_{\pm} := \text{s-lim}_{t \rightarrow \pm\infty} e^{iHt} e^{-iH_0t}$$

exist.

Remark. The Coulomb potential is excluded by this assumption. Its long range requires a modification of the wave operators.

Proof. Since $\|e^{iHt} e^{-iH_0t}\| = 1$, Lemma 5.1 shows that it suffices to prove existence of the limit on $\mathcal{S}(\mathbb{R}^3)$. Let $\varphi \in \mathcal{S}(\mathbb{R}^3)$ and set $\varphi(t) := e^{iHt} e^{-iH_0t} \varphi$.

We use *Cook's argument*, a useful method for comparing strongly continuous unitary groups. By the fundamental theorem of calculus

$$\varphi(t) = \varphi + \int_0^t \varphi'(s) \, ds.$$

The limit as $t \rightarrow +\infty$ exists if and only if the improper integral of $\varphi'(s)$ converges. It is sufficient that

$$\int_T^\infty \|\varphi'(s)\| \, ds < \infty$$

for some fixed lower bound T , chosen conveniently. By the product rule,

$$\varphi'(s) = e^{iHs} i(H - H_0) e^{-iH_0s} \varphi = i e^{iHs} V e^{-iH_0s} \varphi.$$

Here the domains must be checked: $D(H) = D(H_0) = H^2(\mathbb{R}^3)$ and the free evolution preserves $\mathcal{S}(\mathbb{R}^3) \subset H^2(\mathbb{R}^3)$. By unitarity it is sufficient to prove

$$\int_T^\infty \|V e^{-iH_0s} \varphi\| \, ds < \infty.$$

If $V \in L^2(\mathbb{R}^3)$, Corollary 6.2 gives

$$\|V e^{-iH_0s} \varphi\|_2 \leq \|V\|_2 \|e^{-iH_0s} \varphi\|_\infty \leq \frac{\|V\|_2 \|\varphi\|_1}{(2\pi|s|)^{3/2}},$$

which is integrable at infinity.

If $V \notin L^2$, a simple density argument is not enough. Instead, we split V in a time-dependent way:

$$V = V_2^t + V_\infty^t, \quad V_2^t := V \chi_{B_{|t|}(0)}, \quad V_\infty^t := V \chi_{\mathbb{R}^3 \setminus B_{|t|}(0)}.$$

For $|t| > R$,

$$\|V_\infty^t\|_\infty = \operatorname{ess\,sup}_{|x| \geq |t|} |V(x)| \leq \frac{C}{|t|^{1+\varepsilon}}.$$

Without loss of generality we may decrease ε so that $0 < \varepsilon < 1/2$. Using spherical coordinates,

$$\begin{aligned} \|V_2^t\|_2 &\leq \left(\int_{B_R(0)} |V(x)|^2 dx + \int_{B_{|t|}(0) \setminus B_R(0)} \frac{C^2}{|x|^{2(1+\varepsilon)}} dx \right)^{1/2} \\ &\leq (C_1 + C_2(|t|^{1-2\varepsilon} - R^{1-2\varepsilon}))^{1/2} \\ &\leq C_3 \max\{1, |t|^{1/2-\varepsilon}\}. \end{aligned}$$

The constants may change from line to line, but are independent of t . Hölder's inequality, dispersivity, and unitarity now imply

$$\begin{aligned} \|V e^{-iH_0 t} \varphi\|_2 &\leq \|V_2^t\|_2 \|e^{-iH_0 t} \varphi\|_\infty + \|V_\infty^t\|_\infty \|e^{-iH_0 t} \varphi\|_2 \\ &\leq C_\varphi \max\{1, |t|^{1/2-\varepsilon}\} |t|^{-3/2} + C_\varphi |t|^{-1-\varepsilon} \end{aligned}$$

for some constant C_φ that may depend on φ . This is integrable with respect to t at $+\infty$. The argument for $t \rightarrow -\infty$ is the same. $\square$

Theorem 6.4. *Let $H = H^*$ and $H_0 = -\Delta/2$ on $\mathcal{H} = L^2(\mathbb{R}^n)$. If the operators $\Omega_\pm$ exist, then:*

(a) $\Omega_\pm : \mathcal{H} \rightarrow \mathcal{H}$ are isometries: $\|\Omega_\pm \varphi\| = \|\varphi\|$ for all $\varphi \in \mathcal{H}$.

(They need not be surjective though.)

(b) Intertwining:

$$\Omega_\pm e^{-iH_0 t} = e^{-iH t} \Omega_\pm \quad (t \in \mathbb{R}).$$

(c) $\Omega_\pm H_0 \subset H \Omega_\pm$.

(d) $\sigma(H_0) \subset \sigma(H)$.

(e) If $H\varphi = E\varphi$, then $\varphi \perp \operatorname{ran} \Omega_\pm$.

Remark. Intertwining is useful to convert the full evolution into the easier free evolution. It is a property similar to unitary equivalence, which is not applicable here because $\Omega_\pm$ need not be invertible. Part (c) is the infinitesimal version of the intertwining identity.

Part (e) says that eigenstates are not asymptotically free: they are *bound states*.

Proof. (a) By unitarity,

$$\|\Omega_\pm \varphi\| = \lim_{t \rightarrow \pm\infty} \|e^{iH t} e^{-iH_0 t} \varphi\| = \|\varphi\|.$$

(b) For fixed t , substitute $s' = s + t$:

$$\Omega_\pm e^{-iH_0 t} \varphi = \lim_{s \rightarrow \pm\infty} e^{iH s} e^{-iH_0(s+t)} \varphi = \lim_{s' \rightarrow \pm\infty} e^{iH(s'-t)} e^{-iH_0 s'} \varphi = e^{-iH t} \Omega_\pm \varphi.$$

(c) For $\varphi \in D(H_0)$,

$$\frac{i}{\varepsilon} (e^{-iH\varepsilon} - \mathbf{1}) \Omega_\pm \varphi = \Omega_\pm \frac{i}{\varepsilon} (e^{-iH_0\varepsilon} - \mathbf{1}) \varphi \longrightarrow \Omega_\pm H_0 \varphi \quad (\varepsilon \rightarrow 0).$$

Thus $\Omega_{\pm}\varphi \in D(H)$ and $H\Omega_{\pm}\varphi = \Omega_{\pm}H_0\varphi$.

(d) Apply intertwining: Let $\lambda \in \rho(H) \cap \mathbb{R}$. For $\varphi \in D(H_0)$,

$$\begin{aligned} \|(H_0 - \lambda)\varphi\| &= \|\Omega_{\pm}(H_0 - \lambda)\varphi\| = \|(H - \lambda)\Omega_{\pm}\varphi\| \\ &\geq c\|\Omega_{\pm}\varphi\| = c\|\varphi\|, \quad \text{where } c := \|(H - \lambda)^{-1}\|^{-1} > 0. \end{aligned}$$

As in previous arguments, this implies $\lambda \in \rho(H_0)$: $\ker(H_0 - \lambda) = \{0\}$, so self-adjointness gives $\text{ran}(H_0 - \lambda)^{\perp} = \{0\}$. Its range is closed by the lower bound and closedness of H_0 , hence it is all of $\mathcal{H}$. The inverse is bounded by the same estimate. Since both spectra are real, the desired inclusion follows.

(e) Let $H\varphi = E\varphi$ and $\psi \in \mathcal{H}$. Then

$$\begin{aligned} \langle \varphi, \Omega_{\pm}\psi \rangle &= \lim_{t \rightarrow \pm\infty} \langle \varphi, e^{iHt}e^{-iH_0t}\psi \rangle \\ &= \lim_{t \rightarrow \pm\infty} e^{iEt} \langle \varphi, e^{-iH_0t}\psi \rangle = 0 \end{aligned}$$

by the dispersivity from Corollary 6.2. We used $e^{-iHt}\varphi = e^{-iEt}\varphi$, which can be verified by differentiating. $\square$

Lemma 6.5. *If $\Omega : \mathcal{H} \rightarrow \mathcal{H}$ is an isometry, then $\text{ran } \Omega$ is closed and*

$$\Omega^* = \begin{cases} \Omega^{-1} & \text{on } \text{ran } \Omega, \\ 0 & \text{on } (\text{ran } \Omega)^{\perp}. \end{cases}$$

Proof. Isometries are always injective: if $\Omega\psi_1 = \Omega\psi_2$, then

$$0 = \|\Omega(\psi_1 - \psi_2)\| = \|\psi_1 - \psi_2\|.$$

Thus $\Omega : \mathcal{H} \rightarrow \text{ran } \Omega$ is invertible. Its range is closed because a Cauchy sequence $(\Omega\psi_j)$ gives a Cauchy sequence (ψ_j) , whose limit is mapped to the limit of $(\Omega\psi_j)$. By polarization,

$$\langle \varphi, \psi \rangle = \frac{1}{4} \left(\|\varphi + \psi\|^2 - \|\varphi - \psi\|^2 - i\|\varphi + i\psi\|^2 + i\|\varphi - i\psi\|^2 \right),$$

so scalar products are invariant as well $\langle \psi, \varphi \rangle = \langle \Omega\psi, \Omega\varphi \rangle = \langle \psi, \Omega^*\Omega\varphi \rangle$. Hence $\Omega^*\Omega = \mathbf{1}$: Ω^* is a left inverse of Ω .

Is it also a right inverse? If $\varphi \in \text{ran } \Omega$, there exists $\eta \in \mathcal{H}$ such that $\varphi = \Omega\eta$. Then

$$\Omega\Omega^*\varphi = \Omega\Omega^*\Omega\eta = \Omega\eta = \varphi.$$

If $\varphi \in (\text{ran } \Omega)^{\perp}$, then $\langle \Omega\psi, \varphi \rangle = 0$ for every $\psi \in \mathcal{H}$, so $\Omega^*\varphi = 0$. $\square$

Definition (Asymptotic completeness). Let $H = H^*$ and $H_0 = -\Delta/2$ on $L^2(\mathbb{R}^n)$, and assume that $\Omega_{\pm}$ exist. Define the spaces of *scattering states* and *bound states* by

$$\mathcal{H}_{\pm} := \text{ran } \Omega_{\pm}, \quad \mathcal{H}_{\text{B}} := \overline{\text{span}\{\varphi : \varphi \text{ is an eigenvector of } H\}}.$$

We already know that $\mathcal{H}_{\pm}$ are closed and $\mathcal{H}_{\pm} \subset \mathcal{H}_{\text{B}}^{\perp}$. Under the assumptions of Proposition 6.3, one has also *asymptotic completeness*:

$$\mathcal{H}_{+} = \mathcal{H}_{\text{B}}^{\perp} = \mathcal{H}_{-}.$$

Thus every vector orthogonal to the bound states is asymptotically free.

Remark. Asymptotic completeness is a natural expectation: every vector decomposes into a bound component and a scattering component, with no further component. It is generally hard to prove, however, and there are counterexamples, see Figure 5.

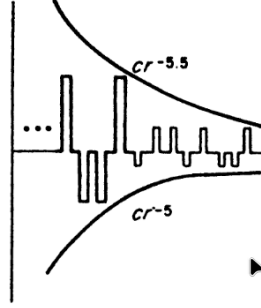


Figure 5: Pearson's potential: an example of a compactly supported, radial potential $V(x) = W(|x|)$ with increasingly narrow, singular oscillations near the origin. The envelopes in the sketch characterize the amplitudes of the bumps. This potential is an example where asymptotic completeness does not hold. See [Reed–Simon Vol. 3, Chapter XI.4] for the details. Among potentials without compact support there are also less pathological examples.

End of Lecture 9

In physics, scattering is described through probabilities of transitions from a specified incoming asymptotic state to a specified outgoing asymptotic state. These probabilities are given by matrix elements of the so-called S -matrix. The following definition makes this precise.

Definition (Scattering operator). Let $\alpha, \beta \in \mathcal{H}$ be normalized. Consider incoming asymptotics $e^{-iH_0 t} \alpha$. What is the probability of observing outgoing asymptotics $e^{-iH_0 t} \beta$? The incoming condition is

$$\|e^{-iHt} \varphi - e^{-iH_0 t} \alpha\| \longrightarrow 0 \quad (t \rightarrow -\infty), \quad \text{so } \varphi = \Omega_- \alpha.$$

By the quantum-mechanical probability rule, the probability to find $e^{-iH_0 t} \beta$ for $t \rightarrow +\infty$ is

$$\begin{aligned} P &= \lim_{t \rightarrow +\infty} \left| \langle e^{-iH_0 t} \beta, e^{-iHt} \varphi \rangle \right|^2 = \lim_{t \rightarrow +\infty} \left| \langle e^{iHt} e^{-iH_0 t} \beta, \Omega_- \alpha \rangle \right|^2 \\ &= |\langle \Omega_+ \beta, \Omega_- \alpha \rangle|^2 = |\langle \beta, \Omega_+^* \Omega_- \alpha \rangle|^2. \end{aligned}$$

The operator

$$S := \Omega_+^* \Omega_-$$

is called the *scattering operator* or *S-matrix*. If asymptotic completeness holds, then S is unitary.

Proofs of asymptotic completeness. Teschl presents Enss's proof for operators $H = -\Delta/2 + V$. For N -body systems, asymptotic completeness was proved much later by Sigal and Soffer using an abstract method, and by Graf in 1990 using a more instructive method.

In the lectures we prove only the simplest case: the potential is so weak that there are no bound states at all. In this case the whole Hilbert space consists of scattering states. In fact, the following theorem shows that in three dimensions, sufficiently weak potentials have no bound states. (This fails in dimensions one and two: attractive potentials can have bound states at arbitrarily small coupling — to be proven later. For the moment, check which part of the proof of Theorem 6.6 fails in one and two dimensions!)

Theorem 6.6. Let $H_0 = -\Delta/2$ on $L^2(\mathbb{R}^3)$, let $\tilde{V} \in L^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ be real-valued, and let $H = H_0 + \lambda \tilde{V}$ with $\lambda \in \mathbb{R}$. Then the wave operators $\Omega_\pm$ exist. Moreover, for $|\lambda|$ sufficiently small,

$$\text{ran } \Omega_\pm = L^2(\mathbb{R}^3).$$

Proof. Since $\tilde{V} \in L^1 \cap L^\infty \subset L^2$, existence follows from the L^2 case of Cook's argument, see Proposition 6.3.

To prove $\text{ran } \Omega_+ = L^2(\mathbb{R}^3)$, we show that

$$\lim_{t \rightarrow +\infty} e^{iH_0 t} e^{-iHt} \varphi$$

exists for every $\varphi \in L^2(\mathbb{R}^3)$. Indeed, if the limit is γ , then

$$e^{iHt} e^{-iH_0 t} \gamma \longrightarrow \varphi, \quad \text{so } \Omega_+ \gamma = \varphi.$$

(This is the general principle of constructing the inverse wave operator; you consider the analogue of existence of the wave operator but with H_0 and H exchanged. If present the bound-state subspace is to be excluded.) By Lemma 5.1 and unitarity, for existence of the strong limit it is sufficient to consider vectors in a dense subset, $\varphi \in \mathcal{S}(\mathbb{R}^3)$.

Set $V := \lambda \tilde{V}$,

$$V(t) := e^{iH_0 t} V e^{-iH_0 t}, \quad \varphi(t) := e^{iH_0 t} e^{-iHt} \varphi.$$

Differentiating gives

$$\frac{d}{dt} \varphi(t) = e^{iH_0 t} i(H_0 - H) e^{-iHt} \varphi = -iV(t)\varphi(t).$$

Integration yields Duhamel's formula/the interaction picture:

$$\varphi(t) = \varphi - i \int_0^t V(t_1) \varphi(t_1) dt_1.$$

Insert the same formula into the right-hand side and iterate. The first iteration gives

$$\varphi(t) = \varphi - i \int_0^t V(t_1) \varphi dt_1 + (-i)^2 \int_0^t dt_1 \int_0^{t_1} dt_2 V(t_1) V(t_2) \varphi(t_2).$$

After N iterations,

$$\begin{aligned} \varphi(t) &= \varphi + \sum_{k=1}^N (-i)^k \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{k-1}} dt_k V(t_1) \cdots V(t_k) \varphi + \mathcal{R}_{N+1}(t), \\ \mathcal{R}_{N+1}(t) &:= (-i)^{N+1} \int_0^t dt_1 \cdots \int_0^{t_N} dt_{N+1} V(t_1) \cdots V(t_{N+1}) \varphi(t_{N+1}). \end{aligned}$$

For fixed $t \geq 0$, unitarity and boundedness of V imply

$$\|\mathcal{R}_{N+1}(t)\|_2 \leq \frac{t^{N+1}}{(N+1)!} \|V\|_\infty^{N+1} \|\varphi\|_2 \longrightarrow 0 \quad (N \rightarrow \infty).$$

Thus the full interacting evolution disappears, leaving only the free evolution in $V(t)$. We obtain the *Dyson series*

$$\varphi(t) = \varphi + \sum_{k=1}^{\infty} \varphi_k(t), \quad \varphi_k(t) := (-i)^k \int_0^t dt_1 \cdots \int_0^{t_{k-1}} dt_k V(t_1) \cdots V(t_k) \varphi.$$

If

$$C_k := \int_0^\infty dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{k-1}} dt_k \|V(t_1) \cdots V(t_k) \varphi\|_2 < \infty,$$

then $\lim_{t \rightarrow +\infty} \varphi_k(t)$ exists. If also $\sum_{k=1}^{\infty} C_k < \infty$, the Dyson series converges uniformly in $t \geq 0$. We may then exchange the limit $t \rightarrow +\infty$ and the summation of the series:

$$\lim_{t \rightarrow +\infty} \varphi(t) = \varphi + \sum_{k=1}^{\infty} \lim_{t \rightarrow +\infty} \varphi_k(t).$$

So it remains to estimate C_k . By unitarity and a change of variables,

$$\begin{aligned}\|V(t_1) \cdots V(t_k)\varphi\|_2 &= \|Ve^{-iH_0(t_1-t_2)}Ve^{-iH_0(t_2-t_3)} \cdots Ve^{-iH_0t_k}\varphi\|_2 \\ &= \|Ve^{-iH_0s_1}Ve^{-iH_0s_2} \cdots Ve^{-iH_0s_k}\varphi\|_2,\end{aligned}$$

where $s_1 = t_1 - t_2, \dots, s_{k-1} = t_{k-1} - t_k, s_k = t_k$.

This is a linear substitution of the integration variables, we find the Jacobi determinant by

$$\begin{pmatrix} s_1 \\ s_2 \\ \vdots \\ s_{k-1} \\ s_k \end{pmatrix} = \underbrace{\begin{pmatrix} 1 & -1 & 0 & \cdots & 0 \\ 0 & 1 & -1 & \cdots & 0 \\ \vdots & & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 1 & -1 \\ 0 & \cdots & 0 & 0 & 1 \end{pmatrix}}_J \begin{pmatrix} t_1 \\ t_2 \\ \vdots \\ t_{k-1} \\ t_k \end{pmatrix}, \quad \det J = 1.$$

So the change of variables is bijective and preserves the measure/volume element. Therefore

$$C_k = \int_0^\infty ds_1 \cdots \int_0^\infty ds_k \|Ve^{-iH_0s_1} \cdots Ve^{-iH_0s_k}\varphi\|_2.$$

Factor the potential as

$$V = V_1V_2, \quad V_1 := \operatorname{sgn}(V)|V|^{1/2}, \quad V_2 := |V|^{1/2}.$$

Since $V \in L^1 \cap L^\infty$, both V_1, V_2 belong to $L^2 \cap L^\infty$. Consequently,

$$\|Ve^{-iH_0s_1} \cdots Ve^{-iH_0s_k}\varphi\|_2 \leq \|V_1\|_\infty \prod_{j=1}^{k-1} \|V_2e^{-iH_0s_j}V_1\|_{\text{op}} \|V_2e^{-iH_0s_k}\varphi\|_2. \quad (15)$$

We now estimate these operator norms.

For small s , unitarity gives, for every $\psi \in L^2$,

$$\|V_2e^{-iH_0s}V_1\psi\|_2 \leq \|V_2\|_\infty \|e^{-iH_0s}V_1\psi\|_2 \leq \|V_2\|_\infty \|V_1\psi\|_2 \leq \|V_2\|_\infty \|V_1\|_\infty \|\psi\|_2.$$

For large s , dispersivity and Hölder's inequality/Cauchy-Schwartz inequality give

$$\begin{aligned}\|V_2e^{-iH_0s}V_1\psi\|_2 &\leq \|V_2\|_2 \|e^{-iH_0s}V_1\psi\|_\infty \\ &\leq \|V_2\|_2 |s|^{-3/2} \|V_1\psi\|_1 \leq \|V_2\|_2 |s|^{-3/2} \|V_1\|_2 \|\psi\|_2.\end{aligned}$$

(We have dropped the harmless factor $(2\pi)^{-3/2} \leq 1$ from the dispersivity estimate.) Combining both bounds,

$$\|V_2e^{-iH_0s}V_1\|_{\text{op}} \leq (\|V_1\|_\infty \|V_2\|_\infty + \|V_1\|_2 \|V_2\|_2) \min\{1, |s|^{-3/2}\}.$$

Similarly for the last factor in (15):

$$\|V_2e^{-iH_0s}\varphi\|_2 \leq (\|V_2\|_\infty \|\varphi\|_2 + \|V_2\|_2 \|\varphi\|_1) \min\{1, |s|^{-3/2}\}.$$

The L^1 norm of φ is finite because $\varphi \in \mathcal{S}(\mathbb{R}^3)$. Writing

$$A := \|V_1\|_\infty \|V_2\|_\infty + \|V_1\|_2 \|V_2\|_2, \quad B_\varphi := \|V_2\|_\infty \|\varphi\|_2 + \|V_2\|_2 \|\varphi\|_1,$$

we obtain

$$C_k \leq \|V_1\|_\infty A^{k-1} B_\varphi \left(\int_0^\infty \min\{1, s^{-3/2}\} ds \right)^k.$$

Each V_j contributes a factor $|\lambda|^{1/2}$, so the total power appearing in C_k is $|\lambda|^k$. Thus, for suitable finite constants independent of k and λ ,

$$C_k \leq |\lambda|^k C_1(\tilde{V})^k C_\varphi \left(\int_0^\infty \min\{1, s^{-3/2}\} ds \right)^k = (|\lambda| C_2(\tilde{V}))^k C_\varphi.$$

Here we used that the time integral is finite (thanks to being in three-dimensional space). If $|\lambda|$ is so small that $|\lambda| C_2(\tilde{V}) < 1$, the series $\sum_{k=1}^\infty C_k$ is bounded by a convergent geometric series.

The analogous argument at $-\infty$ gives the same conclusion for Ω_- . □

End of Lecture 10
