

Mathematical Methods of Quantum Mechanics

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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 $x \neq 0$,

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

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

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

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. □

op:resolvent

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.

lem:neumann

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 $S(\mathbf{1} - T) = \mathbf{1}$. □

thm:analytic

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
