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MATHEMATISCHES INSTITUT

Functional Analysis II

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Lecture Notes WS 2019/2020[1]

[1]These lecture notes are a draft and likely to contain mistakes. Please report any typos, errors, or suggestions to `lampart@math.lmu.de`. Version of January 30, 2020

Contents

1 Linear Operators On Banach Spaces

1.1 Basic Notions

Definition 1.1. A generalised linear operator from Banach spaces X to Y is a pair $A, D(A)$ where

- $D(A) \subset X$ is a linear subspace, and
- $A : D(A) \to Y$ is a linear map.

A linear operator is *densely defined* if $D(A)$ is dense in X.

We will usually consider operators that are densely defined. If $D(A)$ where not dense in X one could just restrict to $\tilde{X} = \overline{D(A)}$ and obtain a densely defined operator, so this is not really a restriction.

Examples 1.2.

a) Let $X = Y = \ell^2$, and

$$D(A) = c_{00} = \{x \in \ell^2 : x_n \neq 0 \text{ for finitely many } n\}. \tag{1.1}$$

Then for *any* sequence $(a_n)_{n\in\mathbb{N}} \in \mathbb{C}^{\mathbb{N}}$, $(Ax)_n = a_n x_n$ is a densely defined operator.

b) Let $X = L^2([0,1])$, $Y = \mathbb{C}$, $D(A) = C([0,1])$ and $Af := f(0)$.

Definition 1.3. A densely defined operator $B, D(B)$ extends $A, D(A)$, if $D(A) \subset D(B)$ and $B|_{D(A)} = A$. We write $A \subset B$.

Definition 1.4. A densely defined operator is called *bounded* if there exists $M \geq 0$ such that

$$\|Ax\|_Y \leq M \|x\|_X \tag{1.2}$$

for all $x \in D(A)$.

Remark 1.5. A is bounded iff A is continuous [FA1, Thm 2.29].

Definition 1.6. Let X, Y be Banach spaces. For a bounded operator A from $D(A) = X$ to Y define the *operator norm*

$$\|A\|_{X\to Y} := \sup_{0\neq x\in X} \frac{\|Ax\|_Y}{\|x\|_X}. \tag{1.3}$$

The Banach space bounded linear maps from X to Y with this norm is denoted by $\mathrm{B}(X, Y)$. The space $\mathrm{B}(X, X)$ is denoted by $\mathrm{B}(X)$.

Proposition 1.7. *If $A, D(A)$ is densely defined and bounded there exists a unique continuous extension $\overline{A}$ with $D(\overline{A}) = X$, i.e. $\overline{A} \in \mathrm{B}(X)$.*

Proof. Let $x \in X$ and $x_n \to x$ be a sequence in $D(A)$ converging to x. By linearity and boundedness Ax_n is Cauchy in Y, so it has a limit y (with $\|y\| \leq M$), and this is unique. Define $\overline{A}x := y$. □

Recall the graph of $A, D(A)$:

$$\mathscr{G}(A) := \{(x, Ax) : x \in D(A)\} \subset D(A) \times Y \subset X \times Y. \tag{1.4}$$

Since A is linear, $\mathscr{G}(A)$ is a linear subspace of $X \oplus Y$.

Definition 1.8. The operator $A, D(A)$ is

- *closed* if the set $\mathscr{G}(A)$ is closed in $X \times Y$ (i.e. for any sequence $(x_n)_{n\in\mathbb{N}}$ in $D(A)$ such that x_n converges to $x \in X$ and Ax_n converges to $y \in Y$, it holds that $x \in D(A)$ and $Ax = y$);
- *closable* if it has a closed extension.

Remarks 1.9.

a) A is closable iff $\overline{\mathscr{G}(A)}$ is the graph of an operator $\overline{A}, D(\overline{A})$. $\overline{A}$ is called the *closure* of A. It is the minimal closed extension:

$$D(\overline{A}) = \bigcap_{\substack{A\subset B \\ B \text{ closed}}} D(B). \tag{1.5}$$

b) If A is closed and $D(A) = X$ then A is bounded, by the Closed Graph Theorem [FA1, Thm.4.13].

Proposition 1.10. *Let $A, D(A)$ be closed and define the graph norm on $D(A)$ by $\|x\|_{D(A)} := \|x\|_X + \|Ax\|_Y$. Then $(D(A), \|\cdot\|_{D(A)})$ is a Banach space and $A : D(A) \to Y$ is continuous w.r.t. this norm. Conversely, If $(D(A), \|\cdot\|_{D(A)})$ is complete then A is closed.*

Proof. $\|\cdot\|_{D(A)}$ defines a norm by linearity of A. Clearly $D(A)$, with this norm, embeds continuously into X. $D(A)$ is complete with this norm, since $(x_n)_\mathbb{N}$ Cauchy in $D(A)$ $\iff$ $(x_n)_\mathbb{N}$ Cauchy in X and $(Ax_n)_\mathbb{N}$ Cauchy in Y $\overset{A \text{ closed}}{\Longrightarrow}$ $x_n \to x \in D(A)$. Continuity of $A : D(A) \to Y$ follows from completeness by the Closed Graph Theorem [FA1, Thm.4.13]. The converse follows from this continuity. □

Examples 1.11.

a) The operator of 1.2a) is always closable, with

$$D(\overline{A}) = \{x \in \ell^2 : (a_n x_n)_\mathbb{N} \in \ell^2\}, \tag{1.6}$$

since the graph norm is equivalent to $\left(\sum_n (1 + |a_n|^2) x_n^2\right)^{1/2}$, which is clearly complete.

b) The operator of 1.2b) is not closable, since $\overline{\mathscr{G}(A)} = L^2([0,1]) \times \mathbb{C}$.

1.2 Resolvent And Spectrum

In this section $A, D(A)$ is a densely defined operator on X, i.e. $X = Y$ and X is a Banach space over $\mathbb{C}$.

Definition 1.12. The set

$$\rho(A) := \{z \in \mathbb{C} : A - z : D(A) \to X \text{ is bijective, and } (A-z)^{-1} \text{ is bounded}\} \tag{1.7}$$

is called the *resolvent set* of A. For $z \in \rho(A)$ the operator

$$R_z(A) := (A-z)^{-1} \tag{1.8}$$

is called the *resolvent*.

Definition 1.13. The complement $\sigma(A) := \mathbb{C} \setminus \rho(A)$ is the *spectrum* of A. We have $\sigma(A) = \sigma_p(A) \dot{\cup} \sigma_c(A) \dot{\cup} \sigma_r(A)$, with

- The *point spectrum*

$$\sigma_p(A) := \{z \in \mathbb{C} : A - z \text{ is not one-to-one}\}$$

- The *continuous spectrum*

$$\sigma_c(A) := \{z \in \mathbb{C} : A - z \text{ is one-to-one, } \operatorname{ran}(A-z) \neq X \text{ but } \overline{\operatorname{ran}(A-z)} = X\}$$

- The *residual spectrum*

$$\sigma_r(A) := \{z \in \mathbb{C} : A - z \text{ is one-to-one but } \overline{\operatorname{ran}(A-z)} \neq X\}.$$

Theorem 1.14. *Let $A, D(A)$ be densely defined on X. The resolvent set $\rho(A)$ is open, and $R_z(A)$ defines an analytic function $\rho(A) \to \mathrm{B}(X)$. Moreover, for $z, w \in \rho(A)$*

$$R_z(A) - R_w(A) = (z-w) R_z(A) R_w(A), \tag{1.9}$$

in particular $R_z(A)$ and $R_w(A)$ commute.

Proof. Like for $A \in \mathrm{B}(X)$, [FA1, Thm.5.22]. $\square$

Example 1.15. Take $X = \ell^2$ and $(Ax)_n = a_n x_n$ as in Example 1.2a). Then $\sigma(A) = \mathbb{C}$, since $\operatorname{ran}(A-z) \subset c_{00} \neq X$. However $\sigma(\overline{A}) = \sigma_p(\overline{A}) = \overline{\cup_n \{a_n\}}$, since for z not an accumulation point of $(a_n)_{\mathbb{N}}$ the formula

$$\Big(R_z(\overline{A})x\Big)_n = (a_n - z)^{-1} x_n \tag{1.10}$$

defines the resolvent. Thus $\sigma(A)$ depends strongly on $D(A)$!

Remarks 1.16.

- If $A \in \mathrm{B}(X)$ then $\sigma(A) \neq \emptyset$. However, there are unbounded operators with empty spectrum, and thus $\rho(A) = \mathbb{C}$ can occur (exercise).
- If $\rho(A) \neq \emptyset$ then A is closed, since $R_z(A) \in \mathrm{B}(X) \implies (A-z)^{-1}$ closed $\implies A$ closed.

1.3 Operators on Hilbert Spaces, Adjoints and Symmetry

We now look at the special case where $X = \mathscr{H}$ is a Hilbert space (over $\mathbb{C}$), that is, it has a scalar product $\langle\cdot,\cdot\rangle : \mathscr{H} \times \mathscr{H} \to \mathbb{C}$ that defines its norm via $\|\varphi\| = \sqrt{\langle\varphi,\varphi\rangle}$.

The Hilbert space structure allows us to define the adjoint operator, which should satisfy the formula

$$\langle\varphi, A\psi\rangle = \langle A^*\varphi, \psi\rangle. \tag{1.11}$$

The question is for what vectors φ, ψ. For $A \in \mathrm{B}(\mathscr{H})$, we can take any $\varphi, \psi \in \mathscr{H}$ and this formula defines $A^* \in \mathrm{B}(\mathscr{H})$ (by the Riesz Representation Theorem). For unbounded A we certainly want $\psi \in D(A)$, but we also need to decide what $D(A^*)$ should be. The following definition chooses $D(A^*)$ in a maximal way so that the formula holds.

Definition 1.17. Let $A, D(A)$ be densely defined on $\mathscr{H}$. We define the *adjoint* A^*, $D(A^*)$ by

$$\begin{aligned} D(A^*) &:= \{\varphi \in \mathscr{H} : \exists \eta_\varphi \in \mathscr{H} \forall \psi \in D(A) : \langle\varphi, A\psi\rangle = \langle\eta_\varphi, \psi\rangle\}, \\ A^* &: D(A^*) \to \mathscr{H}, \\ A^*\varphi &:= \eta_\varphi \end{aligned}$$

Remarks 1.18.

- $A^*\varphi$ is well-defined, since if η_φ exists it is unique, by

$$\forall \psi \in D(A) : \langle\eta_\varphi - \tilde{\eta}_\varphi, \psi\rangle = 0 \implies \eta_\varphi = \tilde{\eta}_\varphi, \tag{1.12}$$

  because $D(A)$ is dense.

- The requirement on $D(A^*)$ can be read as: $\varphi \in D(A^*) \Leftrightarrow$ the linear functional $\langle\varphi, A\psi\rangle$ on $D(A)$ extends continuously to $\mathscr{H}$, since then η exists by the Riesz Representation Theorem. From this it is immediate that for $A \in \mathrm{B}(\mathscr{H})$, $D(A^*) = \mathscr{H}$ and $A^* \in \mathrm{B}(\mathscr{H})$.

- $A \subset B \implies B^* \subset A^*$, since there are fewer conditions to be met in $D(A^*)$, and for $\varphi \in D(B^*) \subset D(A^*)$, $\psi \in D(A) \subset D(B)$

$$\langle B^*\varphi, \psi\rangle = \langle\varphi, B\psi\rangle \overset{A\subseteq B}{=} \langle\varphi, A\psi\rangle = \langle A^*\varphi, \psi\rangle. \tag{1.13}$$

- $D(A^*)$ is *not* always dense.

- *If* $D(A^*)$ is dense we can define $A^{**} = (A^*)^*$.

Theorem 1.19. *Let A, $D(A)$ be densely defined on $\mathscr{H}$.*

a) A^* is closed.

b) $D(A^*)$ is dense iff A is closable.

c) If A is closable then $\overline{A} = A^{**}$ and $A^* = (\overline{A})^*$.

Proof. a) Let $(\varphi_n, \eta_{\varphi_n})$ be in $\mathscr{G}(A^*)$ that converges to $(\varphi, \eta) \in \mathscr{H} \times \mathscr{H}$. Then for all $\psi \in D(A)$:

$$\underbrace{\langle \varphi_n, A\psi \rangle}_{\to \langle \varphi, A\psi \rangle} = \underbrace{\langle \eta_{\varphi_n}, \psi \rangle}_{\to \langle \eta, \psi \rangle},$$

so $\varphi \in D(A^*)$ and $A^*\varphi = \eta$.

b) If A^* is densely defined, then A^{**} extends A, because for every $\varphi \in D(A)$ there exists $\eta = A\varphi \in \mathscr{H}$ such that

$$\forall \psi \in D(A^*) : \langle \varphi, A^*\psi \rangle = \langle \eta, \psi \rangle. \tag{1.14}$$

By a), A^{**} is closed and thus A is closable.

Assume now that A^* is not densely defined and consider $\overline{\mathscr{G}(A)} = (\mathscr{G}(A)^\perp)^\perp$. Note that

$$\mathscr{G}(A^*) = \{(\varphi, \eta) \in \mathscr{H} \times \mathscr{H} : \forall \psi \in D(A) : \langle \varphi, A\psi \rangle - \langle \eta, \psi \rangle = 0\}, \tag{1.15}$$

and since $\langle \varphi, A\psi \rangle - \langle \eta, \psi \rangle = \langle (-\eta, \varphi), (\psi, A\psi) \rangle_{\mathscr{H} \oplus \mathscr{H}}$,

$$\begin{aligned} &\mathscr{G}(A)^\perp \langle \varphi, A\psi \rangle = 0\} \\ &= \{(-A^*\varphi, \varphi) : \varphi \in D(A^*)\}. \end{aligned} \tag{1.16}$$

Now let $0 \neq \xi \in D(A^*)^\perp$, and observe that $(0, \xi) \in (\mathscr{G}(A)^\perp)^\perp$, but certainly not in the graph of any linear operator.

c) We have by (1.15),(1.16)

$$\mathscr{G}(A^{**}) = \{(\varphi, \eta) \in \mathscr{H} \times \mathscr{H} : \forall \psi \in D(A^*) : \langle \eta, \psi \rangle - \langle \varphi, A^*\psi \rangle = 0\} = (\mathscr{G}(A)^\perp)^\perp, \tag{1.17}$$

so $\overline{A} = A^{**}$. This, together with a), implies

$$\overline{A}^* = A^{***} = \overline{A^*} \overset{a)}{=} A^*. \tag{1.18}$$

□

Definition 1.20. A densely defined operator $A, D(A)$ on $\mathscr{H}$ is

- *symmetric* $:\Leftrightarrow A \subset A^*$.
- *self-adjoint* $:\Leftrightarrow A^* = A$.

Remarks 1.21.

a) In terms of the identity

$$\langle \varphi, A\psi \rangle = \langle A^* \varphi, \psi \rangle \stackrel{!}{=} \langle A\varphi, \psi \rangle \tag{1.19}$$

symmetry means that this holds for all $\varphi, \psi \in D(A)$, while self-adjointness means that additionally $D(A^*) = D(A)$.

b) If A is symmetric, it is closable, since A^* is a closed extension. If A is self-adjoint, then $A = A^*$ is closed.

Definition 1.22. Let $A, D(A)$ be symmetric *essentially self-adjoint* if $\overline{A}$ is self-adjoint.
If $A, D(A)$ is symmetric and closed, a subspace $C \subset D(A)$ such that $\overline{A|_C} = A$ is called a *core* for A.

Corollary 1.23. *Let $A, D(A)$ be symmetric. Then A is essentially self-adjoint iff A^* is symmetric. If A has any self-adjoint extension $A \subset B$, then $D(\overline{A}) \subset D(B) \subset D(A^*)$.*

Proof. By Theorem 1.19, A symmetric $\implies$ A closable, and $\overline{A} = A^{**} \subset A^*$ (since A^* is a closed extension of A). Consequently A is essentially self-adjoint iff $A^* \subset A^{**}$. By the same argument $\overline{A} \subset B$, and then $B = B^* \subset A^*$. □

Examples 1.24.

a) Take $\mathscr{H} = \ell^2$ and $(Ax)_n = a_n x_n$ as in Example 1.2a). Then A is symmetric iff $(a_n)_{\mathbb{N}}$ is real. In this case, A is essentially self-adjoint, since $\langle x, Ay \rangle = \sum_{n\in\mathbb{N}} \overline{x_n} a_n y_n$ is a continuous linear functional of $y \in \ell^2$ iff $(a_n x_n)_{\mathbb{N}} \in \ell^2$ (compare Remark 1.11).

b) Let $\mathscr{H} = L^2(\mathbb{R})$, $D(P) = C_0^1(\mathbb{R})$, $P = -i\frac{\mathrm{d}}{\mathrm{d}x}$.
   - P is symmetric: integration by parts;
   - We will later determine P^* and show that P is essentially self-adjoint (Fourier transform).

c) Let $\mathscr{H} = L^2((0,1))$, $D(P_0) = C_0^1((0,1))$, $P_0 = -i\frac{\mathrm{d}}{\mathrm{d}x}$.
   - P_0 is symmetric: integration by parts - there are no boundary terms since $f(0) = f(1) = 0$ for $f \in D(P_0)$.
   - P_0 is not self-adjoint, since $C^1([0,1]) \subset D(P_0^*)$;
   - P_0 is not essentially self adjoint: For $f \in C^1([0,1])$ we have (using the Cauchy-Schwarz inequality)

$$\begin{aligned} |f(0)|^2 &= \int_0^1 |f(0)|^2 \mathrm{d}x = \int_0^1 \left| f(x) - \int_0^x f'(y)\mathrm{d}y \right|^2 \mathrm{d}x \\ &\leq 2\left(\int_0^1 |f(x)|^2 \mathrm{d}x + \int_0^1 |f'(x)|^2 \mathrm{d}x \right) = 2\left(\|f\|_{L^2}^2 + \|P_0^* f\|_{L^2}^2 \right). \end{aligned}$$

   So if $f_n \to f \in D(\overline{P_0}) \cap C^1([0,1]) \subset D(P_0^*)$, then

$$|f(0)|^2 = |f(0) - f_n(0)|^2 \leq 2\,\|f - f_n\|_{D(\overline{P_0})}^2 \,, \tag{1.20}$$

   and thus $f(0) = 0$. Consequently, $D(\overline{P_0}) \neq D(P_0^*)$.

Remark 1.25. We now have a first picture of what can go wrong with self-adjointness. If $D(A)$ is chosen very small, then symmetry will be easy to check, but $D(A^*)$ will be large, so that A^* will no longer be symmetric. If on the other hand $D(A)$ is “too large”, then $D(A)$ might no longer be symmetric (boundary terms).

2 The Fourier Transform

The Fourier transform is an extremely useful tool that will give us many non-trivial examples of operators whose properties (closedness, self-adjointness) and spectrum can easily be established.

2.1 The Fourier Transform on $L^2(\mathbb{R}^d)$

We want to define the Fourier transform of $f \in L^2(\mathbb{R}^d)$, which formally is given by the integral formula

$$\hat{f}(p) = (\mathscr{F} f)(p) \text{``=''} \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \mathrm{e}^{-\mathrm{i}p\cdot x} f(x) \mathrm{d}x. \tag{2.1}$$

However, the integral only converges for $f \in L^1$. Our strategy will be to define $\mathscr{F}$ by the integral formula on a dense subspace of $L^2(\mathbb{R}^d)$, where manipulations of the formula will be easy to justify, and then prove that it has a unique extension to the whole of L^2.

For $\alpha = (\alpha_1 \ldots, \alpha_d) \in \mathbb{N}^d$ denote

$$|\alpha| = \sum_{i=1}^d \alpha_i, \tag{2.2}$$

and

$$\partial_x^\alpha := \prod_{i=1}^d \frac{\partial^{\alpha_i}}{\partial x_i^{\alpha_i}} = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}} \tag{2.3}$$

and for $x \in \mathbb{R}^d$

$$x^\alpha := \prod_{i=1}^d x_i^{\alpha_i} = x_1^{\alpha_1} \cdot \cdots \cdot x_d^{\alpha_d}. \tag{2.4}$$

Definition 2.1. The Schwartz space is

$$\mathscr{S}(\mathbb{R}^d) := \left\{ f \in C^\infty(\mathbb{R}^d) : \forall \alpha, \beta \in \mathbb{N}^d \sup_{x\in\mathbb{R}^d} |x^\alpha \partial_x^\beta f(x)| < \infty \right\}, \tag{2.5}$$

equipped with the coarsest topology such that the maps

$$f \mapsto \|f\|_{\alpha,\beta} := \sup_{x\in\mathbb{R}^d} |x^\alpha \partial_x^\beta f(x)| \tag{2.6}$$

are continuous for every $\alpha, \beta \in \mathbb{N}^d$.

Examples 2.2.

- e^{-x^2},
- $\frac{1}{\cosh x} = \frac{2}{e^x + e^{-x}}$,
- $C_0^\infty(\mathbb{R}^d) \subset \mathscr{S}(R^d)$.

Proposition 2.3.

a) For all $\alpha, \beta \in \mathbb{N}^d$, $\|\cdot\|_{\alpha,\beta}$ defines a semi-norm on $\mathscr{S}(\mathbb{R}^d)$.

b) A sequence $(f_n)_{n\in\mathbb{N}}$ converges to f in $\mathscr{S}(\mathbb{R}^d)$ iff $\|f_n - f\|_{\alpha,\beta} \to 0$ for all $\alpha, \beta \in \mathbb{N}^d$.

c) A function $F : \mathscr{S} \to X$, X a topological space, is continuous iff it is sequentially continuous.

d) The topology of $\mathscr{S}(\mathbb{R}^d)$ is metrisable and $\mathscr{S}(\mathbb{R}^d)$ is complete.

Proof. a): Clear.

b): By definition, convergence in $\mathscr{S}$ implies convergence of $\|\cdot\|_{\alpha,\beta}$. Now the family

$$U_{I,R} := \{g \in \mathscr{S} : \|f - g\|_{\alpha_i,\beta_i} < r_i, i = 1, \dots, n\} \tag{2.7}$$

where $I = ((\alpha_1, \beta_1), \dots, (\alpha_1, \beta_1))$ is a finite collection of indices $(\alpha, \beta) \in (\mathbb{N}^d)^2$ and $R = (r_1, \dots, r_n)$ are positive numbers, is a basis of open neighbourhoods at f (otherwise, the topology would not be the coarsest possible). Then, if $\|f_n - f\|_{\alpha,\beta} \to 0$ for all α, β, the sequence is eventually contained in every $U_{I,R}$, and thus convergent.

c) Since the family of semi-norms is countable, the topology of $\mathscr{S}$ satisfies the first axiom of countability [FA1, Def.1.1]. Continuity is thus equivalent to sequential continuity [FA1, Thm1.6].

d) A metric on $\mathscr{S}(\mathbb{R}^d)$ is given by

$$d(f, g) := \sum_{\alpha,\beta\in\mathbb{N}^d} 2^{-|\alpha|-|\beta|} \frac{\|f - g\|_{\alpha,\beta}}{1 + \|f - g\|_{\alpha,\beta}}. \tag{2.8}$$

Checking that the metric topology is equivalent to the one of Definition 2.1 and completeness is left as an exercise (tutorials). □

Since elements of $\mathscr{S}$ are in particular in L^1, the Fourier transform is clearly well-defined.

Definition 2.4. For $f \in \mathscr{S}(\mathbb{R}^d)$ define the *Fourier transform* as the function $p \mapsto \hat{f}(p)$ given by

$$\hat{f}(p) = (\mathscr{F} f)(p) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{-ip\cdot x} f(x) dx. \tag{2.9}$$

Proposition 2.5. *The linear map $\mathscr{F}$ maps $\mathscr{S}(\mathbb{R}^d)$ continuously to itself. For $f \in \mathscr{S}(\mathbb{R}^d)$, $\alpha \in \mathbb{N}^d$ and $p \in \mathbb{R}^d$ we have the identities*

$$\partial_p^\alpha \hat{f}(p) = (-i)^{|\alpha|} \widehat{x^\alpha f}(p) \quad \text{and} \quad \widehat{\partial_x^\alpha f}(p) = i^{|\alpha|} p^\alpha \hat{f}(p). \tag{2.10}$$

Proof. The first identity follows by differentiating under the integral (which is justified since f and its derivatives are in L^1). The second follows from integration by parts.

Now observe that $\|\hat{f}\|_{0,0} = \|\hat{f}\|_\infty \le (2\pi)^{-d/2}\|f\|_{L^1} < \infty$. Using the two identities, we obtain that $\left\|\hat{f}\right\|_{\alpha,\beta} < \infty$, and $\hat{f} \in \mathscr{S}$.

By Proposition 2.3, continuity is implied by showing that for all α, β $\left\|\hat{f}_n - \hat{f}\right\|_{\alpha,\beta} \to 0$ if $\|f_n - f\|_{\gamma,\delta} \to 0$ for all γ, δ. This follows from the same argument as finiteness of the norms. ☐

Theorem 2.6 (Fourier Inversion Theorem)**.** *The Fourier transform $\mathscr{F} : \mathscr{S}(\mathbb{R}^d) \to \mathscr{S}(\mathbb{R}^d)$ is a bijection. The inverse is continuous and given by the formula*

$$(\mathscr{F}^{-1}g)(x) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}p\cdot x} g(p)\mathrm{d}p. \tag{2.11}$$

Proof. Set $\varphi_\varepsilon := \mathrm{e}^{-\varepsilon x^2/2}$ and note that $\hat{\varphi}_\varepsilon(p) = \varepsilon^{-d/2}\mathrm{e}^{-p^2/(2\varepsilon)}$ (exercise).

We take the formula for "$\mathscr{F}^{-1}$" as a definition and show that it inverts $\mathscr{F}$. By dominated convergence,

$$\begin{aligned}
\mathscr{F}^{-1}\hat{f}(x) &= \lim_{\varepsilon\to 0} \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}p\cdot x}\varphi_\varepsilon(p)\hat{f}(p)\mathrm{d}p \\
&= \lim_{\varepsilon\to 0} \frac{1}{(2\pi)^{d}} \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}p\cdot x}\mathrm{e}^{-ipy}\varphi_\varepsilon(p) f(y)\mathrm{d}y\mathrm{d}p \\
&\overset{\text{Fubini}}{=} \lim_{\varepsilon\to 0} \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \mathscr{F}\left(\varphi_\varepsilon(p)\mathrm{e}^{\mathrm{i}p\cdot x}\right)(y) f(y)\mathrm{d}y \\
&= \lim_{\varepsilon\to 0} \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \varepsilon^{-d/2}\mathrm{e}^{\frac{(y-x)^2}{2\varepsilon}} f(y)\mathrm{d}y \\
&\overset{z=\frac{y-x}{\sqrt{\varepsilon}}}{=} \lim_{\varepsilon\to 0} \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \mathrm{e}^{z^2/2} f(x+\sqrt{\varepsilon}z)\mathrm{d}z \\
&= f(x),
\end{aligned}$$

by dominated convergence and $(2\pi)^{-d/2}\int_{\mathbb{R}^d} \mathrm{e}^{-z^2/2} = \hat{\varphi}_1(0) = 1$. The fact that $\mathscr{F}\mathscr{F}^{-1} = 1$ is proved in the same way. ☐

Corollary 2.7 (Parseval's identity)**.** *Let $f, g \in \mathscr{S}(\mathbb{R}^d)$, then*

$$\int_{\mathbb{R}^d} \overline{\hat{f}(p)}\hat{g}(p)\mathrm{d}p = \int_{\mathbb{R}^d} \overline{f(x)} g(x)\mathrm{d}x. \tag{2.12}$$

Proof. By Fubini and the Fourier inversion formula,

$$\int_{\mathbb{R}^d} \overline{\hat{f}(p)}\hat{g}(p)\mathrm{d}p = \int_{\mathbb{R}^d} \overline{f(x)}(\mathscr{F}^{-1}\hat{g})(x)\mathrm{d}x = \int_{\mathbb{R}^d} \overline{f(x)} g(x)\mathrm{d}x. \tag{2.13}$$

☐

Theorem 2.8. *There exists a unique unitary operator $\mathscr{F}_2$ on $L^2(\mathbb{R}^d)$ such that $\mathscr{F}_2|_{\mathscr{S}} = \mathscr{F}$.*

Proof. As a consequence of Parseval's identity, $\|\mathscr{F}f\|_{L^2} = \|f\|_{L^2}$, $f \in \mathscr{S}$, so if we interpret $\mathscr{F}$ as an operator on $L^2(\mathbb{R}^d)$ defined on the dense domain $D(\mathscr{F}) = \mathscr{S}(\mathbb{R}^d)$, $\mathscr{F}$ is bounded. There thus exists a unique extension $\mathscr{F}_2$ to the whole of $L^2(\mathbb{R}^d)$. The same applies to $\mathscr{F}^{-1}$, and by continuity we have $\mathscr{F}_2\mathscr{F}_2^{-1} = \mathscr{F}_2^{-1}\mathscr{F}_2 = 1$. Parseval's identity also extends to $f, g \in L^2(\mathbb{R}^d)$ by continuity. Consequently, $\mathscr{F}_2$ is a bijective isometry and thus unitary (Exercise 1) □

We will not distinguish $\mathscr{F}$ and $\mathscr{F}_2$ by the notation.

2.2 Sobolev Spaces and Tempered Distributions

Definition 2.9. The space of *tempered distributions* on $\mathbb{R}^d$ is

$$\mathscr{S}'(\mathbb{R}^d) = \{\varphi : \mathscr{S}(\mathbb{R}^d) \to \mathbb{C} \text{ linear and continuous}\} \tag{2.14}$$

with the topology induced by the coarsest topology such that $\varphi \mapsto \varphi(f)$ is continuous for all $f \in \mathscr{S}(\mathbb{R}^d)$ (the weak-$*$ toplogy).

Examples 2.10.

- A function g gives rise to a distribution via $\varphi_g(f) := \int_{\mathbb{R}^d} \overline{g}(x)f(x)\mathrm{d}x$ if $g \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$ and $(1+|x|^2)^{-n}g(x)$ is bounded for some n.
- Finite measures.
- Dirac distribution $\delta_a(f) = f(a)$.

Remarks 2.11.

- The topology of $\mathscr{S}'$ is generated by the semi-norms $\|\varphi\|_f := |\varphi(f)|$, $f \in \mathscr{S}(\mathbb{R}^d)$. A sequence $(\varphi_n)_{\mathbb{N}}$ converges to φ in $\mathscr{S}'$ iff $\varphi_n(f) \to \varphi(f)$ for all $f \in S$.

Lemma 2.12. *Let $T : \mathscr{S}(\mathbb{R}^d) \to \mathscr{S}(\mathbb{R}^d)$ be linear and continuous, then*

$$(T'\varphi)(f) := \varphi(Tf) \tag{2.15}$$

defines a linear continuous map on $T' : \mathscr{S}'(\mathbb{R}^d) \to \mathscr{S}'(\mathbb{R}^d)$.

Proof. T' is clearly well-defined and linear. For continuity, it is sufficient to prove continuity in $0 \in \mathscr{S}'$, by linearity. There, it suffices to show that the pre-images of a neighbourhood basis of zero are open. A neighbourhood basis is given by the sets

$$U_{F,R} = \{\varphi : |\varphi(f_i)| < r_i, i = 1, \dots, n\} \tag{2.16}$$

where $F = (f_1, \dots, f_n)$ is a finite collection of functions in $\mathscr{S}(\mathbb{R}^d)$ and $R = (r_1, \dots, r_n)$ are positive numbers. Then

$$\begin{aligned}(T')^{-1}(U_{F,R}) &= \{(\varphi : T'\varphi \in U_{F,R}\} \\ &= \{(\varphi : |T'\varphi(f_i)| < r_i, i = 1, \dots, n\} \\ &= \{(\varphi : |\varphi(Tf_i)| < r_i, i = 1, \dots, n\} \\ &= U_{TF,R},\end{aligned}$$

with $TF = (Tf_1, \dots, Tf_n)$. □

Examples 2.13.

a) Fourier transform $\mathscr{F}$. For $g \in \mathscr{S}(\mathbb{R}^d) \subset \mathscr{S}'(\mathbb{R}^d)$ we have

$$((\mathscr{F}^{-1})'\varphi_g)(f) = \varphi_g(\mathscr{F}^{-1}f) = \int \overline{g}(x)(\mathscr{F}^{-1}f)(x)\mathrm{d}p \overset{\text{Parseval}}{=} \int \overline{\hat{g}(p)}f(p)\mathrm{d}p = \varphi_{\hat{g}}(f), \tag{2.17}$$

so the action of $(\mathscr{F}^{-1})'$ on $\mathscr{S}'$ extends the one of $\mathscr{F}$ on $\mathscr{S}$. We will also denote this by $(\mathscr{F}^{-1})'\varphi = \mathscr{F}\varphi =: \hat{\varphi}$.

b) Derivative: For any $\alpha \in \mathbb{N}^d$ we have $(\partial^\alpha)' : \mathscr{S}'(\mathbb{R}^d) \to \mathscr{S}'(\mathbb{R}^d)$ linear and continuous. In this way we can define derivatives of all tempered distributions, in particular all L^2-functions.

c) Multiplication by a polynomial: In this case we have $(x^\alpha)'\varphi_g = \varphi_{x^\alpha g} =: x^\alpha\varphi_g$.

Definition 2.14. Let $\alpha \in \mathbb{N}^d$. The α-th *distributional derivative* on $\mathscr{S}'(\mathbb{R}^d)$ is defined as $(\partial^\alpha)_{\mathscr{S}'} := (-1)^{|\alpha|}(\partial^\alpha)'$.

Remark 2.15. The definition of $(\partial^\alpha)_{\mathscr{S}'}$ ensures that its action is compatible with the usual derivative and integration by parts: For $g \in \mathscr{S}(\mathbb{R}^d) \subset \mathscr{S}'(\mathbb{R}^d)$

$$\left((\partial^\alpha)_{\mathscr{S}'}\varphi_g\right)(f) = \int \overline{g(x)}(-1)^{|\alpha|}\partial_x^\alpha f(x)\mathrm{d}x = \int \left(\partial_x^\alpha \overline{g}\right)(x)f(x)\mathrm{d}x = \varphi_{\partial^\alpha g}(f). \tag{2.18}$$

For this reason we will not distinguish $(\partial^\alpha)_{\mathscr{S}'}$ from the usual derivative by the notation. The distributional derivative is a local operation: Let $\varphi \in \mathscr{S}'$ have support in the open set $\Omega \subset \mathbb{R}^d$ (i.e.: $\operatorname{supp} f \subset \Omega^c \implies \varphi(f) = 0$), then $\operatorname{supp} \partial^\alpha\varphi \subset \Omega$.

Also note that f(p))

$$(\mathscr{F}\partial^\alpha\varphi)(f) = \varphi\left((-1)^{|\alpha|}\partial^\alpha\mathscr{F}^{-1}f\right) = \varphi\left(\mathscr{F}^{-1}(-i)^{|\alpha|}\partial^\alpha f\right) = \left((i)^{|\alpha|}p^\alpha\mathscr{F}\varphi\right)(f). \tag{2.19}$$

Definition 2.16. Let $s \in \mathbb{R}$. The *Sobolev space* of order s is the Banach space

$$H^s(\mathbb{R}^d) := \left\{\varphi \in \mathscr{S}'(\mathbb{R}^d) : (1 + |\cdot|^2)^{s/2}\hat{\varphi} \in L^2(\mathbb{R}^d)\right\} \tag{2.20}$$

with the norm

$$\|\varphi\|_{H^s} = \left\|(1 + |\cdot|^2)^{s/2}\hat{\varphi}\right\|_{L^2}. \tag{2.21}$$

The condition $(1+|\cdot|^2)^{s/2}\hat{\varphi} \in L^2(\mathbb{R}^d)$ should be read as "$f \mapsto \hat{\varphi}((1+p^2)^{s/2}f(p))$ defines a continuous linear functional on $L^2(\mathbb{R}^d)$". This implies existence of $g \in L^2_{\mathrm{loc}}$ such that $(1+|p|^2)^{s/2}g(p) \in L^2(\mathbb{R}^d)$ and $\hat{\varphi} = \varphi_g$. Thus, $\hat{\varphi}$ is represented by a function and the norm really is

$$\|\varphi\|_{H^s} = \left(\int_{\mathbb{R}^d}(1+p^2)^s|\hat{\varphi}(p)|^2\mathrm{d}p\right)^{1/2}. \tag{2.22}$$

Remarks 2.17.

a) $H^0 = L^2$ and $H^s \subset H^t$ for $s > t$, so $H^s \subset L^2$ for all $s > 0$.

b) $m \in \mathbb{N}$, then $\varphi \in H^m \Leftrightarrow \varphi \in L^2$ and $\partial^\alpha\varphi \in L^2$ for all $|\alpha| \le m$ (exercise).

c) H^s can be considered as a Hilbert space with the scalar product

$$\langle \varphi, \psi\rangle_{H^s} := \int_{\mathbb{R}^d}(1+p^2)^s\overline{\hat{\varphi}(p)}\hat{\psi}(p)\mathrm{d}p. \tag{2.23}$$

However, it is often more natural to identify $(H^s)'$ not with H^s by Riesz' Theorem, but with H^{-s} via

$$\langle \varphi, \psi\rangle_{H^{-s}\times H^s} := \langle (1+p^2)^{-s/2}\hat{\varphi}, (1+p^2)^{s/2}\hat{\psi}\rangle_{L^2} = \int \overline{\hat{\varphi}}(p)\hat{\psi}(p)\mathrm{d}p, \tag{2.24}$$

which is compatible with the inclusion of L^2 into $\mathscr{S}$.

Examples 2.18.

a) Consider the operation $-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}$ on $L^2(\mathbb{R}^d)$ (cf.Example 1.24). We can define it on the following domains

$$D_{\min} = \mathscr{S}(\mathbb{R}), \tag{2.25}$$

and by using the distributional derivative

$$D_{\max} = \left\{\varphi \in L^2(\mathbb{R}), -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}\varphi \in L^2(\mathbb{R})\right\} = H^1(\mathbb{R}). \tag{2.26}$$

Let $P_{\min} = (-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}, D_{\min})$ and $P_{\max} = (-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}, D_{\max})$.

- $P_{\min}$ is symmetric: Integration by parts.
- $P_{\max} = P^*_{\min}$ and $P_{\max}$ is closed: $\varphi \in D(P^*_{\min}) \Leftrightarrow \psi \mapsto \langle\varphi, P_{\min}\psi\rangle$ is a continuous functional on $L^2(\mathbb{R}^d) \Leftrightarrow \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}\varphi \in L^2(\mathbb{R})$ as a distribution.
- $P_{\max}$ is self-adjoint: Since $P_{\max} = P^*_{\min}$ it is enough to check that $P_{\max}$ is symmetric (cf. Corollary 1.23). But this is clear, since (compare Exercise 2).

$$\langle\varphi, P_{\max}\psi\rangle = \int_{\mathbb{R}}\overline{\hat{\varphi}(p)}p\hat{\psi}(p)\mathrm{d}p. \tag{2.27}$$

b) Let $\mathscr{H} = L^2(\mathbb{R}^d)$, and consider the operator $H = -\Delta$ in the distributional sense, i.e. on $D(H) = H^2(\mathbb{R}^d)$. Then H is self adjoint, since $H = \mathscr{F}^* p^2 \mathscr{F}$ and the multiplication operator by p^2 is self-adjoint on its maximal domain (Exercise 2). We

Definition 2.19. Let $\Omega \subset \mathbb{R}^d$ open and $s > 0$. We define:

- the space of locally H^s-distributions in Ω

$$H^s_{\mathrm{loc}}(\Omega) := \{\varphi \in \mathscr{S}'(\mathbb{R}^d) : \chi\varphi \in H^s(\mathbb{R}^d) \text{ for all } \chi \in C_0^\infty(\Omega)\}; \tag{2.28}$$

- the Space of H^s-distributions in Ω

$$H^s(\Omega) := \{\varphi \in L^2(\Omega) : \exists \tilde{\varphi} \in H^s(\mathbb{R}^d) \text{ with } \tilde{\varphi}|_\Omega = \varphi\}, \tag{2.29}$$

  with the norm

$$\|\varphi\|_{H^s(\Omega)} = \inf_{\tilde{\varphi}|_\Omega = \varphi} \|\tilde{\varphi}\|_{H^s(\mathbb{R}^d)}\,; \tag{2.30}$$

- the space of H^s-distributions in Ω vanishing near the boundary

$$H^s_0(\Omega) := \overline{C_0^\infty(\Omega)}^{\|\cdot\|_{H^s(\mathbb{R}^d)}}, \tag{2.31}$$

  with the norm induced by $H^s(\mathbb{R}^d)$ on this closed subspace.

Remarks 2.20.

a) $H^s_0(\Omega) \subset H^s(\Omega) \subset H^s_{\mathrm{loc}}(\Omega)$ and $H^s_0(\Omega) \subset H^s(\Omega) \subset L^2(\Omega)$.

b) The local H^s-space is not a Banach space. The norm on $H^s(\Omega)$ is the quotient norm on H^s modulo the kernel of the restriction to Ω.

c) All the Sobolev spaces defined here in the L^2-setting can be naturally defined with respect to L^p, $1 \leq p \leq \infty$.

Example 2.21. Let $\mathscr{H} = L^2((0,1))$, $P_0 = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}$, $D(P_0) = C_0^1((0,1))$ (cf. Example 1.24c)). We have already seen that P_0 is not essentially self-adjoint. We will now show that

- $D(\overline{P_0}) = H^1_0((0,1))$,
- $f \in D(P_0^*)$ is continuous up to the boundary, and we have "integration by parts", for $f, g \in D(P_0^*)$

$$\langle f, P_0^* g\rangle = \langle P_0^* f, g\rangle - \mathrm{i}\overline{f(1)}g(1) + \mathrm{i}\overline{f(0)}g(0), \tag{2.32}$$

- $D(P^*) = H^1((0,1))$.

For the first point, let $g \in \mathscr{S}(\mathbb{R})$, $f \in D(P_0)$ and consider

$$\langle f, -\mathrm{i}\tfrac{\mathrm{d}}{\mathrm{d}x} g\rangle_{L^2(\mathbb{R})} = -\mathrm{i}\int_0^1 \overline{f}(x)\tfrac{\mathrm{d}}{\mathrm{d}x} g(x)\mathrm{d}x = \langle P_0 f, g\rangle, \tag{2.33}$$

so

$$\|f\|_{D(P_0)} = \|f\|_{L^2} + \sup_{g\in\mathscr{S}, \|g\|_{L^2}=1} \langle P_0 f, g\rangle = \|f\|_{L^2} + \left\|p\hat{f}(p)\right\|_{L^2} \tag{2.34}$$

is equivalent to the H^1-norm. The closure of $D(P_0)$ in this norm is $H^1_0(0,1)$, by definition.

For the second point, we first argue that $D(P_0^*) \subset H^1_{\mathrm{loc}}(0,1)$. Let $\chi \in C_0^\infty((0,1),[0,1])$ and $f \in D(P_0^*)$. Then $\chi f \in H^1(\mathbb{R})$, since for $g \in \mathscr{S}(\ R)$

$$\langle \chi f, -\mathrm{i}\tfrac{\mathrm{d}}{\mathrm{d}x} g\rangle = \langle f, \chi - \mathrm{i}\tfrac{\mathrm{d}}{\mathrm{d}x} g\rangle = \langle f, P_0 \chi g\rangle_{L^2(0,1)} - \mathrm{i}\langle f, (\tfrac{\mathrm{d}}{\mathrm{d}x}\chi) g\rangle, \tag{2.35}$$

which extends continuously to $g \in L^2(\mathbb{R})$. Note also that the weak derivative equals $-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}\chi f = \chi P_0^* f - \mathrm{i}(\frac{\mathrm{d}}{\mathrm{d}x}\chi) f$. Let $\chi_K = 1$ on $K \subset (0,1)$, then, by locality of the distributional derivative, $-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}\chi_K f|_K = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x} f|_K = P_0^* f$, and by exhausting the interval with compact sets we find

$$\int_0^1 \left|\tfrac{\mathrm{d}}{\mathrm{d}x} f\right|^2 (x)\mathrm{d}x = \|P_0^* f\|^2 . \tag{2.36}$$

Let $K \subset (0,1)$ be a compact interval, and $f_n \in C^1((0,1))$ be a sequence such that such that $\|f_n - f\|_{L^2(K)} + \left\|\frac{\mathrm{d}}{\mathrm{d}x}(f_n - f)\right\|_{L^2(K)} \to 0$ (e.g. convolution with a C_0^∞-function). Then for $x \in K$ (cf. Example 1.24c))

$$|f_n(x) - f_m(x)|^2 \le 2\left(\|f_n - f_m\|^2_{L^2(K)} + \left\|\tfrac{\mathrm{d}}{\mathrm{d}x}(f_n - f_m)\right\|^2_{L^2(K)}\right), \tag{2.37}$$

so f_n converges to f uniformly on K and f is continuous in the interior of $(0,1)$. Moreover, for $0 < a < b < 1$

$$\int_a^b \tfrac{\mathrm{d}}{\mathrm{d}x} f = f_n(b) - f_n(a) + \int_a^b \tfrac{\mathrm{d}}{\mathrm{d}x}(f - f_n)\mathrm{d}x. \tag{2.38}$$

The integral is bounded by $\sqrt{b-a}\left\|\frac{\mathrm{d}}{\mathrm{d}x}(f - f_n)\right\|_{L^2([a,b])}$ by the Cauchy-Schwarz inequality, so f satisfies the formula analogous to the fundamental theorem of calculus (even though f is not C^1).

Now let $(x_n)_{\mathbb{N}}$ be a sequence converging to a boundary point, say $x_n \to 0$. Then for $f \in D(P_0^*)$

$$|f(x_n) - f(x_m)|^2 = \left|\int_{x_n}^{x_m} \tfrac{\mathrm{d}}{\mathrm{d}x} f(y)\mathrm{d}y\right|^2 \overset{\text{Cauchy-Schwarz}}{\le} |x_m - x_n| \int_0^1 \left|\tfrac{\mathrm{d}}{\mathrm{d}x} f(y)\right|^2 \mathrm{d}y, \tag{2.39}$$

so $f(x_n)$ is Cauchy and converges to a limit $y =: f(0)$. The integration-by-parts formula follows from this in the same way as (2.38).

It is clear that $H^1(0,1) \subset D(P_0^*)$. For the reverse inclusion, we need to extend $f \in D(P_0^*)$ to $\tilde{f} \in H^1(\mathbb{R})$. set

$$\tilde{f}(x) = \begin{cases} \mathrm{e}^x f(0) & x \leq 0 \\ f(x) & 0 < x < 1 \\ \mathrm{e}^{1-x} f(1) & x \geq 1. \end{cases}$$

This function is piecewise (weakly) differentiable, and by the integration-by-parts formula for all $g \in \mathscr{S}(\mathbb{R})$:

$$\langle \tilde{f}, \tfrac{\mathrm{d}}{\mathrm{d}x} g \rangle_{L^2(\mathbb{R})} = -\int_{-\infty}^{0} \overline{\tfrac{\mathrm{d}}{\mathrm{d}x}\tilde{f}}(x) g(x) \mathrm{d}x - \int_0^1 \overline{\tfrac{\mathrm{d}}{\mathrm{d}x}\tilde{f}}(x) g(x) \mathrm{d}x - \int_1^\infty \overline{\tfrac{\mathrm{d}}{\mathrm{d}x}\tilde{f}}(x) g(x) \mathrm{d}x, \quad (2.40)$$

since the boundary terms cancel. This extends continuously to $g \in L^2$, so $\tilde{f} \in H^1(\mathbb{R})$.

Remark 2.22. For $m \in \mathbb{N}$ one can define spaces $W^m(\Omega)$ by requiring that the weak derivatives, defined by duality with $C_0^m(\Omega)$ in analogy with (2.18), of $f \in L^2(\Omega)$ be in $L^2(\Omega)$. In the example above, this corresponds to defining $W^1((0,1)) := D(P_0^*)$. One can show that $W^m(\Omega) = H^m(\Omega)$ (with our definition) if the boundary of Ω is sufficiently regular (say C^m, see [AF]). If $d = 1$, then the boundary of a connected open set Ω consists of just finitely many points, and $W^m(\Omega) = H^m(\Omega)$, as we showed in Example 2.21.

Warning: These notations are used with variants of the definitions.

2.2.1 Embedding Theorems

Lemma 2.23 (Riemann-Lebesgue)**.** *Let $C_\infty(\mathbb{R}^d)$ be the Banach space of continuous functions with $\lim_{|x|\to\infty} f(x) = 0$, equipped with the* sup*-norm. Then $\mathscr{F} : L^1(\mathbb{R}^d) \to C_\infty(\mathbb{R}^d)$ defines a bounded operator.*

Proof. It is clear that $\|\mathscr{F} f\|_\infty \leq (2\pi)^{-d/2} \|f\|_{L^1}$, so $\mathscr{F}$ defines a bounded operator $L^1 \to L^\infty$. Now $\mathscr{F}(S) \subset \mathscr{S} \subset C_\infty$ by Proposition 2.5. Then, by continuity and because C_∞ is closed in L^∞, $\mathscr{F}(L^1) \subset \overline{\mathscr{S}} \subset C_\infty$. □

Theorem 2.24 (Sobolev's Lemma)**.** *Every element $\varphi \in H^s(\mathbb{R}^d)$ for $s > d/2$ has a continuous representative, i.e. there exists $f \in C_\infty(\mathbb{R}^d)$ with $\varphi = f$ a.e.. Furthermore, there exists a constant such that for $0 < \gamma \leq 1$, $\gamma < s - d/2$ and $x, y \in \mathbb{R}^d$:*

$$|f(x) - f(y)| \leq C \|f\|_{H^s(\Omega)} |x - y|^\gamma, \quad (2.41)$$

that is, f is Hölder continuous of degree γ.

Proof. For $\varphi \in H^s(\mathbb{R}^d)$, $s > d/2$, we have $\mathscr{F}^{-1}\varphi := \check{\varphi} \in L^1$, because $\check{\varphi}(p) = (1 + p^2)^{-s/2}(1+p^2)^{s/2}\hat{\varphi}(-p)$ is the product of two L^2-functions (the product is L^1 by Cauchy-Schwarz). Then $f := \mathscr{F}\check{\varphi} \in C(\mathbb{R}^d)$ by the Riemann-Lebesgue Lemma and $f = \varphi$ a.e. by Fourier inversion.

Because the exponential function is Hölder-continuous ($|(\mathrm{e}^{ipx} - \mathrm{e}^{ipy})| \leq 2^{1-\gamma}|x - y|^\gamma |p|^\gamma$), we have for $f \in \mathscr{S}$

$$
\begin{aligned}
|f(x) - f(y)| &= \frac{1}{(2\pi)^{d/2}} \left| \int_{\mathbb{R}^d} (\mathrm{e}^{ipx} - \mathrm{e}^{ipy}) \hat{f}(p) \mathrm{d}p \right| \\
&\leq \frac{2^{1-\gamma}}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} |x-y|^\gamma |p|^\gamma |f(p)| \mathrm{d}p \\
&\leq C|x-y|^\gamma \, \| |p|^\gamma |f(p)| \|_{L^1}
\end{aligned}
$$

We conclude as in the first case, since $(1+p^2)^{-s/2+\gamma/2} \in L^2$, because $-s+\gamma < -d/2$. ☐

Corollary 2.25. *Every $\varphi \in H^s(\mathbb{R}^d)$ for $s > d/2 + k$ has a C^k-representative.*

Proof. By applying Sobolev's Lemma to φ and $\mathscr{F}^{-1}(ip)^\alpha \hat{\varphi}$, $|\alpha| \leq k$, we see that φ has a representative with k continuous distributional derivatives. These coincide with the usual derivatives by dominated convergence. ☐

Corollary 2.26. *Let $\Omega \subset \mathbb{R}^d$ be open, then every $\varphi \in H^m_{\mathrm{loc}}(\Omega)$ for $m > d/2 + k$ has a representative in $C^k_b(\Omega)$.*

Proof. Clear, since continuity is a local property. ☐

Recall from [FA1]:

Definition 2.27. Let X, Y be Banach spaces. An operator $T \in \mathrm{B}(X, Y)$ is *compact* if for every bounded set $B \subset X$, $\overline{T(B)}$ is compact in Y (i.e. $T(B)$ is relatively compact).

Since in metric spaces compactness is the same as sequential compactness, this is equivalent to: For every bounded sequence $(x_n)_\mathbb{N}$ in X, the sequence $y_n := Tx_n$ has a convergent subsequence in Y.

Recall also:

Definition 2.28. Let (Ω, d) be a metric space. A set $F \subset C(\Omega)$ is called equi-continuous if

$$\forall x \in \Omega \, \forall \varepsilon > 0 \exists \delta > 0 \, \forall f \in F \, \forall y \text{ with } d(x,y) < \delta : |f(x) - f(y)| < \varepsilon. \tag{2.42}$$

Theorem 2.29 (Arzelà-Ascoli)**.** *Let (Ω, d) be a compact metric space. A set $F \subset C(\Omega)$ is relatively compact iff F is bounded and equi-continuous.*

[FA1, Thm.1.40]

This gives the following:

Corollary 2.30. *Let $\overline{\Omega} \subset \mathbb{R}^d$ be compact and $\gamma > 0$. The inclusion of $C^{0,\gamma}(\overline{\Omega}) \to C(\overline{\Omega})$ is a compact operator.*

Proof. The norm on $C^{0,\gamma}(\overline{\Omega})$ is given by

$$\|f\|_{C^{0,\gamma}} = \|f\|_\infty + \sup_{x\neq y\in\overline{\Omega}} \frac{|f(x)-f(y)|}{|x-y|^\gamma}. \tag{2.43}$$

Thus, bounded sets in $C^{0,\gamma}(\overline{\Omega})$ are mapped to bounded sets in $C(\overline{\Omega})$ and we only need to show that these are equi-continuous. We have for all $x, y \in \overline{\Omega}$

$$|f(x)-f(y)| \leq \|f\|_{C^{0,\gamma}} |x-y|^\gamma, \tag{2.44}$$

so for $\varepsilon > 0$, (2.42) is satisfied with $\delta = (\varepsilon/\|f\|_{C^{0,\gamma}})^{1/\gamma}$, and this proves the claim. □

Corollary 2.31. *Let $\Omega \subset \mathbb{R}^d$ be open with $\overline{\Omega}$ compact and $s > d/2$. Then the embedding*

$$H^s(\Omega) \to C(\overline{\Omega})$$

is a compact operator.

Proof. By definition, $H^s(\Omega)$ is the range of the restriction operator $R_\Omega : H^s(\mathbb{R}^d) \to H^s(\Omega)$, $\varphi \mapsto \varphi|_{\overline{\Omega}}$. Using the Hilbert space structure on H^s, we can write $H^s(\mathbb{R}^d) = \ker(R_\Omega) \oplus \ker(R_\Omega)^\perp$ as an orthogonal sum, and $R_\Omega|_{\ker R_\Omega^\perp}$ is an isometry to $H^s(\Omega)$. It is thus sufficient to prove that that R_Ω is a compact operator on the given spaces.

Let $\tilde{\Omega} \supset \Omega$, then by Sobolev's Lemma $R_{\tilde{\Omega}}$ maps bounded sets in $H^s(\mathbb{R}^d)$ to bounded sets $\in C^{0,\gamma}(\tilde{\Omega})$. Thus $R_\Omega = R_\Omega R_{\tilde{\Omega}}$ maps bounded sets in $H^s(\mathbb{R}^d)$ to bounded sets in $C^{0,\gamma}(\overline{\Omega})$. The claim then
follows from Corollary 2.30. □

All of these statements have generalisations to $s \leq d/2$, where spaces of continuous functions are replaced by L^p-spaces, $p \geq 2$. We will only give the important generalisation of Corollary 2.31 to the L^2-case.

Theorem 2.32 (Rellich's Theorem)**.** *Let $\Omega \subset \mathbb{R}^d$ be open with $\overline{\Omega}$ compact and $s > 0$. Then the embedding*

$$H^s(\Omega) \to L^2(\Omega)$$

is a compact operator.

Proof. As in Corollary 2.31 it is sufficient to prove that the restriction $R : H^s(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ is compact. We will show that $R(B)$ is relatively compact in $L^2(\Omega)$ for the unit ball $B \subset H^m(\mathbb{R}^d)$ by a three-ε-argument.

Let $(\varphi_n)_N$ be a sequence in B. Define $\tilde{\varphi}_{n,k}$ by $\widehat{\tilde{\varphi}_{n,k}}(p) = \hat{\varphi}_n(p)$ for $|p| \leq k$ and $\widehat{\tilde{\varphi}_{n,k}}(p) = 0$ otherwise. Then

$$\|R\tilde{\varphi}_{n,k} - R\varphi_n\|^2_{L^2(\Omega)} \leq \|\tilde{\varphi}_{n,k} - \varphi_n\|^2_{L^2(\mathbb{R}^d)} \leq \int_{|p|>k} |\hat{\varphi}_n(p)|^2 \mathrm{d}p \leq (1+k^2)^{-s/2} < \varepsilon, \tag{2.45}$$

for large enough k. Now $\widehat{\tilde{\varphi}_{n,k}}$ has compact support, so

$$\|\tilde{\varphi}_{n,k}\|_{H^{(d+1)/2}(\mathbb{R}^d)} \leq \|\tilde{\varphi}_{n,k}\|_{L^2(\mathbb{R}^d)} \left(\int_{|p|\leq k} (1+k^2)^{(d+1)/2} \right)^{1/2} \leq C_k. \tag{2.46}$$

Thus, by Corollary 2.31, $R\tilde{\varphi}_{n,k}$ has a convergent subsequence in $C(\overline{\Omega}) \subset L^2(\Omega)$ as $n \to \infty$ (denoted by the same symbols). Then

$$\|R\varphi_n - R\varphi_m\|_{L^2(\Omega)} \leq 2\varepsilon + \|R\tilde{\varphi}_{n,k} - R\tilde{\varphi}_{m,k}\|_{L^2(\Omega)}\,. \tag{2.47}$$

This is less than 3ε for $m, n > N_0$, so $R\varphi_n$ is Cauchy. □

Remark 2.33. As remarked before $H^m(\Omega)$ is the same as the space $W^{m,2}$ of weakly-differentiable functions if Ω is sufficiently regular. Then the compactness results of Corollary 2.31 and Theorem 2.32 transfer to these space under such a regularity condition.

3 Self-Adjoint Operators and the Spectral Theorem

3.1 Criteria for Self-Adjointness

Theorem 3.1. *Let A, $D(A)$ be symmetric. The following are equivalent*

1) $A = A^*$

2) A *is closed and* $\ker(A^* + \mathrm{i}) = \ker(A^* - \mathrm{i}) = \{0\}$

3) $\operatorname{ran}(A + \mathrm{i}) = \operatorname{ran}(A - \mathrm{i}) = \mathscr{H}$.

Proof. 1) $\implies$ 2): $A = A^*$ is closed by Theorem 1.19. If $0 \neq \varphi \in \ker(A^* \pm \mathrm{i})$, then (e.g. for "+")

$$\mathrm{i}\langle\varphi, \varphi\rangle = \langle A^*\varphi, \varphi\rangle = \langle\varphi, A^*\varphi\rangle = -\langle\varphi, \varphi\rangle \tag{3.1}$$

$\implies \varphi = 0$.

2) $\implies$ 3) First note $\ker(A^* + \mathrm{i}) = \operatorname{ran}(A - \mathrm{i})^\perp$:

$$\varphi \in \ker(A^* + \mathrm{i}) \Leftrightarrow \forall\psi \in D(A) : \langle(A^* + \mathrm{i})\varphi, \psi\rangle = 0 \Leftrightarrow \forall\psi \in D(A)\langle\varphi, (A - \mathrm{i})\psi\rangle = 0.$$

Consequently, $\ker(A^*+\mathrm{i}) = \{0\} \implies \overline{\operatorname{ran}(A - \mathrm{i})} = \mathscr{H}$. Now let $\eta \in \mathscr{H}$ with $(A-\mathrm{i})\varphi_n \to \eta$. We have the inequality for all $\psi \in D(A)$:

$$\|(A - \mathrm{i})\psi\|^2 = \langle(A - \mathrm{i})\psi, (A - \mathrm{i})\psi\rangle = \|A\psi\|^2 + \|\psi\|^2 + \mathrm{i}\left(\langle\psi, A\psi\rangle - \langle A\psi, \psi\rangle\right) \geq \|\psi\|^2 ., \tag{3.2}$$

so $(\varphi_n)_{\mathbb{N}}$ is Cauchy, $\varphi_n \to \varphi$. Since A is closed, $\varphi \in D(A)$ and $A\varphi = \eta + \mathrm{i}\varphi$, and $\eta \in \operatorname{ran}(A - \mathrm{i})$.

3) $\implies$ 1) Let $\varphi \in D(A^*)$ and prove that $\varphi \in D(A)$. First, there is $\psi \in D(A)$ s.th. $(A^* - \mathrm{i})\varphi = (A - \mathrm{i})\psi$. Since $A \subset A^*$, we thus have $(A^* - \mathrm{i})(\varphi - \psi) = 0$. Then for every $\eta \in D(A)$:

$$0 = \langle\eta, (A^* - \mathrm{i})(\varphi - \psi)\rangle = \langle(A + \mathrm{i})\eta, (\varphi - \psi)\rangle, \tag{3.3}$$

and thus $\varphi = \psi \in D(A)$ because $\operatorname{ran}(A + \mathrm{i}) = \mathscr{H}$. □

From the proof we obtain directly:

Corollary 3.2. *Let A, $D(A)$ be symmetric. The following are equivalent*

1) A is essentially self-adjoint

2) $\ker(A^* + \mathrm{i}) = \ker(A^* - \mathrm{i}) = \{0\}$

3) $\overline{\operatorname{ran}(A+\mathrm{i})} = \overline{\operatorname{ran}(A-\mathrm{i})} = \mathscr{H}$.

Proof. If A is essentially self-adjoint, then $A^* = \overline{A}$ is self-adjoint, so 1) $\implies$ 2).
2) $\implies$ 3) since $\overline{\operatorname{ran}(A \mp \mathrm{i})} = \ker(A^* \mp \mathrm{i})$.
To see that 3) $\implies$ 1), $(\psi_n)_n$ in $D(A)$ be a sequence such that $(A-\mathrm{i})\psi_n \to (A^*-\mathrm{i})\varphi$. The bound(3.2) implies that ψ_n is Cauchy, and thus converges to some ψ. Then $(\overline{A} - \mathrm{i})\psi \to (A^* - \mathrm{i})\varphi$, and we conclude as in the proof of the Theorem above that $\psi = \varphi$ and $\overline{A} = A^*$. ☐

We can also note the following property of the spectrum:

Corollary 3.3. *Let $A, D(A)$ be symmetric. Then A is self-adjoint iff $\sigma(A) \subset \mathbb{R}$, and in that case*
$$\|R_z(A)\| \leq \operatorname{Im}(z)^{-1}. \tag{3.4}$$

Proof. By Theorem 3.1, A is self-adjoint iff $\{\pm\mathrm{i}\} \subset \rho(A)$. Now $z = \mu + \mathrm{i}\lambda \in \rho(A)$ $\Leftrightarrow \mathrm{i} \in \rho((A-\mu)/\lambda)$, which gives the statement on the spectrum.
For the bound on the resolvent it is sufficient to consider $z = \mathrm{i}\lambda$ (by passing to $A-\mu$), and we have by the calculation (3.2) for $\varphi \in D(A)$
$$\|(A+\lambda\mathrm{i})\varphi\|^2 = \|A\varphi\|^2 + \lambda^2 \|\varphi\|^2 . \tag{3.5}$$
Applying this to $\varphi = (A+\mathrm{i}\lambda)^{-1}\psi$ yields
$$\|\psi\|^2 \geq \lambda^2 \left\|(A+\mathrm{i}\lambda)^{-1}\psi\right\|^2 , \tag{3.6}$$
which proves the claim. ☐

These results give rise to a powerful tool to construct new self-adjoint operators out of known examples.

Definition 3.4. Let $A, D(A)$, $B, D(B)$ be densely defined. B is *bounded relative to A*, for short A-bounded, iff $D(A) \subset D(B)$ and there exist constants $a, b \geq 0$ such that for all $\psi \in D(A)$
$$\|B\psi\| \leq a\|A\psi\| + b\|\psi\| . \tag{3.7}$$
The relative bound of B with respect to A is then the infimum of all $a \geq 0$ such that the inequality holds for some $b \geq 0$.

Theorem 3.5 (Kato-Rellich)**.** *Let $A, D(A)$ be self-adjoint and $B, D(B)$ symmetric. If B is A-bounded with relative bound $a < 1$, then $A + B$ is self-adjoint on $D(A)$ and essentially self-adjoint on any core of A.*

Proof. It is sufficient to show that $\operatorname{ran}(A + B - \mathrm{i}\lambda) = \mathscr{H}$ for some $\lambda > 0$. Using the relative bound and Corollary 3.3 we obtain
$$\|BR_{\mathrm{i}\lambda}(A)\| \leq a\|AR_{\mathrm{i}\lambda}(A)\| + b\|R_{\mathrm{i}\lambda}(A)\| \leq a + \frac{b}{\lambda}. \tag{3.8}$$

If $a + b/\lambda < 1$, the bounded operator $1 + BR_{\mathrm{i}\lambda}(A)$ is thus invertible by a Neumann series ([FA1, Thm.5.18]). Since $A - \lambda\mathrm{i}$ is onto, then so is

$$(1 + BR_{\mathrm{i}\lambda}(A))\,(A - \lambda\mathrm{i}) = A + B - \lambda\mathrm{i}. \tag{3.9}$$

If we work instead of $D(A)$ on any core $C(A)$ of A, then $\mathrm{ran}(A - \lambda\mathrm{i})|_{C(A)}$ is dense, and by continuity and bijectivity of $1 + BR_{\mathrm{i}\lambda}(A)$ so is the range of $(A + B - \lambda\mathrm{i})\,|_{C(A)}$. □

Corollary 3.6 (Second Resolvent Formula)**.** *Let $A, D(A)$ be self-adjoint and $B, D(B)$ symmetric and A-bounded with relative bound $a < 1$. Denote by $A + B$ the self-adjoint operator on $D(A)$ given by the Kato-Rellich Theorem. Then for every $z \in \rho(A{+}B) \cap \rho(A)$ we have*

$$R_z(A + B) - R_z(A) = -R_z(A)BR_z(A + B) = -R_z(A + B)BR_z(A). \tag{3.10}$$

Proof. Since $A + B$ is self-adjoint, we have $\mathbb{C} \setminus \mathbb{R} \subset \rho(A)$. In (3.9) we showed that for $|\lambda|$ large enough

$$\begin{aligned} R_{\mathrm{i}\lambda}(A + B) &= R_{\lambda\mathrm{i}} \sum_{n=0}^{\infty} (-1)^n (BR_{\lambda\mathrm{i}})^n \\ &= R_{\lambda\mathrm{i}} - R_{\lambda\mathrm{i}} BR_{\lambda\mathrm{i}} \sum_{n=0}^{\infty} (-1)^n (BR_{\lambda\mathrm{i}})^n = R_{\lambda\mathrm{i}} - R_{\lambda\mathrm{i}} BR_{\mathrm{i}\lambda}(A + B). \end{aligned}$$

This establishes the desired equality on two semi-infinite strips on the imaginary axis. By analytic continuation it must then hold for all $z \in \mathbb{C} \setminus \mathbb{R}$, and then also for all remaining points in $\rho(A) \cap \rho(A + B)$, which are in the closure of $\mathbb{C} \setminus \mathbb{R}$.

The second equality follows from the same reasoning applied to $A = A + B - B$. □

Example 3.7 (Schrödinger operators)**.** The Schrödinger equation is the partial differential equation

$$\mathrm{i}\partial_t \psi(t, x) = -\Delta\psi(t, x) + V(x)\psi(t, x), \tag{3.11}$$

where V is a real function (we denote the multiplication operator by the same symbol).

An important example is $V(x) = -\frac{1}{|x|}$ in $d = 3$ dimensions. It corresponds to a model of an electron in $\mathbb{R}^3$ interacting with a nucleus (fixed at $x = 0$) via electrostatic interactions – a model for the hydrogen atom.

The function $\psi(t, \cdot)$ is called the wave-function and accounts for the sate of the electron at time t. The square modulus $|\psi(t, \cdot)|^2$ is the probability distribution of the position of the electron (Born's rule). It is thus natural to consider the Schrödinger equation on $L^2(\mathbb{R}^d)$, where it takes the abstract form

$$\mathrm{i}\partial_t \psi(t) = H\psi(t), \tag{3.12}$$

where $H, D(H)$ is an unbounded operator. Since the total probability $\|\psi(t)\|_{L^2}$ should be equal to one for all times, we are interested in solutions that preserve this norm. This implies that H must be symmetric since

$$\tfrac{\mathrm{d}}{\mathrm{d}t} \|\psi(t)\|^2 = 2\mathrm{Re}(\langle\psi(t), -\mathrm{i}H\psi\rangle) = -2\mathrm{Im}(\langle\psi, H\psi\rangle). \tag{3.13}$$

In particular, if $\lambda \in \sigma_p(H)$ is a real eigenvalue with eigenfunction φ, then $\psi(t) = \mathrm{e}^{-\mathrm{i}t\lambda}\varphi$ is a periodic solution to the Schrödinger equation. The probability distribution $|\psi|^2$ for this solution does not change, so it is interpreted as a stationary state.

We will later see that the equation has a good existence theory if and only if H is self-adjoint. With the tools we have now, we can prove this self-adjointness for many cases, e.g. $d = 3$ and $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Since the electrostatic potential $1/|x|$ is square-integrable for $x \leq 1$ and bounded for $x \geq 1$, this applies to the Hamiltonian operator for the Hydrogen atom. We claim that V is $-\Delta$-bounded with relative bound zero, which implies that

$$H = -\Delta + V(x) \tag{3.14}$$

is self-adjoint on $D(H) = D(-\Delta) = H^2(\mathbb{R}^3)$. We have $H^s(\mathbb{R}^3) \subset L^\infty(\mathbb{R}^3)$ for $s > 3/2$ (by Sobolev's Lemma 2.24), and, for $s < 2$ and $\varepsilon > 0$

$$|p|^s \leq \begin{cases} \varepsilon^{s/(s-2)} & |p| \leq \varepsilon^{1/(s-2)} \\ \varepsilon p^2 & |p| > \varepsilon^{1/(s-2)}, \end{cases} \tag{3.15}$$

so $|p|^s \leq \varepsilon p^2 + \varepsilon^{s/(s-2)}$.

Consequently,

$$\|\psi\|_{L^\infty} \leq \varepsilon \|{-\Delta\psi}\|_{L^2} + C_\varepsilon \|\psi\|_{L^2} . \tag{3.16}$$

Now decompose $V = V_2 + V_\infty$ with $V_p \in L^p(\mathbb{R}^3)$, then

$$\begin{aligned} \|V\psi\|_{L^2} &\leq \|V_2\|_{L^2} \|\psi\|_{L^\infty} + \|V_\infty\|_{L^\infty} \|\psi\|_{L^2} \\ &\leq \varepsilon \|V_2\|_{L^2} \|{-\Delta\psi}\|_{L^2} + (\|V_2\|_{L^2} C_\varepsilon + \|V_\infty\|_{L^\infty}) \|\psi\|_{L^2} , \end{aligned} \tag{3.17}$$

so V is $-\Delta$-bounded with relative bound zero.

From the proof of the Kato-Rellich Theorem we also see that $\lambda \in \rho(H)$ for $\lambda << 0$ sufficiently small (exercise). This means that H has no eigenvalues smaller than some $\lambda_{\min} \leq 0$. This means that the electron cannot have arbitrarily small energy, even though the interaction can be very negative. This implies stability of the Hydrogen atom, which was a puzzle in the early 20th century.

3.1.1 Quadratic Forms

Definition 3.8. A *form* on a Hilbert space $\mathscr{H}$ with form-domain $\mathscr{Q} \subset \mathscr{H}$ is a sesquilinear form

$$q : \mathscr{Q} \times \mathscr{Q} \to \mathbb{C}. \tag{3.18}$$

- q is *densely defined* if $\mathscr{Q}$ is dense in $\mathscr{H}$.
- q is *symmetric* if $q(\psi, \varphi) = \overline{q(\varphi, \psi)}$
- q is *bounded from below* if q is symmetric and there exists $M \geq 0$ such that

  $$\forall \psi \in \mathscr{Q} : q(\psi, \psi) \geq -M \|\psi\|^2_{\mathscr{H}} \tag{3.19}$$

  and *non-negative* if $M = 0$.

- q is *closed* if it is bounded from below and $\mathscr{Q}$ with the scalar product
$$\langle\cdot,\cdot\rangle_{\mathscr{Q}} := q(\cdot,\cdot) + (M+1)\langle\cdot,\cdot\rangle_{\mathscr{H}} \tag{3.20}$$
is a Hilbert space.
- q is *closable* if there exists a closed form $\tilde{q}$ with domain $\widetilde{\mathscr{Q}}$, $\mathscr{Q} \subset \widetilde{\mathscr{Q}} \subset \mathscr{H}$ that restricts to q. If $\widetilde{\mathscr{Q}}$ is the completion of the pre-Hilbert space $(\mathscr{Q}, \langle\cdot,\cdot\rangle_{\mathscr{Q}})$, then $\tilde{q}$ is called the *closure* of q and denoted by $\overline{q}$.

Remarks 3.9.

a) By polarisation any symmetric form is uniquely determined by the associated *quadratic* form $\psi \mapsto q(\psi,\psi)$, i.e.
$$q(\varphi,\psi) = \tfrac{1}{4}\left(q(\varphi+\psi,\varphi+\psi) - q(\varphi-\psi,\varphi-\psi)\right) + \tfrac{\mathrm{i}}{4}\left(q(\varphi+\mathrm{i}\psi,\varphi+\mathrm{i}\psi) - q(\varphi-\mathrm{i}\psi,\varphi-\mathrm{i}\psi)\right). \tag{3.21}$$

b) A form is symmetric iff $q(\psi,\psi)$ is real.

Example 3.10.

a) Let A, $D(A)$ be a symmetric operator, then
$$q_A(\psi,\varphi) := \langle A\psi,\varphi\rangle \tag{3.22}$$
defines a form on $D(A)$. We call A bounded from below if this form is bounded from below.

b) Let $\mathscr{Q} = C_0(\mathbb{R}) \subset L^2(\mathbb{R})$, then
$$q(f,g) := \overline{f}(0)g(0) \tag{3.23}$$
is a densely defined form with domain $\mathscr{Q}$. This form is non-negative since $q(f,f) = |f(0)|^2 \geq 0$.

Proposition 3.11. *Let A, $D(A)$ be symmetric and bounded from below. Then the associated form q_{A} is closable.*

Proof. Let $\mathscr{Q}_A$ be the completion of $D(A)$ w.r.t. $\langle\cdot,\cdot\rangle_{\mathscr{Q}_A}$. We need to show that this can be identified with a subspace of $\mathscr{H}$. The inclusion $\iota : D(A) \to \mathscr{H}$ extends to a continuous map since $D(A)$ is dense in $\mathscr{Q}_A$. We need to show that this extension is one-to-one. Assume that $\iota\psi = 0$, $\psi \in \mathscr{Q}_A$ and take a sequence $(\psi_n)_{\mathbb{N}}$ in $D(A)$ converging to ψ in $\mathscr{Q}_A$. Then $(\iota\psi_n)_{\mathbb{N}} = (\psi_n)_{\mathbb{N}}$ converges to zero in $\mathscr{H}$, and
$$\|\psi\|^2_{\mathscr{Q}_A} = \lim_{n\to\infty}\lim_{m\to\infty}\left(\langle A\psi_n,\psi_m\rangle_{\mathscr{H}} + (M+1)\langle\psi_n,\psi_m\rangle_{\mathscr{H}}\right) = 0, \tag{3.24}$$
so $\psi = 0$. This ι is injective and $\iota\mathscr{Q}_A \subset \mathscr{H}$ is the domain of the closure
$$\overline{q}_A(\iota\psi,\iota\varphi) = \langle\psi,\varphi\rangle_{\mathscr{Q}_A} - (M+1)\langle\iota\psi,\iota\varphi\rangle_{\mathscr{H}}. \tag{3.25}$$
□

For A, $D(A)$ symmetric and bounded from below we call the domain of $\overline{q_A}$ the form-domain of A, and denote it by $Q(A)$.

Example 3.12. Let q be the form of Example 3.10 b). This form is neither closed nor closable: We can find a sequence $(f_n) \in C_0(\mathbb{R})$ with $f_n(0) = q(f_n, f_n) = 1$, $f_n \to 0$ in $L^2(\mathbb{R})$. Then $(f_n)_{\mathbb{N}}$ is Cauchy in the norm $\|\cdot\|_{\mathscr{Q}}$, since

$$\|f_n - f_m\|^2_{\mathscr{Q}} = \underbrace{q(f_n - f_m, f_n - f_m)}_{=0} + \|f_n - f_m\|^2_{\mathscr{H}}\,. \tag{3.26}$$

Consequently the inclusion $\iota : C_0(\mathbb{R}) \to L^2(\mathbb{R})$ does not extend to an injective map from the completion $\overline{\mathscr{Q}}$ to $L^2(\mathbb{R})$. The Proposition thus implies that this form is not associated with an operator.

Theorem 3.13 (Riesz-Friedrichs)**.** *Let q be a densely defined, bounded from below, and closed form with domain $\mathscr{Q}$. Then there exists a unique self-adjoint operator A, $D(A) \subset \mathscr{Q}$ on $\mathscr{H}$ such that $q = \overline{q_A}$.*

Proof. Without loss of generality $q = \langle \cdot, \cdot \rangle_{\mathscr{Q}}$. Let

$$\Gamma := \{(\psi, \varphi) \in \mathscr{Q} \times \mathscr{H} : \forall \eta \in \mathscr{Q} : q(\psi, \eta) = \langle \varphi, \eta \rangle_{\mathscr{H}}\}, \tag{3.27}$$

and

$$D := \{\psi \in \mathscr{Q} : \exists \varphi \in \mathscr{H} : (\psi, \varphi) \in \Gamma\}. \tag{3.28}$$

We start by showing that Γ is the graph of an operator A with dense domain $D := D(A)$.

Clearly Γ is a linear subspace of $\mathscr{Q} \times \mathscr{H}$. To see that it is a graph, we need to check that for any $\psi \in \mathscr{Q}$ there exists at most one $\varphi \in \mathscr{H}$ such that $(\psi, \varphi) \in \Gamma$. But if (ψ, φ) and $(\psi, \tilde{\varphi})$ are both in Γ, then also $(0, \varphi - \tilde{\varphi})$, and $\langle \varphi - \tilde{\varphi}, \eta \rangle_{\mathscr{H}} = 0$ for all $\eta \in \mathscr{Q}$. Since $\mathscr{Q}$ is dense, this implies $\varphi = \tilde{\varphi}$.

We have thus shown that Γ is the graph of an operator A with domain D. This operator is onto, for if $\varphi \in \mathscr{H}$ is arbitrary, then $\eta \mapsto \langle \varphi, \eta \rangle_{\mathscr{H}}$ is a continuous linear functional on $\mathscr{Q}$, and by Riesz' Theorem there is $\psi \in \mathscr{Q}$ s.th. $\langle \varphi, \eta \rangle_{\mathscr{H}} = \langle \psi, \eta \rangle_{\mathscr{Q}}$, i.e. $(\psi, \varphi) \in \Gamma$.

To show that D is dense, it is sufficient to prove that D is dense in $\mathscr{Q}$. Take $\eta \in D(A)^\perp$ (w.r.t. $\mathscr{Q}$). By surjectivity, there is $\psi \in D$ s.th. $A\psi = \eta$. Then

$$0 = \langle \psi, \eta \rangle_{\mathscr{Q}} = \|\eta\|^2_{\mathscr{H}} \tag{3.29}$$

so $\eta = 0$ and D is dense.

Clearly, A is symmetric, as for $\psi, \eta \in D(A)$

$$\langle A\psi, \eta \rangle_{\mathscr{H}} = \langle \psi, \eta \rangle_{\mathscr{Q}} = \overline{\langle \eta, \psi \rangle_{\mathscr{Q}}} = \overline{\langle A\eta, \psi \rangle_{\mathscr{H}}} = \langle \psi, A\eta \rangle_{\mathscr{H}}. \tag{3.30}$$

We also know that A is injective, since $\langle A\psi, \psi \rangle_{\mathscr{H}} = \|\psi\|^2_{\mathscr{Q}}$, and surjective – so $0 \in \rho(A)$. Since the resolvent set is open (see Theorem 1.14), there exists $\lambda \in \mathbb{R}$ s.th. $\{\pm \mathrm{i}\lambda\} \subset \rho(A)$, so A is self-adjoint by Theorem 3.1.

By construction, q is a closed extension of q_A, and since $D(A)$ is dense in $(\mathscr{Q}, \|\cdot\|_{\mathscr{Q}})$ it is equal to the closure $\overline{q_A}$.

It remains to prove uniqueness, so let $B, D(B)$ satisfy the required properties. By the definition of Γ, A extends B, but since both are self-adjoint this implies $A = B$. □

Remark 3.14. We see that self-adjoint and bounded from below operators are in one-to one correspondence with closed and bounded-from-below forms.

However, a form may be symmetric but have no closed extensions. A symmetric operator is automatically closable, but may have no self-adjoint extensions.

Corollary 3.15 (The Friedrichs Extension)**.** *Let A, $D(A)$ be symmetric and bounded from below and let $Q(A)$ be its form-domain (that exists by Proposition 3.11). Then there exists a unique self-adjoint extension A_F of A such that*

$$D(A) \subset D(A_F) \subset Q(A). \tag{3.31}$$

Moreover, $q_{A_F} = \overline{q_A}$.

Example 3.16 (The Dirichlet Laplacian)**.** Let $\Omega \subset \mathbb{R}^d$ be open, and define the quadratic form

$$q(f, f) = \int_\Omega |\nabla f(x)|^2 \mathrm{d}x \tag{3.32}$$

on $\mathscr{Q} = H^1_0(\Omega)$. For $f \in C_0^\infty(\Omega)$ we have

$$q(f, f) = -\int_\Omega \overline{f(x)} \Delta f(x) \mathrm{d}x. \tag{3.33}$$

Hence q is the closure of the quadratic form of $(-\Delta, C_0^\infty(\Omega))$.

This form is clearly symmetric and non-negative, so there is a unique self-adjoint extension of $(-\Delta, C_0^\infty(\Omega))$ with $D(-\Delta) \subset H^1_0(\Omega)$. This extension is called the *Dirichlet Laplacian*, or the Laplacian with *Dirichlet boundary conditions*.

If $\overline{\Omega}$ is compact, then this operator has compact resolvent: We have that $R_z(-\Delta) \to H^1_0(\Omega) \subset D(-\Delta)$ is bounded, and the embedding $\iota : H^1_0(\Omega) \to L^2(\Omega)$ is compact, by Rellich's Theorem. Thus $R_z(-\Delta) = \iota R_z(-\Delta)$ is compact. By Exercise T09, we thus have that $\sigma(-\Delta) = \sigma_p(-\Delta)$ is a discrete subset of $\mathbb{R}$. Since $q > 0$, $\sigma_p(-\Delta) \subset \mathbb{R}_+$, and since $-\Delta$ is not bounded, $\sigma_p(-\Delta)$ contains a sequence tending to infinity.

Formulated as a result in PDEs, this proves that if $\overline{\Omega}$ is compact, the equation

$$\begin{cases} (-\Delta + \lambda) f = g & \text{in } \Omega \\ f = 0 & \text{on } \partial\Omega \end{cases} \tag{3.34}$$

with $g \in L^2(\Omega)$ has a unique solution $f = R_{-\lambda}(-\Delta) g$ in $H^1(\Omega)$, except for λ in some discrete set, the spectrum of $-\Delta$.

If the boundary of Ω is sufficiently regular (say C^2) then $D(-\Delta) = H^1_0(\Omega) \cap H^2(\Omega)$. In this case the solution f above is an element of $H^2(\Omega)$.

Example 3.17 (Elliptic operators with rough coefficients)**.** We can go further and consider the form

$$q(f, f) = \int_\Omega a(x)|\nabla f(x)|^2 \mathrm{d}x \tag{3.35}$$

with $a \in L^\infty(\Omega)$, $a(x) \geq \gamma > 0$, on C_0^∞. This form is closable (since $\|\cdot\|_{\mathscr{Q}}$ is equivalent to the norm of $H^1(\Omega)$), so by the Riesz-Friedrichs Theorem it is associated to a non-negative self-adjoint operator with domain contained in $H_0^1(\Omega)$. However, its domain can be very complicated, as $\sum_{i=1}^d \partial_x^i a(x) \partial_x^i$ is not necessarily defined from $H^2(\Omega)$ (or $C^2(\Omega)$) to $L^2(\Omega)$, if a is not differentiable.

Example 3.18 (Robin boundary conditions on $\mathbb{R}_+$)**.** Let $\mathscr{H} = L^2(\mathbb{R}_+)$ and consider the operator $A_\theta := -\Delta$ on

$$D_\theta := \{f \in H^2(\mathbb{R}_+) : \cos(\pi\theta) f(0) - \sin(\pi\theta)(\tfrac{\mathrm{d}}{\mathrm{d}x} f)(0) = 0\} \tag{3.36}$$

for some $\theta \in [0, 1)$ (the boundary condition makes sense by Sobolev's Lemma). Note that $\theta = 0$ corresponds to the Dirichlet-condition $f(0) = 0$ and $\theta = 1/2$ to the Neumann condition $(\frac{\mathrm{d}}{\mathrm{d}x} f)(0) = 0$. Through integration by parts, we can express the quadratic form as

$$q_{A_\theta}(f, f) = \int_0^\infty |\tfrac{\mathrm{d}}{\mathrm{d}x} f(x)|^2 \mathrm{d}x - \begin{cases} \dfrac{-|f(0)|^2}{\tan(\pi\theta)} & \text{for } \theta \notin \{0, 1/2\} \\ 0 & \text{for } \theta \in \{0, 1/2\}. \end{cases} \tag{3.37}$$

The operator A is thus symmetric and bounded from below. There is thus a self-adjoint extension of A_θ for all θ. Its domain is contained in the domain of $\overline{q_{A_\theta}}$. This is

$$\mathscr{Q}_\theta = \begin{cases} H^1(\mathbb{R}_+) & \text{for } \theta \neq 0 \\ H_0^1(\mathbb{R}_+) & \text{for } \theta = 0. \end{cases} \tag{3.38}$$

We observe that the difference between the operators A_θ, which originally lies in the boundary conditions, is reflected in different ways on the form-level. In particular for the Neumann case $\theta = 1/2$ it is not evident how θ enters at all!

Theorem 3.19 (The KLMN Theorem)**.** *Let A, $D(A)$ be a self-adjoint operator and bounded from below. Let q be a densely symmetric form on $\mathscr{Q} \supset Q(A)$ and suppose there exist $b \geq 0$ and $0 < a < 1$ such that for all $\psi \in D(A)$*

$$|q(\psi, \psi)| \leq a q_A(\psi, \psi) + b \|\psi\|_{\mathscr{H}}^2 . \tag{3.39}$$

Then there exists a unique self-adjoint operator $B, D(B)$ with $Q(B) = Q(A)$ and

$$q_B = q_A + q. \tag{3.40}$$

Proof. We will show that $q_A + q$ has a closed extension to $Q(A)$, the result then follows from the Riesz-Friedrichs Theorem.

Without loss of generality A is positive. Define the form $\beta = q_A + q$ with domain $Q(A)$. β is clearly symmetric. We have, using the bound in the hypothesis,

$$\beta(\psi,\psi) \geq (1-a)q_A(\psi,\psi) - b\,\|\psi\|^2_{\mathscr{H}} \geq -b\,\|\psi\|^2\,, \tag{3.41}$$

so β is bounded from below by $-b$. Furtheremore

$$\beta(\psi,\psi) + (b+1)\,\|\psi\|^2 \leq a q_A(\psi,\psi) + (2b+1)\,\|\psi\|^2_{\mathscr{H}} \leq (2b+1)\,\|\psi\|^2_{Q(A)}\,, \tag{3.42}$$

and, by (3.41),

$$\|\psi\|^2_{Q(A)} = q_A(\psi,\psi) + \|\psi\|^2_{\mathscr{H}} \leq \frac{1}{1-a}\left(\beta(\psi,\psi) + (b+1)\,\|\psi\|^2\right), \tag{3.43}$$

so the norms induced by q_A and β are equivalent. Hence $Q(A)$ with the norm induced by β is complete and β is closed. By the Riesz-Friedrichs Theorem there thus exists a unique self-adjoint operator B, $D(B) \subset Q(A)$ with $\beta = q_B$. □

Example 3.20. Let $\mathscr{H} = L^2(\mathbb{R})$ and define a quadratic form on $H^2(\mathbb{R})$ by

$$\int |\tfrac{\mathrm{d}}{\mathrm{d}x} f|^2 \mathrm{d}x + |f(0)|^2, \tag{3.44}$$

i.e. the sum of the form of $-\Delta$ and the form from example (3.10) b). This is well defined because $H^2(\mathbb{R}) \hookrightarrow C(\mathbb{R})$ by Sobolev's Lemma. It satisfies the hypothesis of the KLMN theorem for the same reason (and interpolation, as in Example 3.7). Consequently, there is an associated self-adjoint and bounded below operator, even though part of the from is not associated with an operator.

3.1.2 Classification of Self-Adjoint Extensions

We now turn to the Classification of self-adjoint extensions of a symmetric operator A, $D(A)$. From Theorem 3.1 we already know that the spaces

$$\ker(A^* \mp \mathrm{i}) = \mathrm{ran}(A \pm \mathrm{i})^\perp \tag{3.45}$$

play an important role.

Definition 3.21. Let A, $D(A)$ be symmetric. We call

$$K_\pm := \ker(A^* \mp \mathrm{i}) \tag{3.46}$$

the *defect-spaces* of A, and

$$N_\pm := \dim K_\pm \tag{3.47}$$

the *defect indices.*

We know that A is essentially self-adjoint iff $N_+ = N_- = 0$. We will now show that A has self-adjoint extensions iff K_+ and K_- are isomorphic, so essentially if $N_+ = N_-$.

Definition 3.22. Let A, $D(A)$ be symmetric. We call

$$\begin{aligned} C_A &: \operatorname{ran}(A+\mathrm{i}) \to \operatorname{ran}(A-\mathrm{i}) \\ C_A &:= (A-\mathrm{i})(A+\mathrm{i})^{-1} \end{aligned}$$

the *Cayley transform* of A.

Note that C_A is not necessarily densely defined.

Lemma 3.23. *For any symmetric A, $D(A)$, the Cayley transform is isometric and onto.*

Proof. We have for all $\psi \in D(A)$

$$\|(A+\mathrm{i})\psi\|^2 = \|A\psi\|^2 + \|\psi\|^2 = \|(A-\mathrm{i})\psi\|^2 . \tag{3.48}$$

Thus, for $\varphi = (A+\mathrm{i})\psi \in \operatorname{ran}(A+\mathrm{i})$, we have $C_A\varphi = (A-\mathrm{i})\psi$, so C_A is onto, and

$$\|C_A\varphi\| = \|(A-\mathrm{i})\psi\| = \|(A+\mathrm{i})\psi\| = \|\varphi\| , \tag{3.49}$$

so C_A is isometric. □

Proposition 3.24. *A symmetric operator A, $D(A)$ is self-adjoint if and only if C_A is unitary.*

Proof. If A is self-adjoint, then C_A is a surjective isometry from $\operatorname{ran}(A+\mathrm{i}) = \mathscr{H}$ to $\operatorname{ran}(A-\mathrm{i}) = \mathscr{H}$ and thus unitary.

If C_A is unitary, then in particular $\operatorname{ran}(A \pm \mathrm{i}) = \mathscr{H}$, and A is self-adjoint. □

Lemma 3.25. *If $\tilde{A}$ is a symmetric extension of A then $C_{\tilde{A}}$ is an isometric extension of C_A. Conversely, for any isometric extension $\tilde{C}$ of C_A there is a symmetric extension $\tilde{A}$ of A.*

Proof. Let $A \subset \tilde{A}$. Then $\operatorname{ran}(A+\mathrm{i}) \subset \operatorname{ran}(\tilde{A}+\mathrm{i})$. Moreover, for $\varphi = (A+\mathrm{i})\psi$, $\psi \in D(A) \subset D(\tilde{A})$

$$C_{\tilde{A}}\varphi = (\tilde{A}-\mathrm{i})(\tilde{A}+\mathrm{i})^{-1}\varphi = (\tilde{A}-\mathrm{i})\psi = (A-\mathrm{i})\psi = C_A\varphi, \tag{3.50}$$

so $C_{\tilde{A}}$ extends C_A.

For the converse, let $\tilde{C} : L_+ \to L_-$ be an isometry with $\operatorname{ran}(A \pm \mathrm{i}) \subset L_\pm$. We claim that

$$\tilde{A} = \mathrm{i}(\tilde{C}+1)(\tilde{C}-1)^{-1} \tag{3.51}$$

$$D(\tilde{A}) = \operatorname{ran}(\tilde{C}-1) \tag{3.52}$$

is a symmetric extension of A. First, we show that this is well-defined by proving that $\tilde{C}-1$ is one-to-one. Assume that $\tilde{C}\psi = \psi$, then for $\varphi \in D(A)$:

$$\begin{aligned} -2\mathrm{i}\langle\psi,\varphi\rangle &= \langle\psi, ((A-\mathrm{i})-(A+\mathrm{i}))\,\varphi\rangle \\ &= \langle\psi, (C_A-1)(A+\mathrm{i})\varphi\rangle \\ &= \langle\psi, (\tilde{C}-1)(A+\mathrm{i})\varphi\rangle \\ &= \langle\tilde{C}\psi, \tilde{C}(A+\mathrm{i})\varphi\rangle - \langle\psi, (A+\mathrm{i})\varphi\rangle \\ &\overset{\text{isom.}}{=} 0. \end{aligned}$$

This implies $\psi = 0$ as $D(A)$ is dense.

This calculation shows that for $\varphi \in D(A)$

$$\varphi = \tfrac{\mathrm{i}}{2}(\tilde{C} - 1)(A + \mathrm{i})\varphi. \tag{3.53}$$

Using this, we see that $\tilde{A}$ extends A, since

$$\tilde{A}\varphi = \tfrac{\mathrm{i}}{2}\tilde{A}(\tilde{C} - 1)(A+\mathrm{i})\varphi = -\tfrac{1}{2}(\tilde{C}+1)(A+\mathrm{i})\varphi \overset{C_A \subset \tilde{C}}{=} -\tfrac{1}{2}(C_A+1)(A+\mathrm{i})\varphi = A\varphi. \tag{3.54}$$

To check symmetry of $\tilde{A}$, consider $\varphi = (\tilde{C} - 1)\psi \in D(\tilde{A})$, and compute

$$\langle \varphi, \tilde{A}\varphi\rangle = \mathrm{i}\langle(\tilde{C} - 1)\psi, (\tilde{C} + 1)\psi\rangle \overset{\text{isom.}}{=} \mathrm{i}\left(\langle \tilde{C}\psi, \psi\rangle - \langle \tilde{\psi}, \tilde{C}\psi\rangle\right) = 2\mathrm{Im}(\langle\psi, \tilde{C}\psi\rangle, \tag{3.55}$$

which is real, and by polarisation $\tilde{A}$ is symmetric. $\square$

Remark 3.26. Note that $\overline{C_A} = C_{\overline{A}}$, since if $\varphi_n = (A + \mathrm{i})\psi_n$ is convergent, the so is ψ_n (see also Theorem 3.1) and thus $(A+\mathrm{i})\psi_n \to (\overline{A}+\mathrm{i})\psi$. Consequently $\overline{C_A}$ maps $\mathrm{ran}(\overline{A}+\mathrm{i})$ isometrically to $\mathrm{ran}(\overline{A} + \mathrm{i})$, and since the isometric extension of C_A is unique it must equal $C_{\overline{A}}$.

Theorem 3.27. *Let A, $D(A)$ be symmetric, then there is a one-to-one correspondence between unitary maps from K_+ to K_- and self-adjoint extensions of A.*

Proof. Let $U : K_+ \to K_-$ be unitary. Then we define

$$\tilde{C} : \mathscr{H} = \overline{\mathrm{ran}(A + \mathrm{i})} \oplus K_+ \to \overline{\mathrm{ran}(A - \mathrm{i})} \oplus K_- \tag{3.56}$$

by $(\varphi, k) \mapsto (C_{\overline{A}}\varphi, Uk)$ (where C_A is extended to the closure by continuity, where it equals $C_{\overline{A}}$ as remarked above). Since the sum is orthogonal this defines a unitary extension of C_A, and by Lemma 3.25 a symmetric extension of A. This is self-adjoint by Proposition 3.24.

For the converse, let B be a self-adjoint extension of A. Then C_B is a unitary extension of C_A by Lemma 3.25 and Proposition 3.24. Thus $C_B|_{K_+}$ is a surjective isometry to its range. Since C_B is isometric and extends C_A, $\mathrm{ran}\, C_B|_{K_+} \subset K_-$, and since C_B is onto we must have equality. We thus have a surjective isometry $C_B : K_+ \to K_-$, and this is unitary by Exercise 01. $\square$

Corollary 3.28. *A symmetric operator A, $D(A)$ with finite deficiency indices has self-adjoint extensions if and only if $N_+ = N_-$. The self-adjoint extensions are then parametrised by the elements of $U(K_+, K_-) \cong U(N)$. The extension A_U corresponding to $U \in U(K_+, K_-)$ given by*

$$D(A_U) = D(\overline{A}) \oplus \mathrm{span}\{U\varphi_+ - \varphi_+ : \varphi_+ \in K_+\} \subset D(A) \oplus K_+ \oplus K_- \tag{3.57}$$

$$A_U(\psi + U\varphi_+ - \varphi_+) = \overline{A}\psi + \mathrm{i}(U\varphi_+ + \varphi_+). \tag{3.58}$$

Proof. Clearly there exist unitary maps between the finite dimensional spaces $K_\pm$ iff their dimensions are equal. By Lemma 3.25 the domain of the extension associated with U is

$$D(A_U) = \operatorname{ran}(C_U - 1) = \operatorname{ran}(\overline{C_A} - 1) \oplus \operatorname{ran}(U - 1). \tag{3.59}$$

Now $\operatorname{ran}(U-1) = \{U\varphi_+ - \varphi_+ : \varphi_+ \in K_+\}$ and $\operatorname{ran}(\overline{C_A} - 1) = D(\overline{A})$. The action of A_U on $\operatorname{ran}(U-1)$ is given by

$$A_U(U\varphi_+ - \varphi_+) = \mathrm{i}(C_U + 1)(C_U - 1)^{-1}(U\varphi_+ - \varphi_+) = \mathrm{i}(U\varphi_+ + \varphi_+). \tag{3.60}$$

□

Examples 3.29.

a) Let $P_+ = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}$ with $D(P_+) = C_0^1(\mathbb{R}_+) \subset L^2(\mathbb{R}^+)$. P_+ is symmetric, and we have $D(P_+^*) = H^1(\mathbb{R}_+)$. To calculate $K_\pm = \ker(P_+^* \mp \mathrm{i})$, consider the differential equations

$$-\mathrm{i}\tfrac{\mathrm{d}}{\mathrm{d}x} f(x) = \pm \mathrm{i} f(x), \qquad x > 0. \tag{3.61}$$

Their unique solutions are $f(x) = f(0)\mathrm{e}^{\mp x}$, which is an element of $L^2(\mathbb{R}_+)$ only for one of the possible signs. To relate this to P_+^*, use Sobolev's Lemma to see that $f(0)$ is well-defined, and since also $P_+^* f = \pm \mathrm{i} f$, $f \in K_\pm$ implies that $f \in H^2(\mathbb{R}_+) \subset C^1(\mathbb{R}_+)$. We deduce that $f \in K_\pm$ is a classical solution to the differential equation, and thus $N_+ = 1$, $N_- = 0$. There are no self-adjoint extensions of P_+.

b) Let $\mathscr{H} = L^2((0,1))$, $D(P_0) = C_0^1((0,1))$, $P_0 = -i\frac{\mathrm{d}}{\mathrm{d}x}$ (see Example 1.24 c), 2.21). We showed that $D(P_0^*) = H^1((0,1))$, and we have the identity

$$\langle f, P_0^* g\rangle - \langle P_0^* f, g\rangle = \mathrm{i}\left(\overline{f(1)}g(1) - \overline{f(0)}g(0)\right). \tag{3.62}$$

We will now classify all self-adjoint extensions of P_0 in terms of boundary conditions, first by elementary methods and then by applying Theorem 3.27.

Let $P_0 \subset A \subset P_0^*$ be a self-adjoint extension of P_0. Symmetry implies that for all $f \in D(A)$ we have $|f(0)|^2 = |f(1)|^2$, so there exists $\alpha \in S^1$ s.th. $f(0) = \alpha f(1)$. Hence

$$D(A) \subset \{f \in H^1(0,1) : f(0) = \alpha f(1)\} =: D(P_\alpha). \tag{3.63}$$

We will now prove that $P_\alpha = P_0^*|_{D(P_\alpha)}$ is self-adjoint for all $\alpha \in S^1$, and thus $A = P_\alpha$ (for some α).

Take $g \in D(P_\alpha) \subset D(P_0^*)$, then for every $f \in D(P_\alpha)$

$$\langle g, P_\alpha^* f\rangle = \langle P_0^* g, f\rangle + f(1)\left(\overline{g(1)} - \alpha\overline{g(0)}\right). \tag{3.64}$$

The right hand side defines a continuous linear functional of $f \in L^2((0,1))$ iff $\overline{g(1)} - \alpha\overline{g(0)} = 0$, so we must have we also have $g(0) = \overline{\alpha}^{-1} g(1) = \alpha g(1)$ and thus $g \in D(P_\alpha)$.

The operators P_α for $\alpha \in S^1$ are thus all self-adjoint extensions of P_0.

Now we will use the formalism of Theorem 3.27. We must first determine $K_\pm$. If $f \in H^1(0,1)$ is a solution of $-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x} f = \pm \mathrm{i} f$, then the weak derivative of f is continuous, so f is C^1. Since the unique solutions to the differential equation (with $f(0) = 1$) are $\mathrm{e}^{\mp x}$, and normalising in L^2 we set

$$f_+(x) := \frac{\sqrt{2}}{\sqrt{1-\mathrm{e}^{-2}}}\mathrm{e}^{-x}, \qquad f_-(x) := \frac{\sqrt{2}}{\sqrt{e^2-1}}\mathrm{e}^{x}. \tag{3.65}$$

We thus have $K_\pm = \operatorname{span}(f_\pm)$ and $N_+ = N_- = 1$. The unitary maps $K_+ \to K_-$ are of course parametrised by $U_\gamma f_+ = \gamma f_-$, $\gamma \in S^1$. Let A_γ be the self-adjoint extension associated to U_γ. By (3.52),

$$\begin{aligned} D(A_\gamma) = \operatorname{ran}(C_{A_\gamma} - 1) &= \operatorname{ran}(C_{\overline{P_0}} - 1) \oplus \operatorname{span}\left(U_\gamma f_+ - f_+\right) \\ &= H^1_0(0,1) \oplus \operatorname{span}\left(\gamma f_- - f_+\right). \end{aligned}$$

Consequently, $f \in D(A_\gamma)$ satisfies

$$\frac{f(0)}{f(1)} = \frac{\gamma - \mathrm{e}}{\mathrm{e}\gamma - 1} =: \alpha \qquad (\in S^1). \tag{3.66}$$

Hence $A_\gamma \subset P_\alpha$, and by self-adjointness we have equality.

Corollary 3.30 (Von Neumann's Theorem)**.** *Let J be a conjugation on $\mathscr{H}$, i.e. an anti-linear isometry with $J^2 = 1$. If A, $D(A)$ is a densely defined symmetric operator that commutes with J, then A has at least one self-adjoint extension.*

Proof. Note that commutation requires that $JD(A) \subset D(A)$ as well as $AJ = JA$. By $J = J^{-1}$ we then have $JD(A) = D(A)$. Now let $\psi \in K_+$. Then for all $\varphi \in D(A)$,

$$0 = \langle (A^* - \mathrm{i})\psi, \varphi\rangle \overset{\text{polarisation}}{=} \overline{\langle J\psi, J(A+\mathrm{i})\varphi\rangle} \overset{J \text{ anti-linear}}{=} \overline{\langle J\psi, (A-\mathrm{i})J\varphi\rangle}. \tag{3.67}$$

Since $J : D(A) \to D(A)$ is onto, this implies that $J\psi \in K_- = \operatorname{ran}(A-\mathrm{i})^\perp$. Since $J^2 = 1$ we obtain $JK_+ = K_-$, and the map $\psi \mapsto \langle J\psi, \cdot\rangle$ is a *linear*, surjective isometry from K_+ to K_-'. Thus, K_+ is isomorphic to K_-' and then also K_-, as Hilbert spaces. Hence, there exist unitary operators $K_+ \to K_-$, and by Theorem 3.27 self-adjoint extensions of A. □

3.2 The Spectral Theorem

We will start by discussing different ways of generalising the spectral theorem in finite dimensions and prove the equivalence of these generalisations. We will then prove the spectral theorem by proving one of the variants in Section 3.2.2.

The finite-dimensional spectral theorem can be formulated as:

Theorem. Let $\mathscr{H}$ be a finite-dimensional complex Hilbert space of dimension n and $A : \mathscr{H} \to \mathscr{H}$ be a self-adjoint linear map. There exists a unitary map $U : \mathscr{H} \to \mathbb{C}^n$ such that UAU^* is a diagonal matrix.

This can be reformulated in a way that is more amenable to generalisation as follows: We can think of an element of $\mathbb{C}^{\dim(\mathscr{H})}$ as a function from the finite set $f : \{1, \ldots, n\} \to \mathbb{C}$. The scalar product is then given by the standard form $\langle f, g\rangle = \sum_{j=1}^{n} \overline{f(j)}g(j)$. The sum is the integral with respect to the counting measure ζ, so we can identify $\mathbb{C}^n = L^2(\{1, \ldots, n\}, \zeta)$. A diagonal matrix $D = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$ then corresponds to the multiplication operator $Df = (j \mapsto \lambda_j f(j))$.

We thus have the equivalent formulation

Theorem. Let $\mathscr{H}$ be a finite-dimensional complex Hilbert space of dimension n and $A : \mathscr{H} \to \mathscr{H}$ be a self-adjoint linear map. There exists a unitary map $U : \mathscr{H} \to L^2(\{1, \ldots, n\}, \zeta)$ and a function $\lambda : \{1, \ldots, n\} \to \mathbb{R}$ such that UAU^* equals the operator of multiplication by λ.

Here it is more clear where we can modify the statement to accommodate more general cases by allowing for more general L^2-spaces. Consider the example of the Laplacian of $\mathscr{H} = L^2(\mathbb{R}^d)$, $H = -\Delta$, $D(H) = H^2(\mathbb{R})$. In this case, there exists a unitary map $U = \mathscr{F}$, $U : \mathscr{H} \to L^2(\mathbb{R}^d)$ such that $\mathscr{F}^{-1}H\mathscr{F}$ is multiplication by the function $p \mapsto p^2$. Hence, a modification of the theorem holds also for the unbounded operator H that has no eigenvalues.

Formulating the statement in this way, we immediately obtain the ability to define arbitrary functions of A, by composition with the function λ:

Corollary. Let $\mathscr{H}$ be a finite-dimensional complex Hilbert space of dimension n and $A : \mathscr{H} \to \mathscr{H}$ be a self-adjoint linear map. Let $\mathcal{A}$ be the algebra of functions from $\sigma(A)$ to $\mathbb{C}$. There exists a unique map

$$\Phi : \mathcal{A} \to \mathrm{B}(\mathscr{H}) \tag{3.68}$$

satisfying

i) Φ is a homomorphism of algebras,

ii) $\Phi(\overline{f}) = \Phi(f)^*$,

iii) $\Phi(1) = 1_{\mathscr{H}}$ and $\Phi(x \mapsto x) = A$.

Existence of Φ is clear, since $\Phi(f) = U^*(f \circ \lambda)U$ satisfies all the properties (note that $\sigma(A) = \operatorname{ran}(\lambda)$, so the composition makes sense exactly for functions f defined on $\sigma(A)$). Uniqueness follows from the fact that the polynomial functions $x \mapsto x^r$, $r = 0, \ldots, |\sigma(A)| - 1$ form a basis of the space of all functions on $\sigma(A)$, and by multiplicativity we must have $\Phi(x^r) = A^r$.

The map Φ is called the functional calculus, and we write $\Phi(f) =: f(A)$. Note that for an arbitrary linear map on $\mathscr{H}$ we can only define $f(A)$ if f is analytic near $\sigma(A)$, by power series.

On the other hand, the existence of a functional calculus implies that A is equivalent to multiplication operator, as we will now show.

Consider the linear map $f \mapsto \overline{\langle v, \Phi(f)v \rangle}$. By duality, there is an element $m_v \in \mathbb{C}^{\sigma(A)}$ such that $\langle v, \Phi(f)v \rangle = \sum_{a \in \sigma(A)} m_v(a) f(a)$. By *ii)*, m_v is real, and since for any non-negative $f = g^2$, $\langle v, \Phi(f)v \rangle_{\mathscr{H}} = \|\Phi(g)v\|^2 \geq 0$, m_v is non-negative. We can thus think of m_v as a measure.

Let $v \in \mathscr{H}$ be any vector and define the *cyclic subspace generated by* v as

$$\mathscr{H}_v := \operatorname{span}\{\Phi(f)v : f : \sigma(A) \to \mathbb{C}\}. \tag{3.69}$$

The vector v is called a cyclic vector (for A) if $\mathscr{H}_v = \mathscr{H}$. Then the map $f \mapsto \Phi(f)v$ induces an isomorphism from $L^2(\sigma(A), m_v)$ to $\mathscr{H}_v$, since it is onto by definition and

$$\langle \Phi(g)v, \Phi(f)v \rangle = \langle v, \Phi(\overline{g})\Phi(f)v \rangle = \langle v, \Phi(\overline{g}f)v \rangle = \sum_{a \in \sigma(A)} m_v(a)\overline{g}(a)f(a) = \langle g, f \rangle_{L^2(\sigma(A), m_v)}, \tag{3.70}$$

so in particular it is isometric.

If we denote this unitary map by U_v, then

$$(U_v^* A U_v f)(x) = (U_v^* \Phi(x \mapsto x)\Phi(f)v)(x) = (U_v^* \Phi(x \mapsto xf(x))v)(x) = xf(x), \tag{3.71}$$

so $U_v^* A U_v$ acts as multiplication by $x \in \sigma(A)$. Since $\mathscr{H}$ is finite dimensional, there are finitely many $v_1, \dots, v_k$ such that

$$\mathscr{H} = \bigoplus_{j=1}^{k} \mathscr{H}_{v_j}, \tag{3.72}$$

the map

$$U^* := \bigoplus_{j=1}^{k} U_v^* : \mathscr{H} \to L^2\left(\sigma(A) \times \{1, \dots, k\}, m_{v_1} \otimes \cdots \otimes m_{v_k}\right) \tag{3.73}$$

is unitary, and $U^* A U$ acts as multiplication with $x \in \sigma(A)$. We see that A is equivalent to a multiplication operator if and only if A has a functional calculus. Note also that depending on the starting point we find different representations of A as a multiplication operator on different spaces, so this is not unique.

There is a different way to formulate the spectral theorem:

Theorem. Let $\mathscr{H}$ be a finite-dimensional complex Hilbert space and $A : \mathscr{H} \to \mathscr{H}$ be a self-adjoint linear map. Then there exists an orthonormal basis of $\mathscr{H}$ consisting of eigenvectors of A.

Of course, an operator on an infinite dimensional space may not have eigenvectors at all, so this will not generalise as such. More abstractly, we can forget about the eigenvectors and just consider the corresponding subspaces, or their orthogonal projections. We have the following properties:

- For every Borel subset $B \subset \mathbb{R}$, there exists an orthogonal projection $P(B)$ on $\mathscr{H}$ $(= \sum_{a \in B \cap \sigma(A)} P_a)$.

- If $B_1, B_2 \subset \mathbb{R}$ are disjoint, then $P(B_1) + P(B_2) = P(B_1 \cup B_2)$,
- $P(\mathbb{R}) = 1$

So we can think of the family $(P_B)_{B \in \mathscr{B}(\mathbb{R})}$ as a measure on $\mathbb{R}$ (σ-additivity is easy to check), taking values in the orthogonal projections on $\mathscr{H}$ – a projection-valued-measure (PVM). This PVM is called the *spectral measure* of A. For all $v \in \mathscr{H}$, $B \mapsto \langle v, P(B)v\rangle$ defines an actual measure μ_v. The operator A then has the representation

$$\langle v, Av\rangle = \sum_{a \in \sigma(A)} \langle v, aP_a v\rangle = \int a\mu_v(\mathrm{d}a). \tag{3.74}$$

The measure μ_v is called the *spectral measure* of v with respect to A. By polarisation, the formula above together with knowledge of μ_v for all $v \in \mathscr{H}$ completely determine A and the family of projections $(P_B)_{B \in \mathscr{B}(\mathbb{R})}$. We thus write

$$A = \int_{\mathbb{R}} aP(\mathrm{d}a). \tag{3.75}$$

Our reformulation of the spectral theorem in terms of PVM's is then

Theorem. Let $\mathscr{H}$ be a finite-dimensional complex Hilbert space and $A : \mathscr{H} \to \mathscr{H}$ be a self-adjoint linear map. There exists a unique projection-valued measure $P : \mathscr{B}(\mathbb{R}) \to \mathrm{B}(\mathscr{H})$ such that

$$A = \int_{\mathbb{R}} aP(\mathrm{d}a). \tag{3.76}$$

Moreover, for any real function $f \in C(\mathbb{R})$, the formula

$$\forall v \in \mathscr{H} : \langle v, \Phi(f)v\rangle = \int_{\mathbb{R}} f(a)\mu_v(\mathrm{d}a) \tag{3.77}$$

determines $\Phi(f)$, and thus the functional calculus of A.

Now consider the example of the Laplacian on $\mathbb{R}^d$ as above. For any Borel set $B \subset \mathbb{R}$, we define the corresponding projection $P(B)$ as the projection to those functions whose Fourier transform has support in $\{p \in \mathbb{R}^d : p^2 \subset B\}$, i.e.,

$$P(B) = \mathscr{F}^{-1}\chi_B(p^2)\mathscr{F}, \tag{3.78}$$

where χ is the operator of multiplication by the characteristic function. This clearly satisfies the properties listed above (σ-additivity is not clear, we will see in what sense it holds later). Let $f \in D(H) = H^2(\mathbb{R}^d)$, then

$$\begin{aligned}
\mu_f(B) = \langle f, P(B)f\rangle &= \int_{\mathbb{R}^d} \chi_B(p^2)|\hat{f}(p)|^2\mathrm{d}p \\
&= \int_0^\infty \chi_B(p^2) \int_{S^{d-1}} |\hat{f}(\omega p)|^2 \mathrm{d}\omega r^{d-1}\mathrm{d}r \\
&= \int_B \left(\int_{S^{d-1}} |\hat{f}(\omega\sqrt{a})|^2\mathrm{d}\omega\right) \tfrac{1}{2}a^{(d-2)/2}\mathrm{d}a,
\end{aligned}$$

so μ_f is absolutely continuous w.r.t. to the Lebesgue measure on $\mathbb{R}$ with density given above. Thus by the same integral transformations

$$\langle f, Hf\rangle = \int_{\mathbb{R}^d} p^2|\hat{f}(p)|^2 \mathrm{d}p = \int_{\mathbb{R}} a\mu_f(\mathrm{d}a) \tag{3.79}$$

holds.

3.2.1 Variants of the Spectral Theorem and Their Equivalence

We will now formulate more precisely the variants of the spectral theorem discussed above and prove their equivalence according to the following scheme

$$\begin{aligned}&\exists \text{ functional calculus } \Longrightarrow \text{ equivalence to multiplication operator}\\ &\Longrightarrow \exists \text{ spectral measure } \Longrightarrow \exists \text{ funct. calc.}\end{aligned}$$

Definition 3.31. Let $\mathcal{A}$ be a subalgebra of B^∞ (the bounded Borel-measureable functions from $\mathbb{R}$ to $\mathbb{C}$ *without* identification on null sets) that is invariant under complex conjugation. A map $\Phi : \mathcal{A} \to \mathrm{B}(\mathscr{H})$ is a continuous $*$-morphism if

a) Φ is linear,

b) Φ is multiplicative: $\forall f, g \in \mathcal{A}$: $\Phi(fg) = \Phi(f)\Phi(g)$,

c) Φ is involutive: $\forall f \in \mathcal{A}$: $\Phi(\overline{f}) = \Phi(f)^*$,

d) if the constant function $x \mapsto 1$ is in $\mathcal{A}$, then $\Phi(1) = 1_{\mathscr{H}}$,

e) Φ is bounded: $\|\Phi(f)\|_{\mathrm{B}(\mathscr{H})} \leq \|f\|_\infty$.

Note that if Φ is bounded at all, then the constant must be one, for if there exists a function f, with $|f| \leq 1$ and $\|\Phi(f)\psi\|_{\mathscr{H}} > 1$ for some normalised ψ, then $|f|^2 \leq 1$, and

$$\left\|\Phi(|f|^2)\psi\right\|_{\mathscr{H}} = \sup_{\|\eta\|=1} \langle \eta, \Phi(f)^*\Phi(f)\psi\rangle \geq \|\Phi(f)\psi\|^2 . \tag{3.80}$$

Hence if the bound on Φ is larger than $a > 1$, then it is also larger than $a^2 > a > 1$, and thus infinity.

Definition 3.32. Let A, $D(A)$ be a closed operator and $\sigma(A) \subset \mathbb{R}$. A *continuous functional calculus* for A is a continuous $*$-morphism $\Phi : C_\infty(\mathbb{R}) \to \mathrm{B}(\mathscr{H})$ such that for $z \in \mathbb{C} \setminus \mathbb{R}$, $\Phi((x-z)^{-1}) = R_z(A)$.

Theorem 3.33. *Let A, $D(A)$ be a closed operator on $\mathscr{H}$ with $\sigma(A) \subset \mathbb{R}$ that admits a continuous functional calculus. There exists a measure space (Ω, Σ, μ), a function $\lambda : \Omega \to \mathbb{R}$ and and a unitary map $U : L^2(\Omega, \mu) \to \mathscr{H}$ such that*

- *$U^*D(A) = D(M_\omega) = \{f \in L^2(\Omega) : \omega \mapsto \lambda(\omega)f(\omega) \in L^2(\Omega)\}$.*
- *$U^*AU = M_\lambda$, the operator of multiplication by λ.*

In particular, A is self-adjoint. If $\mathscr{H}$ is separable then μ is σ-finite.

Proof. Let $\psi \in \mathscr{H}$ be a normalised vector, and define a linear functional on $C_\infty(\mathbb{R})$ by

$$\ell_\psi(f) = \langle \psi, f(A)\psi \rangle_{\mathscr{H}}, \tag{3.81}$$

where $f(A) := \Phi(f)$ is defined by the functional calculus. This linear functional is continuous and positive, since

$$\ell_\psi(|f|^2) = \|f(A)\psi\|^2 \geq 0. \tag{3.82}$$

By the Riesz-Markov Theorem [RS1, Thm.IV.18] there exists a unique measure μ_ψ on $\mathbb{R}$ such that

$$\ell_\psi(f) = \int_{\mathbb{R}} f(x)\mu_\psi(\mathrm{d}x) \tag{3.83}$$

The measure of an open set $V \subset \mathbb{R}$ is given by

$$\mu_\psi(V) = \sup\{\ell_\psi(f) : f \in C_\infty(\mathbb{R}) \text{ with } f|_{V^c} = 0 \text{ and } f|_V \leq 1\}, \tag{3.84}$$

so in particular $\mu_\psi(\mathbb{R}) \leq \|\psi\|^2 = 1$. Now define the cyclic subspace generated by ψ as

$$\mathscr{H}_\psi := \overline{\{f(A)\psi : f \in C_\infty(\mathbb{R})\}}. \tag{3.85}$$

We claim that $f \mapsto f(A)\psi$ induces a unitary

$$U_\psi : L^2(\mathbb{R}, \mu_\psi) \to \mathscr{H}_\psi \tag{3.86}$$

This is well defined, since if $f(A)\psi = g(A)\psi$, then

$$0 = \|f(A)\psi - g(A)\psi\|^2_{\mathscr{H}} = \int |f(x) - g(x)|^2 \mu_\psi(\mathrm{d}x), \tag{3.87}$$

so $f(x) = g(x)$ for μ_ψ-a.e. x. The map is clearly isometric and onto, so it is unitary.

If $\mathscr{H}_\psi = \mathscr{H}$, then we are almost finished, since on the dense set spanned by the elements $\varphi = f(A)\psi$,

$$U(x-z)^{-1}U^*\varphi = U(x-z)^{-1}U^*f(A)\psi = U(x-z)^{-1}f(x) = R_z(A)f(A)\psi = R_z(A)\varphi, \tag{3.88}$$

and thus

$$U\{f \in L^2(\mathbb{R}, \mu_\psi) : xf(x) \in L^2(\mathbb{R}, \mu_\psi)\} = U\mathrm{ran}(x - \mathrm{i})^{-1} = \mathrm{ran}\, R_{\mathrm{i}}(A) = D(A), \tag{3.89}$$

and

$$(U^*AU - \mathrm{i})\,(x - \mathrm{i})^{-1} = U^*(A - \mathrm{i})R_z(A) = 1 = (x - \mathrm{i})^{-1}\,(U^*AU - \mathrm{i})\,. \tag{3.90}$$

To finish the proof if $\mathscr{H} \neq \mathscr{H}_\psi$, first note that, by the reasoning above,

$$f(A)\mathscr{H}_\psi \subset \mathscr{H}_\psi \tag{3.91}$$

for all $f \in C_\infty(\mathbb{R})$. Then also $f(A)\mathscr{H}_\psi^\perp \subset \mathscr{H}_\psi^\perp$, since for every $\varphi \in \mathscr{H}_\psi = (\mathscr{H}_\psi^\perp)^\perp$ and $\eta \in \mathscr{H}_\psi^\perp$

$$\langle \varphi, f(A)\eta\rangle = \langle \overline{f}(A)\varphi, \eta\rangle = 0.$$

The domain $D(A) \cap \mathscr{H}_\psi^\perp = \operatorname{ran} R_z(A)|_{\mathscr{H}_\psi^\perp}$ is thus dense, and $A|_{\mathscr{H}_\psi^\perp}$ admits a continuous functional calculus, and we can iterate our argument. To complete the proof, we must thus show that $\mathscr{H}$ is a direct sum of A-invariant cyclic subspaces $\mathscr{H}_{\psi_i}$. We will do this using Zorn's Lemma.

Let $\mathcal{I}$ be the subset of the set of collections of closed linear subspaces of $\mathscr{H}$ such that for all $I \in \mathcal{I}$

- $V, W \in I \implies V \perp W$,
- $V \in I \implies \exists \psi \in \mathscr{H}$: $V = \mathscr{H}_\psi$ is the A-cyclic subspace generated by ψ.

The set $\mathcal{I}$ is partially ordered by inclusion. Now let $\mathcal{J} \subset \mathcal{I}$ be a totally ordered set, then

$$K = \bigcup_{J \in \mathcal{J}} J = \{V \subset \mathscr{H} : \exists J \in \mathcal{J} \text{ with } V \in J\}. \tag{3.92}$$

The elements of K are clearly A-cyclic subspaces of $\mathscr{H}$. They are mutually orthogonal, since if $V, W \in K$, $V \in J \in \mathcal{J}$, $W \in I \in \mathcal{J}$, then either $I \subset J$ or $J \subset I$, since $\mathcal{J}$ is totally ordered, and thus $V \perp W$. Hence, $K \in \mathcal{I}$ and $J \leq K$ for all $J \in \mathcal{J}$, i.e. every totally ordered set has an upper bound in $\mathcal{I}$. Thus, by Zorn's Lemma, there exists a maximal element $M \in \mathcal{I}$. Setting

$$\mathscr{H}_M := \bigoplus_{V \in M} V, \tag{3.93}$$

we must have $\mathscr{H}_M = \mathscr{H}$, since otherwise there exists $0 \neq \psi \in \mathscr{H}_M^\perp$ and $M \cup \{\mathscr{H}_\psi\} \supset M$. Note that the direct sum is in the sense of Hilbert spaces, i.e. we take the completion (or closure in $\mathscr{H}$) of the linear span. Then, by definition of $\mathcal{I}$ (and choice), there exists a subset $C \subset \mathscr{H}$ such that

$$\mathscr{H} = \bigoplus_{V \in M} V = \bigoplus_{\psi \in C} \mathscr{H}_\psi. \tag{3.94}$$

Then

$$U := \bigoplus_{\psi \in C} U_\psi : \bigoplus_{\psi \in C} L^2(\mathbb{R}, \mu_\psi) \to \mathscr{H} \tag{3.95}$$

is unitary. We have

$$\bigoplus_{\psi \in C} L^2(\mathbb{R}, \mu_\psi) = L^2(\mathbb{R} \times C, \mu) \tag{3.96}$$

by the identification $f(x)_\psi := f(x, \psi)$, where the measure is given by

$$\mu(E) = \sum_{\psi \in C} \mu_\psi(\pi_{\mathbb{R}}(E \cap (\mathbb{R} \times \{\psi\}))), \tag{3.97}$$

where $\pi_{\mathbb{R}} : \mathbb{R} \times S \to \mathbb{R}$ is the projection to the first factor (as σ-algebra one can take the product of the Borel sets on $\mathbb{R}$ and the σ-algebra generated by finite subsets of C).

If $\mathscr{H}$ is separable, then the set C can be at most countable, so μ is σ-finite because the μ_ψ are finite. □

Corollary 3.34 (Measurable functional Calculus)**.** *Let A, $D(A)$ admit a continuous functional calculus. There exists a continuous $*$-morphism $\Phi : B^\infty(\mathbb{R}) \to \mathrm{B}(\mathscr{H})$ such that $\forall z \in \mathbb{C} \setminus \mathbb{R}$: $\Phi((x-z)^{-1}) = R_z(A)$. Moreover, for every bounded sequence $(f_n)_{n\in\mathbb{N}}$ that converges point-wise to f, $\Phi(f_n)$ converges to $\Phi(f)$ in the strong operator topology.*

Proof. In view of Theorem 3.33, we define the measurable functional calculus by

$$f(A) := U M_{f\circ\lambda} U^*. \tag{3.98}$$

Then $\|(f_n(A) - f(A))\psi\|_{\mathscr{H}} = \|((f_n - f)\circ\lambda)U^*\psi\|_{L^2(\Omega,\mu)}$, and for a bounded sequence f_n,

$$\lim_{n\to\infty} \|(f_n - f)\circ\lambda U^*\psi\|^2_{L^2(\Omega,\mu)} = \lim_{n\to\infty} \int_{\mathbb{R}} |f_n(\lambda(\omega)) - f(\lambda(\omega))|^2 \mu_\psi(\mathrm{d}\omega) = 0, \tag{3.99}$$

by dominated convergence, since μ_ψ is a finite measure. □

Remark 3.35. The extension of the functional calculus from continuous functions to measurable functions is unique (this follows from Lusin's theorem).

Definition 3.36. A *projection-valued-measure* (PVM) is a map $P : \mathscr{B}(\mathbb{R}) \to \mathrm{B}(\mathscr{H})$ satisfying

1. $\forall B \in \mathscr{B}(\mathbb{R})$, $P(B)$ is an orthogonal projection, i.e. $P(B)^2 = P(B) = P(B)^*$;
2. $P(\mathbb{R}) = 1_{\mathscr{H}}$ and $P(\varnothing) = 0$;
3. P is strongly σ-additive: For every disjoint family of Borel sets $(B_n)_{n\in\mathbb{N}}$ and every $\psi \in \mathscr{H}$
$$P\left(\bigcup_{n\in\mathbb{N}} B_n\right)\psi = \lim_{N\to\infty} \sum_{n=1}^{N} P(B_n)\psi \tag{3.100}$$

Proposition 3.37. *Let A, $D(A)$ admit a measurable functional calculus. Then $B \mapsto P_A(B) := \chi_B(A)$ defines a PVM. Moreover,*

$$D(A) = \{\psi \in \mathscr{H} : \int \lambda^2 \mu_\psi(\mathrm{d}\lambda) < \infty\}, \tag{3.101}$$

and

$$\langle \psi, A\psi\rangle := \int \lambda \mu_\psi(\mathrm{d}\lambda). \tag{3.102}$$

Proof. The map $\chi_B(A)$, where χ_B is the characteristic function of B, defines an orthogonal projection because χ_B is real and $\chi_B^2 = \chi_B$. Strong σ-additivity follows from Corollary 3.34, since for a disjoint family of sets, $\sum_{n=1}^N \chi_{B_n}$ converges point-wise to $\chi_{\cup_n B_n}$ and is bounded by one.

The Isomorphism $U_\psi : L^2(\mathbb{R}, \mu_\psi) \to \mathscr{H}_\psi$ from the proof of Theorem 3.33 maps the constant function $f \equiv 1$ to ψ, so $\psi \in D(A) \Leftrightarrow \int \lambda^2 \mu_\psi(\mathrm{d}\lambda) < \infty$. The representation of A then follows from the fact that $U_\psi^* A U_\psi = M_\lambda$. □

Definition 3.38. Let P be a PVM and for any $\varphi, \psi \in \mathscr{H}$ define the complex measure

$$\mu_{\varphi,\psi}(B) := \langle \varphi, P(B)\psi \rangle. \tag{3.103}$$

For any $f \in B^\infty(\mathbb{R})$ the integral of f with respect to P, denoted $\int f(x)P(\mathrm{d}x)$ is defined to be the unique bounded operator such that for every $\varphi, \psi \in \mathscr{H}$

$$\langle \varphi, \int f(x)P(\mathrm{d}x)\psi \rangle := \int f(x)\mu_{\varphi,\psi}(\mathrm{d}x). \tag{3.104}$$

Of course, the measures $\mu_{\varphi,\psi}$ can be obtained from the measures $\mu_\psi = \mu_{\psi,\psi}$ by polarisation:

$$\mu_{\varphi,\psi} = \tfrac{1}{4}(\mu_{\psi+\varphi} - \mu_{\psi-\varphi}) - \tfrac{\mathrm{i}}{4}(\mu_{\psi+\mathrm{i}\varphi} - \mu_{\psi-\mathrm{i}\varphi}). \tag{3.105}$$

Proposition 3.39. *Let P be a PVM on $\mathscr{H}$. Then $\Phi(f) := \int f(\lambda)P(\mathrm{d}\lambda)$ defines a continuous $*$-morphism from $B^\infty(\mathbb{R})$ to $\mathrm{B}(\mathscr{H})$ and there exists a unique self-adjoint operator A, $D(A)$ such that $\Phi((x-z)^{-1}) = R_z(A)$.*

Proof. Linearity follows directly from the properties of the integral. Boundedness follows from the fact that $\mu_\psi(\mathbb{R}) = \|\psi\|^2$ by

$$\begin{aligned} \|\Phi(f)\| &= \sup_{\varphi,\psi\in\mathscr{H}, \|\varphi\|=\|\psi\|=1} |\langle \varphi, \Phi(f)\psi\rangle| \\ &\leq \|f\|_\infty \tfrac{1}{4} \left(\mu_{\psi+\varphi}(\mathbb{R}) + \mu_{\psi-\varphi}(\mathbb{R}) + \mu_{\psi+\mathrm{i}\varphi}(\mathbb{R}) + \mu_{\psi-\mathrm{i}\varphi}(\mathbb{R})\right) \\ &\leq 4\|f\|_\infty . \end{aligned}$$

For multiplicativity, consider first characteristic functions χ_B. Clearly $\Phi(\chi_B) = P(B)$. Since

$$P(B_1)P(B_2) = P(B_1 \cap B_2) = \Phi(\chi_{B_1 \cap B_2}) = \Phi(\chi_{B_1}\chi_{B_2}), \tag{3.106}$$

multiplicativity holds for (multiples of) characteristic functions. By linearity, it then holds for simple functions, and then by continuity for all functions in $B^\infty(\mathscr{H})$, since these can be approximated uniformly by step functions. The same argument shows that $\Phi(f)^* = \Phi(\overline{f})$, since this also holds for χ_B. With multiplicativity and involutivity we then obtain the improved bound

$$\|\Phi(f)\psi\|^2 = \langle \psi, \Phi(f)^*\Phi(f)\psi\rangle = \langle \psi, \Phi(|f|^2)\psi\rangle \leq \|f\|_\infty^2 \mu_\psi(\mathbb{R}) = \|f\|_\infty^2 \|\psi\|^2 . \tag{3.107}$$

We have thus shown that the integral w.r.t. P defines a continuous $*$-morphism.

It remains to show that the family of operators $\Phi(f)$ is associated with a self-adjoint operator A. This follows from the Lemma below if we can show that there is no nonzero $\psi \in \mathscr{H}$ that is contained in all of the kernels of $\Phi((x-z)^{-1})$, $z \in \mathbb{C} \setminus \mathbb{R}$. Assume to the contrary that there exist such ψ. Then for all $\lambda \neq 0$

$$0 = \lambda \langle \psi, \Phi((x - \mathrm{i}\lambda)^{-1}\psi) \rangle = \int \frac{\lambda}{x - \mathrm{i}\lambda} \mu_\psi(\mathrm{d}x). \tag{3.108}$$

But by dominated convergence

$$\lim_{\lambda\to\infty} \int \frac{\lambda}{x - \mathrm{i}\lambda} \mu_\psi(\mathrm{d}x) = \mathrm{i} \int \mu_\psi = \mathrm{i}\, \|\psi\|^2 \,, \tag{3.109}$$

so $\psi = 0$. The claim now follows from the Lemma below. □

Lemma 3.40. *Let $U \subset \mathbb{C}$ be an open set and invariant under complex conjugation. Let $\{R(z), z \in U\}$ be a family of bounded operators on $\mathscr{H}$ satisfying*

1. *$\forall z \in U$:$R(z)^* = R(\overline{z})$,*
2. *$\forall z, w \in U$: $R(z) - R(w) = (z - w)R(z)R(w)$*
3. *$\bigcap_{z\in U} \ker R(z) = \{0\}$.*

Then there exists a unique self-adjoint operator A, $D(A)$ on $\mathscr{H}$ such that $U \subset \rho(A)$ and $R(z) = R_z(A)$.

Proof. By 2), we have $\ker R(z) = \ker R(w)$, so all of the $R(z)$ are injective. We thus tentatively define $D(A) = \operatorname{ran} R(z_0)$ for some $z_0 \in U$. This is independent of z_0, since for all $w \in U$

$$R(z_0)\psi = R(w)\psi + (z_0 - w)R(w)R(z_0)\psi \in \operatorname{ran} R(w), \tag{3.110}$$

It is also dense, since if $\psi \in D(A)^\perp$, then $\psi \in \ker R(z_0)^* = \ker R(\overline{z_0}) = \{0\}$.

Now set $A(z) := R(z)^{-1} + z$, which is well-defined on $D(A)$. To see that this is independent of z, we use again 2) and the fact that $A(z)R(z) = 1 + zR(z)$ in

$$\begin{aligned} A(z)R(w) &= A(z)R(z) + (w - z)A(z)R(z)R(w) \\ &= 1 + zR(z) + (w - z)(1 + zR(z))R(w) \\ &= 1 + zR(z) + (w - z)R(w) + z(R(w) - R(z)) \\ &= 1 + wR(w) = A(w)R(w). \end{aligned}$$

This shows that $A(z)R(w)\psi = A(w)R(w)\psi$ for all $\psi \in \mathscr{H}$, so $A(w) = A(z)$. This implies that A is symmetric, since for $\varphi = R(\overline{z})\tilde{\varphi}, \psi \in D(A)$

$$\langle \varphi, A\psi \rangle = \langle R(\overline{z})\tilde{\varphi}, (R(z)^{-1} + z)\psi \rangle = \langle \tilde{\varphi}, \psi \rangle + \langle \overline{z} R(\overline{z})\tilde{\varphi}, \psi \rangle = \langle (R(\overline{z})^{-1} + \overline{z})\varphi, \psi \rangle, \tag{3.111}$$

and $R(\overline{z})^{-1} + \overline{z} = A$. Since $\operatorname{ran} A - z = \operatorname{ran} R(z)^{-1} = \mathscr{H}$ for all $z \in U$. Since U is invariant by conjugation this proves that A is self-adjoint, by Theorem 3.1. Uniqueness of A is clear since the inverse is unique. □

3.2.2 Proof of the Spectral Theorem

We will now prove the spectral theorem. To this end, we first prove existence of a functional calculus for continuous functions. We then state the spectral theorem in multiplication operator form, and in PVM form, as follows from the equivalence shown in the previous section.

Definition 3.41. The *one-point compactification* of $\mathbb{R}$ is the set $\overline{\mathbb{R}} := \mathbb{R} \cup \{\infty\}$ with the topology such that $U \subset \overline{\mathbb{R}}$ is open iff

- $U \subset \mathbb{R}$ is open, or
- there exists a compact set $K \subset \mathbb{R}$ such that $U = \overline{\mathbb{R}} \setminus K (= \{\infty\} \cup \mathbb{R} \setminus K)$.

Note that $\overline{\mathbb{R}}$ is homeomorphic to the circle S^1 via stereographic projection. Let $\mathcal{A}$ be the algebra of continuous functions such that their limits for $x \to \pm\infty$ exist and are equal. Then $\mathcal{A}$ is isomorphic to $C(\overline{\mathbb{R}})$ by setting $f(\infty) = \lim_{x\to\pm\infty} f(x)$.

Theorem 3.42 (Continuous Functional Calculus)**.** *Let A, $D(A)$ be a self-adjoint operator on a complex Hilbert space $\mathscr{H}$. There exists a unique continuous $*$-morphism $\Phi : C(\overline{\mathbb{R}}) \to \mathrm{B}(\mathscr{H})$ such that for $z \in \mathbb{C} \setminus \mathbb{R}$, $\Phi((x-z)^{-1}) = R_z(A)$. In particular, A admits a continuous functional calculus.*

For the proof, recall (see [RS1, Thm.IV.10])

Theorem (Stone-Weierstrass)**.** Let X be a compact Hausdorff space and $\mathcal{A} \subset C(X)$ a subalgebra. Suppose that

- $\mathcal{A}$ separates points: $\forall x \neq y \in X\ \exists f \in \mathcal{A}$: $f(x) \neq f(y)$,
- $\mathcal{A}$ is invariant under conjugation: $f \in \mathcal{A} \implies \overline{f} \in \mathcal{A}$
- $1 \in \mathcal{A}$,

then $\overline{\mathcal{A}} = C(X)$.

Proof of Theorem 3.42. Let $\mathcal{A} \subset C(\overline{\mathbb{R}})$ be the algebra generated by the constant function $x \mapsto 1$ and the functions $x \mapsto (x-z)^{-1}$ for $z \in \mathbb{C} \setminus \mathbb{R}$. This algebra consists of finite linear combinations of finite products of generating elements. By the requirements that $\Phi(1) = 1_{\mathscr{H}}$ and $\Phi((x-z)^{-1}) = R_z(A)$ (which exists by self-adjointness of A 3.3) together with multiplicativity, we must have

$$\Phi\left(\prod_{j=1}^{m}(x-z_j)^{-1}\right) = \prod_{j=1}^{m} R_{z_j}(A). \tag{3.112}$$

This is well-defined because $R_z(A)$ and $R_w(A)$ commute, by the resolvent formula. By linearity, this extends uniquely to a homomorphism $\Phi : \mathcal{A} \to \mathrm{B}(\mathscr{H})$. This homomorphism is involutive since $R_z(A)^* = R_{\overline{z}}(A)$, because A is self-adjoint.

If this is continuous, then it extends to the closure of $\mathcal{A}$ in $C(\overline{\mathbb{R}})$. By the Stone-Weierstrass Theorem, this equals $C(\overline{\mathbb{R}})$. This gives existence, and since Φ is uniquely determined on the dense set $\mathcal{A}$ also uniqueness.

We thus only need to prove boundedness of Φ. We deduce this from the fact that if $f \in \mathcal{A}$ is a non-negative function, then $f = |g|^2$ for some $g \in \mathcal{A}$, which is proved in Lemma 3.43 below.

Consider now the non-negative function $x \mapsto \|f\|_\infty^2 - |f(x)|^2$. By Lemma 3.43 there exists $g \in \mathcal{A}$ such that $\|f\|_\infty^2 - |f(x)|^2 = |g(x)|^2$. We then have

$$\Phi(|f|^2) = \Phi(f)^*\Phi(f) = \Phi(\|f\|_\infty^2 - |g|^2) = \|f\|_\infty^2 - \Phi(g)^*\Phi(g), \tag{3.113}$$

and thus for all $\psi \in \mathscr{H}$

$$\|\Phi(f)\psi\|^2 = \langle \psi, \|f\|_\infty^2 \psi\rangle - \|\Phi(g)\psi\|^2 \leq \|f\|_\infty^2 \|\psi\|^2 . \tag{3.114}$$

□

It remains to prove the existence of the "square root" of positive elements of $\mathcal{A}$.

Lemma 3.43. *Let $\mathcal{A} \subset C(\overline{\mathbb{R}})$ be the algebra generated by the constant function $x \mapsto 1$ and the functions $x \mapsto (x-z)^{-1}$ for $z \in \mathbb{C} \setminus \mathbb{R}$. If $f \in \mathcal{A}$ is a non-negative function, then there exists $g \in \mathcal{A}$ with $f = |g|^2$.*

Proof. Let $f \in \mathcal{A}$ be a generic element. By bringing all terms to a common denominator, we can write

$$f(x) = \frac{P(x)}{Q(x)} \tag{3.115}$$

with complex polynomials P, Q such that $\deg P \leq \deg Q$ and Q has no real roots. We can reduce this fraction so that P and Q have no common roots and Q is normalised. Writing

$$P(x) = c \prod_{j=1}^{J} (x - a_j)^{m_j} \prod_{k=1}^{K} (x - w_k)^{p_k}, \tag{3.116}$$

where a_j, $j = 1, \dots, J$ are the real roots of P and w_k, $k = 1, \dots, K$ the roots in $\mathbb{C} \setminus \mathbb{R}$, and

$$Q(x) = \prod_{\ell=1}^{L} (x - z_\ell)^{q_\ell}. \tag{3.117}$$

Then f is a real function if and only if for all $x \in \mathbb{R}$ $\overline{P(x)}Q(x) = P(x)\overline{Q(x)}$, i.e.,

$$\overline{c} \prod_{k=1}^{K} (x - \overline{w}_k)^{p_k} \prod_{\ell=1}^{L} (x - z_\ell)^{q_\ell} = c \prod_{k=1}^{K} (x - w_k)^{p_k} \prod_{\ell=1}^{L} (x - \overline{z}_\ell)^{q_\ell}. \tag{3.118}$$

This implies that c, the coefficient of the highest-order term, is real. Furthermore, since P and Q have no common roots, this also shows that for all $k = 1, \dots, K$, $\overline{w}_k$ is a root of P with the same multiplicity as w_k, and the same for Q. Hence, a real function $f \in \mathcal{A}$ has the form (after re-numbering the roots)

$$f(x) = c \prod_{j=1}^{J} (x - a_j)^{m_j} \frac{\prod_{k=1}^{K/2} |x - w_k|^{2p_r}}{\prod_{\ell=1}^{L/2} |x - z_\ell|^{2q_\ell}}. \tag{3.119}$$

This function is non-negative iff all the m_j are even and $c \geq 0$, and in that case $f(x) = |g(x)|^2$ with

$$g(x) = \sqrt{c} \prod_{j=1}^{J} (x - a_j)^{m_j/2} \frac{\prod_{k=1}^{K/2} (x - w_k)^{p_r}}{\prod_{\ell=1}^{L/2} (x - z_\ell)^{q_\ell}}. \tag{3.120}$$

By partial fraction decomposition, g is an element of $\mathcal{A}$ and the proof is complete. □

In view of the equivalences of the previous section, we have now proved the following two variants of the spectral theorem.

Theorem 3.44 (Spectral Theorem in Multiplication Operator Form)**.** *Let A, $D(A)$ be a self-adjoint operator on a complex Hilbert space $\mathscr{H}$. There exists a measurable space (Ω, Σ), a measure μ on $(\sigma(A) \times \Omega, \mathscr{B}(\mathbb{R}) \otimes \Sigma)$ and a unitary map $U : L^2(\sigma(A) \times \Omega, \mu) \to \mathscr{H}$ such that*

- $U^* D(A) = D(M_\lambda) = \{f \in L^2(\sigma(A) \times \Omega) : (\lambda, \omega) \mapsto \lambda f(\lambda, \omega) \in L^2(\sigma(A) \times \Omega)\}$.
- $U^* A U = M_\lambda$, *the operator of multiplication by* $(\lambda, \omega) \mapsto \lambda$.

If $\mathscr{H}$ is separable then Ω is countable and μ is σ-finite.

Proof. This follows from the existence of the functional calculus by Theorem 3.33, since $C_\infty(\mathbb{R}) \subset C(\overline{\mathbb{R}})$. □

Theorem 3.45 (Spectral Theorem in PVM form)**.** *Let $\mathscr{H}$ be a Hilbert space. The densely defined self-adjoint operators on $\mathscr{H}$ are in one-to-one correspondence with the PVMs on $\mathscr{H}$.*

More precisely, for any self-adjoint operator A, $D(A)$, the functional calculus defines a PVM by $B \mapsto P_A(B) := \chi_B(A)$. We have

$$D(A) = \{\psi \in \mathscr{H} : \int \lambda^2 \mu_\psi(\mathrm{d}\lambda) < \infty\}, \tag{3.121}$$

and

$$\langle \psi, A\psi \rangle := \int \lambda \mu_\psi(\mathrm{d}\lambda). \tag{3.122}$$

Conversely, for any PVM P, choosing $D(A)$ and A as above defines a self-adjoint operator A, $D(A)$, and $\chi_B(A) = P(B)$.

Proof. This follows from the Spectral Theorem in Multiplication Operator Form and Propositions 3.37, 3.39. □

3.3 Applications of the spectral theorem

3.3.1 Unitary groups

Let A, $D(A)$ be a self-adjoint operator and consider the abstract Schrödinger equation:

$$\begin{cases} \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}\psi(t) = A\psi(t) \\ \quad \psi(0) = \psi_0. \end{cases} \tag{3.123}$$

We can define by the functional calculus the operator $\mathrm{e}^{-\mathrm{i}tA}$. Formally $t \mapsto \psi(t) = \mathrm{e}^{-\mathrm{i}tA}\psi_0$ is a solution to the abstract Schrödinger equation. Since the functional calculus is multiplicative, we have

$$\mathrm{e}^{-\mathrm{i}(t+s)A} = \mathrm{e}^{-\mathrm{i}tA}\mathrm{e}^{-\mathrm{i}sA}, \tag{3.124}$$

and

$$(\mathrm{e}^{-\mathrm{i}tA})^{-1} = \mathrm{e}^{\mathrm{i}tA} = (\mathrm{e}^{-\mathrm{i}tA})^*, \tag{3.125}$$

so for every t this operator is unitary. This is called the unitary group generated by A (and A is called the generator).

We will now explain in which sense exactly these groups solve the Schrödinger equation, and the question of uniqueness of this solution.

Lemma 3.46. *Let A, $D(A)$ be a self-adjoint and $U(t) := \mathrm{e}^{-\mathrm{i}tA}$ be the unitary group generated by A. We have*

1. $\forall t, s \in \mathbb{R}$: $U(t)U(s) = U(t+s)$
2. $\forall t \in \mathbb{R}$: $U(-t) = U(t)^*$
3. $U(0) = 1_{\mathscr{H}}$
4. *U is strongly continuous:* $\forall \psi \in \mathscr{H}$: $\lim_{t\to 0} U(t)\psi = \psi$.
5. $\forall t \in \mathbb{R}$: $U(t)D(A) \subset D(A)$
6. *U is strongly differentiable on $D(A)$ and solves* (3.123)*:* $\forall \psi \in D(A)$*:*

$$\frac{\mathrm{d}}{\mathrm{d}t}U(t)\psi := \lim_{h\to 0} \frac{U(t+h)\psi - U(t)\psi}{h} = -\mathrm{i}AU(t)\psi. \tag{3.126}$$

Proof. Properties 1)-3) follow directly from the functional calculus. Since $\mathrm{e}^{-\mathrm{i}t\lambda}$ converges to one point-wise as $t \to 0$ and is bounded, 4) follows from continuity of the calculus w.r.t. such limits, see Corollary 3.34. Note that by the group property 1) this implies continuity in all $t \in \mathbb{R}$, not just $t = 0$.

5) is clear since for a multiplication operator with a real function $D(A) = D(A\mathrm{e}^{-\mathrm{i}tA})$.

For 6) it is again enough to prove this for $t = 0$. There we have, by the same argument as in Corollary 3.34,

$$\left\| \left(h^{-1}(U(h) - 1) + \mathrm{i}A \right) \psi \right\|^2_{\mathscr{H}} = \int |h^{-1}(\mathrm{e}^{-\mathrm{i}h\lambda} - 1) + \mathrm{i}\lambda|^2 \mu_\psi(\mathrm{d}\lambda). \tag{3.127}$$

This tends to zero by dominated convergence if $\lambda^2 \in L^1(\mathbb{R}, \mu_\psi)$, which by the Spectral Theorem (in PVM form) is equivalent to $\psi \in D(A)$. $\square$

For general $\psi \in \mathscr{H}$, $\mathrm{e}^{-\mathrm{i}tA}\psi$ is not differentiable but only continuous. It is still a solution to the Schrödinger equation in the following weak sense: Let $\varphi \in D(A)$, then

$$\langle \varphi, \mathrm{e}^{-\mathrm{i}tA}\psi \rangle = \langle \mathrm{e}^{\mathrm{i}tA}\varphi, \psi \rangle \tag{3.128}$$

is differentiable in t, and the derivative equals

$$-\mathrm{i}\langle A\varphi, \psi \rangle. \tag{3.129}$$

We interpret this as a linear functional on $D(A)$, which is a Banach space with the graph norm. Hence, $\mathrm{e}^{-\mathrm{i}tA}\psi$ is differentiable when interpreted as a function $t \mapsto D(A)'$, and its derivative equals $\varphi \mapsto -\mathrm{i}\langle A\varphi, \psi \rangle$. We call any function $t \mapsto \psi(t)$ with this property a weak solution to the Schrödinger equation.

Proposition 3.47. *Let $I \subset \mathbb{R}$ be an open interval containing zero and $\psi(t) \in C(I, \mathscr{H}) \cap C^1(I, D(A)')$ be a weak solution to the Schrödinger equation with $\psi(0) = \psi_0$. Then $\psi(t) = \mathrm{e}^{-\mathrm{i}At}\psi_0$.*

Proof. Let $\varphi_0 \in D(A)$ and consider the quantity $f(t) = \langle \mathrm{e}^{-\mathrm{i}tA}\varphi_0, \psi(t) \rangle$. We have $f \in C^1(I)$, and using the equations satisfied by $\psi(t)$ and $\mathrm{e}^{-\mathrm{i}tA}\varphi_0$

$$\tfrac{\mathrm{d}}{\mathrm{d}t} f(t) = \mathrm{i}\langle A\mathrm{e}^{-\mathrm{i}tA}\varphi_0, \psi(t) \rangle - \mathrm{i}\langle A\mathrm{e}^{-\mathrm{i}tA}\varphi_0, \psi(t) \rangle = 0. \tag{3.130}$$

Consequently $f(t) = f(0) = \langle \varphi_0, \psi_0 \rangle$, and

$$\langle \varphi_0, \mathrm{e}^{\mathrm{i}At}\psi(t) - \psi_0 \rangle = 0 \tag{3.131}$$

for all $\psi \in D(A)$, whence $\mathrm{e}^{\mathrm{i}At}\psi(t) = \psi_0$ and $\psi(t) = \mathrm{e}^{-\mathrm{i}At}\psi_0$. $\square$

Example 3.48. In quantum mechanics, the evolution of a system is described by the Schrödinger equation with a self-adjoint operator of the form

$$H = -\Delta + V, \tag{3.132}$$

where V is a multiplication operator (cf. Example 3.7).

We have now established that, under the hypothesis ensuring that H is self-adjoint on some domain $D(H) \subset L^2(\mathbb{R}^d)$ this equation has a unique solution. The solution operator $U(t)$ maps the initial condition to the state at time t. The unitarity of this map is important, since $|\psi(t)|^2$ is to be interpreted as a probability density (Born's rule), so unitarity ensures that total probability is conserved.

We will now prove that any linear "dynamical system" in $\mathscr{H}$ that is implemented by unitary maps comes from a solution to an abstract Schrödinger equation.

Theorem 3.49 (Stone's Theorem)**.** *Let $t \mapsto U(t) \in \mathrm{B}(\mathscr{H})$ be a strongly continuous unitary group, that is*

1. *$\forall t, s \in \mathbb{R}$: $U(t)U(s) = U(t+s)$*

2. *$U(0) = 1_{\mathscr{H}}$*

3. *U is strongly continuous: $\forall \psi \in \mathscr{H}$: $\lim_{t\to 0} U(t)\psi = \psi$.*

Then there exists a self-adjoint operator A, $D(A)$ on $\mathscr{H}$ such that $U(t) = \mathrm{e}^{-\mathrm{i}tA}$.

Proof. The idea is to define $A = \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}U|_{t=0}$, the main challenge being to find a suitable dense domain.

Set

$$D := \{\psi \in \mathscr{H} : \exists \lim_{h\to 0} h^{-1}(U(h)-1)\psi\}. \tag{3.133}$$

We start by proving that D is dense. For this, let $\psi \in \mathscr{H}$ be arbitrary and consider for $\varepsilon > 0$ the vector ψ_ε defined by

$$\forall \varphi \in \mathscr{H} : \langle \varphi, \psi_\varepsilon \rangle = \frac{1}{\varepsilon}\int_0^\varepsilon \langle \varphi, U(t)\psi\rangle \mathrm{d}t. \tag{3.134}$$

We will show that $\psi_\varepsilon \to \psi$ as $\varepsilon \to 0$ and $\psi_\varepsilon \in D$. For the first point, note that by dominated convergence

$$\frac{1}{\varepsilon}\int_0^\varepsilon \langle \varphi, U(t)\psi\rangle \mathrm{d}t = \int_0^1 \langle \varphi, U(\varepsilon t)\psi\rangle \mathrm{d}t \to \langle \varphi, \psi\rangle, \tag{3.135}$$

so $\psi_\varepsilon \rightharpoonup \psi$ weakly in $\mathscr{H}$. Since also

$$\|\psi_\varepsilon\|^2 = \frac{1}{\varepsilon^2}\int_0^\varepsilon\int_0^\varepsilon \langle U(s)\psi, U(t)\psi\rangle \mathrm{d}s\mathrm{d}t = \int_0^1\int_0^1 \langle \psi, U(\varepsilon(t-s))\psi\rangle \mathrm{d}s\mathrm{d}t \to \|\psi\|^2, \tag{3.136}$$

we have $\psi_\varepsilon \to \psi$ in norm (compare Exercise T00.3).

Now to see that $\psi_\varepsilon \in D$ for fixed $\varepsilon > 0$ and $h < \varepsilon$, consider

$$\begin{aligned}
\langle \varphi, h^{-1}(U(h)-1)\psi_\varepsilon\rangle &= \frac{1}{h\varepsilon}\int_0^\varepsilon \langle \varphi, U(t+h) - U(t)\psi\rangle \mathrm{d}t \\
&= \frac{1}{h\varepsilon}\int_h^{h+\varepsilon} \langle \varphi, U(t)\psi\rangle - \frac{1}{h\varepsilon}\int_0^\varepsilon \langle \varphi, U(t)\psi\rangle \mathrm{d}t \\
&= \frac{1}{h\varepsilon}\int_0^h \langle \varphi, U(t+\varepsilon)\psi\rangle - \frac{1}{h\varepsilon}\int_0^h \langle \varphi, U(t)\psi\rangle \mathrm{d}t.
\end{aligned}$$

By the argument that shows $\psi_\varepsilon \to \psi$, the vector defined by the first term converges to $\varepsilon^{-1}U(\varepsilon)\psi$, and the second to $-\varepsilon^{-1}\psi$ as $h \to 0$, so in particular the limit exists and $\psi_\varepsilon \in D$.

We will now prove that $A := \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}U|_{t=0}$ is essentially self-adjoint on D. To check that A is symmetric, let $\varphi, \psi \in D$, then

$$\langle \varphi, A\psi\rangle = \lim_{h\to 0}\langle \varphi, \mathrm{i}h^{-1}(U(h)-1)\psi\rangle = \lim_{h\to 0}\langle \mathrm{i}h^{-1}(1-U(-h))\varphi, \psi\rangle = \langle A\varphi, \psi\rangle. \tag{3.137}$$

To prove essential self-adjointness, suppose that $\varphi \in \ker(A + \mathrm{i})$ (the argument for $-\mathrm{i}$ is the same). Then for $\psi \in D(A)$:

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\langle\varphi, U(t)\psi\rangle = \langle\varphi, -\mathrm{i}AU(t)\psi\rangle = \langle\varphi, U(t)\psi\rangle. \tag{3.138}$$

The unique solution to the differential equation above then is $\langle\varphi, U(t)\psi\rangle = \mathrm{e}^t\langle\varphi, \psi\rangle$. But since U is an isometry this gives for all $t \in \mathbb{R}$

$$\mathrm{e}^t\langle\varphi, \psi\rangle \leq \|\varphi\|\,\|\psi\|\,, \tag{3.139}$$

whence $\langle\varphi, \psi\rangle = 0$ for all $\psi \in D(A)$, and thus $\varphi = 0$. Hence, A is essentially self-adjoint on D and $\overline{A}$ is self-adjoint (actually A is already closed, but we will not show this). Then $\mathrm{e}^{-\mathrm{i}\overline{A}t}\psi$ and $U(t)\psi$ are both solutions to the abstract Schrödinger equation for $\psi \in D$. By the uniqueness of this solution, Proposition 3.47, we thus have $U(t) = \mathrm{e}^{-\mathrm{i}\overline{A}t}$, first on D and then by continuity on $\mathscr{H}$. □

Remark 3.50. Stone's theorem can be read as a classification of all unitary representations of the group $(\mathbb{R}, +)$ subject to the condition of strong continuity.

Without the continuity condition there are additional representations. For example, let $\mathscr{H} = \mathbb{C}$ and $F : \mathbb{R} \to \mathbb{R}$ be $\mathbb{Q}$-linear (i.e., we view $\mathbb{R}$ as a vector space over $\mathbb{Q}$). Then $U(t) = \mathrm{e}^{\mathrm{i}F(t)}$ is a unitary representation of $\mathbb{R}$, which continuous only if F is a multiple of the identity.

Examples 3.51.

- **The translation group on** $\mathbb{R}$. Define on $L^2(\mathbb{R})$, $(U(t)f)(x) := f(x-t)$. This is clearly a strongly continuous unitary group. For $f \in \mathscr{S}(\mathbb{R})$ we can calculate the generator
$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} f(x-t) = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}f. \tag{3.140}$$
Hence the generator is a self-adjoint extension of the operator $P_{\min}$ of Example 2.18 a). But this operator is essentially self-adjoint, with unique self-adjoint extension P given by $(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}, H^1(\mathbb{R}))$. We thus have
$$f(x-t) = (\mathrm{e}^{-\mathrm{i}tP}f)(x) = (\mathrm{e}^{-t\frac{\mathrm{d}}{\mathrm{d}x}}f)(x). \tag{3.141}$$

- **Translations on** $[0,1]$. If we want to define a unitary translation on the interval $[0,1]$ we have to make sure that no mass is lost at the boundaries. This can be achieved by identifying the boundary points and setting for $0 \leq t \leq 1$
$$(U(t)f)(x) = \begin{cases} f(x-t) & 1 \geq x-t > 0 \\ f(x-t+1) & 0 > x-t \geq -1. \end{cases} \tag{3.142}$$
More generally, we can set for $\theta \in [0, 2\pi)$
$$(U_\theta(t)f)(x) = \begin{cases} f(x-t) & 1 \geq x-t > 0 \\ \mathrm{e}^{-\mathrm{i}\theta}f(x-t+1) & 0 \geq x-t \geq -1. \end{cases} \tag{3.143}$$

The generator is always given by the local expression $-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}$, but the domain depends on θ. Note that the set of functions with $f(1) = \mathrm{e}^{-\mathrm{i}\theta} f(0)$ is invariant under U_θ. U_θ is thus the group generated by P_α from Example 3.29 b) with $\alpha = \mathrm{e}^{\mathrm{i}\theta}$.

Geometrically, all of these groups correspond to translations on a vector bundle over the circle, with different identifications of the fibres at $x = 0$ and $x = 1$. The operators P_α are different connections on the vector bundle $S^1 \times \mathbb{R}$.

- **Right Translation on** $\mathbb{R}_+$. Define an isometry $T(t) : L^2(\mathbb{R}_+) \to L^2(\mathbb{R}_+)$ by

$$(T(t)f)(x) := \begin{cases} 0 & x \le t \\ f(x-t) & x > t. \end{cases} \tag{3.144}$$

By differentiating one can see that this solves the equation

$$\frac{\mathrm{d}}{\mathrm{d}t} f = -\frac{\mathrm{d}}{\mathrm{d}x} T(t) f, \tag{3.145}$$

but the derivative can exist in $x = 0$ only if $f(x) = 0$, so the generator is $(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}, H_0^1(\mathbb{R}_+))$. We saw in Example 3.29 a) that this is not self-adjoint. This is reflected in the fact that $T(t)$ is not unitary as $\operatorname{ran}(T(t)) \subset L^2(t, \infty)$.

We also have a perturbation theory for unitary groups:

Theorem 3.52. *Suppose $A, D(A)$, $B, D(B)$ are self-adjoint and $A + B$ self-adjoint on $D(A + B) = D(A) \cap D(B)$. Then for all $t \in \mathbb{R}$*

$$\mathrm{e}^{-\mathrm{i}(A+B)t} = \mathrm{s} - \lim_{n\to\infty} \left(\mathrm{e}^{-\mathrm{i}\frac{t}{n}A} \mathrm{e}^{-\mathrm{i}\frac{t}{n}B} \right)^n \tag{3.146}$$

Proof. Since the difference of the two expressions is uniformly bounded (by two), it is sufficient to prove strong convergence on the dense set $D((A+B)^2)$. Now set $\tau = \frac{t}{n}$ and note that

$$\left(\mathrm{e}^{-\mathrm{i}\tau A}\mathrm{e}^{-\mathrm{i}\tau B}\right)^n - \mathrm{e}^{-\mathrm{i}(A+B)t} = \sum_{j=0}^{n-1} \left(\mathrm{e}^{-\mathrm{i}\tau A}\mathrm{e}^{-\mathrm{i}\tau B}\right)^{n-1-j} \left(\mathrm{e}^{-\mathrm{i}\tau A}\mathrm{e}^{-\mathrm{i}\tau B} - \mathrm{e}^{-\mathrm{i}(A+B)\tau}\right) \left(\mathrm{e}^{-\mathrm{i}(A+B)\tau}\right)^j . \tag{3.147}$$

Consequently

$$\left\| \left(\mathrm{e}^{-\mathrm{i}\tau A}\mathrm{e}^{-\mathrm{i}\tau B}\right)^n - \mathrm{e}^{-\mathrm{i}(A+B)t}\psi \right\| \le |t| \max_{s \le t} F_\tau(s) \tag{3.148}$$

with

$$F_\tau(s) = \left\| \tfrac{1}{\tau} \left(\mathrm{e}^{-\mathrm{i}\tau A}\mathrm{e}^{-\mathrm{i}\tau B} - \mathrm{e}^{-\mathrm{i}(A+B)\tau} \right) \mathrm{e}^{-\mathrm{i}(A+B)s}\psi \right\| . \tag{3.149}$$

For $\varphi \in D(A + B)$,

$$\lim_{\tau\to 0} \tfrac{1}{\tau} \left(\mathrm{e}^{-\mathrm{i}\tau A}\mathrm{e}^{-\mathrm{i}\tau B} - \mathrm{e}^{-\mathrm{i}(A+B)\tau} \right) \varphi = 0, \tag{3.150}$$

so we have convergence of $F_\tau(s) \to 0$, for every s. To improve this to uniform convergence in s, note that in particular we have a bound

$$\left\| \tfrac{1}{\tau} \left(\mathrm{e}^{-\mathrm{i}\tau A}\mathrm{e}^{-\mathrm{i}\tau B} - \mathrm{e}^{-\mathrm{i}(A+B)\tau} \right) \varphi \right\| \le C_\varphi . \tag{3.151}$$

Now $D(A+B)$ with the graph norm is a Banach space, so by the uniform boundedness principle, there exists a constant such that

$$\left\| \tfrac{1}{\tau} \left(\mathrm{e}^{-\mathrm{i}\tau A} \mathrm{e}^{-\mathrm{i}\tau B} - \mathrm{e}^{-\mathrm{i}(A+B)\tau} \right) \varphi \right\| \leq C \left\| \varphi \right\|_{D(A+B)} . \tag{3.152}$$

Consequently,

$$\begin{aligned} |F_\tau(s) - F_\tau(r)| &\leq \left\| \tfrac{1}{\tau} \left(\mathrm{e}^{-\mathrm{i}\tau A} \mathrm{e}^{-\mathrm{i}\tau B} - \mathrm{e}^{-\mathrm{i}(A+B)\tau} \right) \left(\mathrm{e}^{-\mathrm{i}(A+B)s} - \mathrm{e}^{-\mathrm{i}(A+B)r} \right) \psi \right\| \\ &\leq C \left\| \left(1 - \mathrm{e}^{-\mathrm{i}(A+B)(s-r)} \right) \psi \right\|_{D(A+B)} \leq C' |s-r|, \end{aligned}$$

as $\psi \in D((A+B)^2)$. Now assume that

$$\limsup_{\tau \to 0} \max_{s \leq t} F_\tau(s) > 0. \tag{3.153}$$

Then there exists a sequence $\tau_n \to 0$ and $s(\tau_n)$ such that

$$\limsup_{n \to \infty} F_{\tau_n}(s_n) > 0. \tag{3.154}$$

But the sequence s_n has a convergent subsequence $s_n \to s$, and since $\lim_{n \to \infty} F_{\tau_n}(s) = 0$ and $|F_{\tau_n}(s_n) - F_{\tau_n}(s)| < C|s_n - s|$ we must have convergence to zero. This shows that

$$\lim_{\tau \to 0} \max_{s \leq t} F_\tau(s) = 0. \tag{3.155}$$

□

3.3.2 Spectrum and Dynamics

If ψ is an eigenfunction of a self-adjoint operator A, $D(A)$, then the action of the unitary group $\mathrm{e}^{-\mathrm{i}tA}$ is very simple – the orbit $\mathrm{e}^{-\mathrm{i}tA}$ is periodic. We will now discuss a more sophisticated way of relating the spectrum of A to the dynamics.

Definition 3.53. Let μ be a finite measure on $(\mathbb{R}, \mathscr{B}(\mathbb{R}))$. We define:

- μ is *supported on* a set M if $\mu(M^c) = 0$;
- the *support* of μ is

$$\operatorname{supp}(\mu) = \{x \in \mathbb{R} | \forall \varepsilon > 0 : \mu((x-\varepsilon, x+\varepsilon) > 0\} = \bigcap \{C \subset \mathbb{R} \text{ closed} : \mu(C^c) = 0\}. \tag{3.156}$$

- μ is *pure-point* if μ is supported on a finite or countable set;
- μ is *continuous* (w.r.t. the Lebesgue measure) if μ and has no atoms, i.e. for all $x \in \mathbb{R}$: $\mu(\{x\}) = 0$;
- μ is *absolutely continuous* (w.r.t. the Lebesgue measure) if every Lebesgue null set is a μ null set,

- μ is *singular* (w.r.t. the Lebesgue measure) if μ is supported on a set of Lebesgue measure zero;
- μ is *singular-continuous* (w.r.t. the Lebesgue measure) if μ is singular and has no atoms. Then μ is supported on an uncountable set of Lebesgue measure zero (such as the Cantor set).

Remark 3.54. In terms of the function $F(t) = \mu((0, t])$ this means:

- μ continuous $\Leftrightarrow$ F continuous;
- μ absolutely continuous $\Leftrightarrow$ F absolutely continuous, i.e. $f = F'$ exists a.e. and $\int_0^t f(s)\mathrm{d}s = F(t)$ (cf. the Radon-Nikodym Theorem);

We have the Lebesgue decomposition decompose any measure μ as $\mu = \mu_{pp} + \mu_{ac} + \mu_{sc}$, with measures having the respective properties. We can also decompose $\mathbb{R} = M_{pp} \cup M_{ac} \cup M_{sc}$, such that $\mu_\bullet$ is supported on $M_\bullet$. However, this decomposition is not unique.

Now let $\psi \in \mathscr{H}$ and let μ_ψ denote the spectral measure of ψ w.r.t A.

Definition 3.55. Let A, $D(A)$ be a self-adjoint operator on $\mathscr{H}$. We define the following subspaces of $\mathscr{H}$:

- $\mathscr{H}_{pp} := \{\psi \in \mathscr{H} : \mu_\psi \text{ is pure-point}\}$
- $\mathscr{H}_{c} := \{\psi \in \mathscr{H} : \mu_\psi \text{ is continuous}\}$
- $\mathscr{H}_{ac} := \{\psi \in \mathscr{H} : \mu_\psi \text{ is absolutely continuous}\}$
- $\mathscr{H}_{sc} := \{\psi \in \mathscr{H} : \mu_\psi \text{ is singular continuous}\}$

Proposition 3.56. *The following hold true:*

a) $\mathscr{H}_{pp} = \overline{\mathrm{span}\{\psi \in \mathscr{H} : \psi \textit{ is an eigenvector of } A\}}$*,*

b) $\mathscr{H}_c = \mathscr{H}_{pp}^\perp$*,*

c) $\mathscr{H}_{sc} = \{\psi \in \mathscr{H}_c : \exists \textit{ Leb. null set } M : P_A(M)\psi = \psi\}$ *and this subspace is closed,*

d) $\mathscr{H}_{ac} = \mathscr{H}_c \cap \mathscr{H}_{sc}^\perp$*.*

In particular, $\mathscr{H} = \mathscr{H}_{pp} \oplus \mathscr{H}_{ac} \oplus \mathscr{H}_{sc}$ *and this sum is orthogonal.*

Proof. a): "$\supset$" If ψ is in the closure of the span of eigenvectors, there exist normalised mutually orthogonal eigenvectors $(\psi_n)_{\mathbb{N}}$ and coefficients $(a_n)_{\mathbb{N}}$ so that $\psi = \sum_{n=1}^\infty a_n \psi_n$. Let M be the corresponding countable set of eigenvalues. Then the spectral measure of ψ_n is supported on a single point in M and

$$\mu_\psi(M) = \langle \psi, P_A(M)\psi\rangle = \sum_{n=1}^\infty |a_n|^2 \langle \psi_n, P_A(M)\psi_n\rangle = \sum_{n=1}^\infty |a_n|^2 = \|\psi\|^2 = \mu_\psi(\mathbb{R}). \tag{3.157}$$

Thus $\operatorname{supp}(\mu_\psi) \subset M$ is countable and $\psi \in \mathscr{H}_{pp}$.

"$\subset$" Let $C = \operatorname{supp}(\mu_\psi)$ be the countable set of atoms. Then

$$\mu_\psi = \sum_{\lambda \in C} \mu_\psi(\{\lambda\}) = \sum_{\lambda \in C} \langle \psi, P_A(\{\lambda\})\psi \rangle = \sum_{\lambda \in C} \|P_A(\{\lambda\})\psi\|^2 . \tag{3.158}$$

The spectral measure of $P_A(\{\lambda\})\psi$ is clearly supported on the point λ, so $AP_A(\{\lambda\})\lambda\psi$ is an eigenvector of A with eigenvalue λ. For $\lambda \neq \lambda'$ these are orthogonal, so $\psi = \sum_{\lambda \in C} P_A(\{\lambda\})\psi$ is a sum of eigenvectors.

$\underline{b)}$: If μ_ψ is continuous, then $\|P_A(\{\lambda\})\psi\|^2 = \mu_\psi(\{\lambda\}) = 0$ for all $\lambda \in \mathbb{R}$. Since by the proof of a) $\varphi \in \mathscr{H}_{pp}$ can be written as a sum of $P_A(\{\lambda\})\varphi$ and the $P_A(\{\lambda\})$ are orthogonal projections, we have $\langle \psi, \varphi \rangle = 0$ and thus $\mathscr{H}_c \subset \mathscr{H}_{pp}^\perp$. If on the other hand $\psi \in \mathscr{H}_{pp}^\perp$, then $P_A(\{\lambda\})\psi$ for all $\lambda \in \mathbb{R}$ and thus $\mu_\psi(\{\lambda\}) = 0$ and $\psi \in \mathscr{H}_c$.

$\underline{c)}$: If $\psi \in \mathscr{H}_{sc}$ the $\psi \in \mathscr{H}_c$ by b). The support of μ_ψ is then a Lebesgue null set with $P_A(\operatorname{supp}(\mu_\psi))\psi = \psi$. If $\psi \in \mathscr{H}_c$ and M has Lebesgue measure zero and satisfies $P_A(M)\psi = \psi$, then $\operatorname{supp}(\mu_\psi) \subset M$, and μ_ψ is singular continuous.

To see that $\mathscr{H}_{sc}$ is closed, let $(\psi_n)_\mathbb{N}$ be sequence in $\mathscr{H}_{sc}$ converging to $\psi \in \mathscr{H}$ and let $(M_n)_\mathbb{N}$ be a corresponding sequence of null sets. Then $M = \cup_{n=1}^\infty M_n$ has measure zero, and

$$P_A(M)\psi = \lim_{n\to\infty} P_A(M)\psi_n = \lim_{n\to\infty} \psi_n = \psi, \tag{3.159}$$

so $\psi \in \mathscr{H}_{sc}$.

$\underline{d)}$: Exercise! $\square$

Corollary 3.57. *Let $P_\bullet$ be the orthogonal projector to $\mathscr{H}_\bullet$ for $\bullet \in \{pp, c, ac, sc\}$. Then $AP_\bullet = P_\bullet AP_\bullet$ and $A = P_\bullet AP_\bullet + P_\bullet^\perp AP_\bullet^\perp$*

Proof. If μ_ψ is supported by M, then so is $\mu_{A\psi}$. Hence $AP_\bullet \subset \mathscr{H}_\bullet$. The statement then follows from the fact that $P_\bullet$ is an orthogonal projection. $\square$

In view of this corollary we define

Definition 3.58. Let A, $D(A)$ be self-adjoint. We call

- $\sigma_{pp}(A) := \sigma(P_{pp}AP_{pp})$ the *pure-point spectrum* of A,
- $\sigma_{ac}(A) := \sigma(P_{ac}AP_{ac})$ the *absolutely continuous spectrum* of A,
- $\sigma_{sc}(A) := \sigma(P_{sc}AP_{sc})$ the *singular continuous spectrum* of A.

Proposition 3.59. *Let A, $D(A)$ be self-adjoint. Then*

a) $\sigma(A) = \sigma_{pp}(A) \cup \sigma_{ac}(A) \cup \sigma_{sc}(A)$,

b) $\sigma_{pp}(A) = \overline{\{\lambda \in \mathbb{R} : \ker(A - \lambda) \neq \{0\}\}}$,

c) $\sigma_{ac}(A)$ *is either empty or has positive Lebesgue measure,*

d) $\sigma_{sc}(A)$ *is either empty or uncountable.*

Proof. By Corollary 3.57 we have

$$A - \lambda = P_{pp}(A-\lambda)P_{pp} + P_{ac}(A-\lambda)P_{ac} + P_{sc}(A-\lambda)P_{sc}. \tag{3.160}$$

a) In the decomposition $\mathscr{H} = \mathscr{H}_{pp} \oplus \mathscr{H}_{ac} \oplus \mathscr{H}_{sc}$ this is a block-diagonal matrix, which is invertible iff each block is invertible. Hence $\rho(A) = \rho(P_{pp}AP_{pp}) \cap \rho(P_{ac}AP_{ac}) \cap \rho(P_{sc}AP_{sc})$, and the spectrum is the union of the spectra.

b) If $\lambda \in \mathbb{R}$ can be approximated by eigenvalues, there exists a sequence of normalised eigenvectors $\psi_n \in \mathscr{H}_{pp}$ such that $\|(A-\lambda)\psi_n\| \le |\lambda_n - \lambda| \to 0$, so $\lambda \in \sigma(A|_{\mathscr{H}_{pp}})$ by Weyl's criterion (Exercise 11).

If on the other hand $\lambda \in \sigma_{pp}(A)$. Then there exists a Weyl sequence for λ in $\mathscr{H}_{pp}$ and in particular a normalised element $\psi_\delta \in \mathscr{H}_{pp}$ with $\|(A-\lambda)\psi_\delta\| \le \delta$, for any $\delta > 0$. Assume now that $|\lambda - \mu| > \delta$ for every eigenvalue of A and some $\delta > 0$. Write $\psi_\delta = \sum_\gamma a_n \psi_n$ with orthonormal eigenvectors ψ_n and a sequence $\sum_{n=1}^\infty |a_n|^2 = 1$. Then

$$\|(A-\lambda)\psi_\delta\|^2 = \sum_{n=1}^\infty |a_n|^2 \, \|(A-\lambda)\psi_n\|^2 = \sum_{n=1}^\infty |a_n|^2 |\mu_n - \lambda|^2 > \delta, \tag{3.161}$$

a contradiction.

c) Assume $\sigma_{ac}(A) = N$ is a set of zero Lebesgue measure. Then, by Exercise 23 $1_{\mathscr{H}_{ac}} = \chi_N(P_{ac}AP_{ac})$, and thus for every $\psi \in \mathscr{H}_{ac}$

$$\|\psi\|^2 = \mu_\psi(\mathbb{R}) = \int \chi_N(P_{ac}AP_{ac})\mu_\psi(\mathrm{d}x) = \mu_\psi(N) = 0, \tag{3.162}$$

so $\mathscr{H}_{ac} = \{0\}$ and $\sigma_{ac}(A) = \varnothing$ (since $\mathrm{B}(\{0\}) = \{1\}$).

d) Same as c). $\square$

Examples 3.60.

a) Let $\mathscr{H} = L^2(\mathbb{R}) \oplus \mathbb{C}$ and $A(f,\gamma) = (x^2 f(x), \gamma)$, then $\mathscr{H}_{ac} = L^2(\mathbb{R}) \oplus \{0\}$, $\sigma_{ac} = \mathbb{R}_+$, $\mathscr{H}_{pp} = \{0\} \oplus \mathbb{C}$, $\sigma_{pp} = \{1\}$.

b) Let $\alpha : \mathbb{N} \to \mathbb{Q} \cap [0,1]$ be a bijection and $(\psi_n)_\mathbb{N}$ a complete orthonormal set in $\mathscr{H}$. Then

$$\varphi \mapsto A\varphi = \sum_{n=1}^\infty \alpha(n)\psi_n\langle\psi_n, \varphi\rangle \tag{3.163}$$

defines a bounded self-adjoint operator. We clearly have $\mathscr{H}_{pp} = \mathscr{H}$ and thus $\sigma(A) = \sigma_{pp}(A) = \overline{\mathbb{Q} \cap [0,1]} = [0,1]$.

c) For $\bullet \in \{pp, c, ac, sc\}$ one can obtain an operator such that $\sigma(A) = \sigma_\bullet(A)$ and $\mathscr{H}_\bullet = \mathscr{H}$ by taking a measure μ from the respective class and letting A be the multiplication operator by $x \mapsto x$ on $L^2(\mathbb{R}, \mu)$. The spectrum is then exactly the support of the measure.

The decomposition of the spectrum by properties of the spectral measure can be related to the dynamical behaviour under $U(t) := \mathrm{e}^{-\mathrm{i}At}$. Let $\varphi, \psi \in \mathscr{H}$ be normalised vectors. Then

$$\langle \varphi, U(t)\psi\rangle = \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}t\lambda} \mu_{\varphi,\psi}(\mathrm{d}\lambda) = \hat{\mu}_{\varphi,\psi} \tag{3.164}$$

is just the Fourier transform of the associated spectral measure (as an element of $\mathscr{S}'$). This implies, for example, that if $\mu_{\varphi,\psi}$ is absolutely continuous (i.e. if $\varphi, \psi \in \mathscr{H}_{ac}$), then $\lim_{t\to\infty}\langle \varphi, U(t)\psi\rangle = 0$, by the Riemann-Lebesgue Lemma. More generally, we have

Theorem 3.61 (Wiener's Theorem)**.** *Let μ be a finite complex Borel measure and $\hat{\mu}$ its Fourier transform. Then the Cèsaro mean of $|\hat{\mu}(t)|^2$ is convergent and*

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T |\hat{\mu}(t)|^2 \mathrm{d}t = \sum_{\lambda\in\mathbb{R}:\mu(\{\lambda\})>0} |\mu(\{\lambda\})|^2 \tag{3.165}$$

Proof. By Fubini we have

$$\begin{aligned}\frac{1}{T}\int_0^T |\hat{\mu}(t)|^2 \mathrm{d}t &= \frac{1}{T}\int_0^T \int_{\mathbb{R}}\int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}\eta t}\mathrm{e}^{\mathrm{i}\lambda t}\mu(\mathrm{d}\eta)\mu^*(\mathrm{d}\lambda)\mathrm{d}t \\ &= \int_{\mathbb{R}}\int_{\mathbb{R}} \left(\frac{1}{T}\int_0^T \mathrm{e}^{\mathrm{i}t(\lambda-\eta)}\mathrm{e}^{\mathrm{i}\lambda t}\mathrm{d}t\right)\mu(\mathrm{d}\eta)\mu^*(\mathrm{d}\lambda).\end{aligned}$$

The function in parenthesis converges pointwise to $\chi_{\{0\}}(\eta-\lambda)$ and is bounded by one, so by dominated convergence the whole expression tends to

$$\int_{\mathbb{R}}\int_{\mathbb{R}} \chi_{\{0\}}(\eta-\lambda)\mu(\mathrm{d}\eta)\mu^*(\mathrm{d}\lambda) = \int_{\mathbb{R}} \mu(\{\lambda\})\mu^*(\mathrm{d}\lambda) = \sum_{\lambda:\mu(\{\lambda\})>0} |\mu(\{\lambda\})|^2. \tag{3.166}$$

□

Corollary 3.62. *Let A, $D(A)$ be self-adjoint and $\psi \in \mathscr{H}_c$. Then*

$$\frac{1}{T}\int_0^T \mathrm{e}^{-\mathrm{i}At}\psi \mathrm{d}t \tag{3.167}$$

converges weakly to zero as $T\to\infty$. If $\psi \in \mathscr{H}_{ac}$ this holds without the mean.

Proof. As noted above, we have

$$\Big|\Big\langle \varphi, \frac{1}{T}\int_0^T \mathrm{e}^{-\mathrm{i}At}\psi\mathrm{d}t\Big\rangle\Big|^2 = \Big|\frac{1}{T}\int_0^T \hat{\mu}_{\varphi,\psi}(t)\mathrm{d}t\Big|^2 \le \frac{1}{T}\int_0^T |\hat{\mu}_{\varphi,\psi}|^2(t)\mathrm{d}t. \tag{3.168}$$

Now since $\psi = P_c\psi$, $\mu_{\varphi,\psi} = \mu_{P_c\varphi,\psi}$ has no atoms, this converges to zero as $T\to\infty$. The statement for $\psi \in \mathscr{H}_{ac}$ follows from the Riemann Lebesgue Lemma. □

This means that if $\psi_0 \in \mathscr{H}_{ac}$, $\psi(t) = \mathrm{e}^{-\mathrm{i}At}$ eventually becomes (essentially) orthogonal to any φ. It is also of interest to follow what happens e.g. to the support of $\psi(t)$ for large times. For this we will the following notion.

Definition 3.63. Let A, $D(A)$ be self-adjoint. An operator K, $D(K)$ with $D(A) \subset D(K)$ is called *relatively compact* with respect to A (or A-compact) if $KR_{\mathrm{i}}(A)$ is compact.

Example 3.64. Let $\chi \in C_\infty(\mathbb{R}^d)$. Then multiplication by χ is not a compact operator on $\mathscr{H} = L^2(\mathbb{R}^d)$ (except for $\chi = 0$). However, χ is $-\Delta$-compact by Exercise 09.

Proposition 3.65. *Let A, $D(A)$ be self-adjoint and K relatively compact. Then for every $\psi \in D(A)$*

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \left\| K \mathrm{e}^{-\mathrm{i}tA} P_c \psi \right\|^2 \mathrm{d}t = 0 \tag{3.169}$$

and

$$\lim_{t\to\infty} \left\| K \mathrm{e}^{-\mathrm{i}tA} P_{ac} \psi \right\| = 0. \tag{3.170}$$

If K is bounded then the statement holds for all $\psi \in \mathscr{H}$.

Proof. Let $\psi \in \mathscr{H}_c$, resp. $\mathscr{H}_{ac}$. If K is a rank-one operator, i.e. $K\psi = \varphi_1 \langle \varphi_2, \psi \rangle$, then

$$\left\| K \mathrm{e}^{-\mathrm{i}tA} \psi \right\|^2 = \|\varphi_1\|^2 \, |\langle \varphi_2, \mathrm{e}^{-\mathrm{i}tA}\psi \rangle|^2 = \|\varphi_1\|^2 \, |\hat{\mu}_{\varphi_2,\psi}(t)|^2 \tag{3.171}$$

and the statement follows from Wiener's Theorem, resp. the Riemann-Lebesgue Lemma. The statement thus holds for any finite-rank operator, and by approximation for any compact K.

For relatively compact K, take $\psi \in \mathscr{H}_\bullet \cap D(A)$. Then $\psi = R_{\mathrm{i}}\psi_0$ for some $\psi_0 \in \mathscr{H}_\bullet$ since these spaces are A-invariant. The statement thus follows from the argument above since $R_{\mathrm{i}}(A)$ commutes with $\mathrm{e}^{-\mathrm{i}tA}$.

If K is bounded and $\psi \in \mathscr{H}_\bullet$, we can find $\psi_n \in D(A) \cap \mathscr{H}_\bullet$ with $\|\psi - \psi_n\| < 1/n$, and then

$$\left\| K \mathrm{e}^{-\mathrm{i}tA} \psi \right\| \le \left\| K \mathrm{e}^{-\mathrm{i}tA} \psi_n \right\| + \|K\| / n. \tag{3.172}$$

Choosing first n and then T, resp. t, sufficiently large concludes the proof. $\square$

Example 3.66. Let $H = -\Delta$ and $\chi \in C_\infty(\mathbb{R}^d)$. Then $\mathscr{H} = \mathscr{H}_{ac}$ and thus for all $\psi \in H^2(\mathbb{R}^d) = D(H)$

$$\lim_{t\to\infty} \left\| \chi(x) \mathrm{e}^{-\mathrm{i}tH} \psi \right\| = 0, \tag{3.173}$$

i.e. the support of $\mathrm{e}^{-\mathrm{i}tH}\psi$ "moves to infinity". The solution disperses (as can also be seen from the explicit solution).

We have the following characterisation of spectral types by the long-time behaviour of the dynamics due to Ruelle, Amrein, Georgescu and Enß.

Theorem 3.67 (RAGE)**.** *Let A, $D(A)$ be self-adjoint and $(K_n)_{\mathbb{N}}$ a sequence of bounded relatively compact operators converging strongly to the identity. Then*

$$\mathscr{H}_c = \Big\{ \psi \in \mathscr{H} : \lim_{n\to\infty} \lim_{T\to\infty} \frac{1}{T} \int_0^T \left\| K_n \mathrm{e}^{-\mathrm{i}tA} \psi \right\| \mathrm{d}t = 0 \Big\},$$

$$\mathscr{H}_{pp} = \Big\{ \psi \in \mathscr{H} : \lim_{n\to\infty} \sup_{t\ge 0} \left\| (1 - K_n) \mathrm{e}^{-\mathrm{i}tA} \psi \right\| = 0 \Big\}.$$

Proof. We start with the first equation. By the previous theorem and Cauchy-Schwarz we have for $\psi \in \mathscr{H}_c$

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \left\| K_n \mathrm{e}^{-\mathrm{i}tA}\psi \right\| \mathrm{d}t \le \lim_{T\to\infty} \left(\frac{1}{T}\int_0^T \left\| K_n \mathrm{e}^{-\mathrm{i}tA}\psi \right\|^2 \mathrm{d}t \right)^{1/2} = 0. \tag{3.174}$$

For the converse it is sufficient to show that if $P_{pp}\psi \neq 0$, then $\left\| K_n \mathrm{e}^{-\mathrm{i}tA} P_{pp}\psi \right\| > \varepsilon$ for t sufficiently large. We will achieve this by showing that

$$\lim_{n\to\infty} \sup_{t\ge 0} \left\| (1-K_n)\mathrm{e}^{-\mathrm{i}tA} P_{pp}\psi \right\| = 0. \tag{3.175}$$

To see this, write $P_{pp}\psi = \sum_{j=1}^\infty \alpha_j \psi_j$ with orthonormal eigenvectors ψ_j of A (cf. Proposition 3.56). The sequence of operators K_n is bounded, and it converges in norm on any finite dimensional subspace, e.g. the span of $\psi_1, \dots, \psi_N$. Thus denoting by P_N the projection to this span, with is invarriant under $\mathrm{e}^{-\mathrm{i}tA}$,

$$\begin{aligned} &\left\| (1-K_n)\mathrm{e}^{-\mathrm{i}tA} P_{pp}\psi \right\|_{\mathscr{H}} \\ &\le \left\| (1-K_n)P_N \right\|_{\mathrm{B}(\mathscr{H})} \left\| \mathrm{e}^{-\mathrm{i}tA} P_{pp}\psi \right\| + \left\| 1-K_n \right\|_{\mathrm{B}(\mathscr{H})} \left\| (1-P_N)\mathrm{e}^{-\mathrm{i}tA} P_{pp}\psi \right\| \end{aligned} \tag{3.176}$$

converges to zero uniformly by choosing first N and then n sufficiently large. This completes the proof of the first equality, and the inclusion of the left hand side in the right for the second equality.

To complete the proof, we have to show that $\lim_{n\to\infty}\sup_{t\ge 0} \left\| (1-K_n)\mathrm{e}^{-\mathrm{i}tA}\psi \right\| \neq 0$ if $P_c\psi \neq 0$. But if this is zero, then we have

$$\begin{aligned} 0 &= \lim_{n\to\infty}\lim_{T\to\infty} \frac{1}{T}\int_0^T \left\| (1-K_n)\mathrm{e}^{-\mathrm{i}tA} P_c\psi \right\| \mathrm{d}t \\ &\ge \left\| P_c\psi \right\| - \lim_{n\to\infty}\lim_{T\to\infty} \frac{1}{T}\int_0^T \left\| K_n\mathrm{e}^{-\mathrm{i}tA} P_c\psi \right\| \mathrm{d}t = \left\| P_c\psi \right\|, \end{aligned}$$

a contradiction. □

Proposition 3.68. *Let A, $D(A)$ be self-adjoint and K relatively compact. Then for every $\psi \in D(A)$*

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \mathrm{e}^{\mathrm{i}tA} K \mathrm{e}^{-\mathrm{i}tA}\psi \mathrm{d}t = \sum_{\lambda\in\sigma_p(A)} P_A(\{\lambda\}) K P_A(\{\lambda\})\psi. \tag{3.177}$$

If K is bounded then the statement holds for all $\psi \in \mathscr{H}$.

Proof. By replacing K with $KR_{\mathrm{i}}(A)$ as in the proof of Proposition 3.65, it is sufficient to prove the statement for bounded K. By compactness of K, it is then sufficient to show weak convergence, i.e. that we have (3.177) after taking the scalar product with any $\varphi \in \mathscr{H}$. Writing $1 = P_{pp} + P_c$, Proposition 3.65 implies that the contributions of $P_c\psi$ and $P_c\varphi$ vanish. It thus remains to calculate

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \mathrm{e}^{\mathrm{i}tA} P_{pp} K \mathrm{e}^{-\mathrm{i}tA} P_{pp}\psi \mathrm{d}t = \sum_{\lambda,\eta\in\sigma_p(A)} \lim_{T\to\infty} \frac{1}{T}\int_0^T \mathrm{e}^{\mathrm{i}t(\eta-\lambda)} P_A(\{\lambda\}) K P_A(\{\eta\})\psi \mathrm{d}t, \tag{3.178}$$

which yields the claim by the argument from the proof of Wiener's Theorem. □

We can also directly obtain the projections onto $\mathscr{H}_\bullet$ from the dynamics.

Corollary 3.69. *Let A, $D(A)$ be self-adjoint and $(K_n)_{\mathbb{N}}$ a sequence of bounded relatively compact operators converging strongly to the identity. Then*

$$\lim_{n\to\infty}\lim_{T\to\infty} \frac{1}{T}\int_0^T \mathrm{e}^{\mathrm{i}tA} K_n \mathrm{e}^{-\mathrm{i}tA}\psi \mathrm{d}t = P_{pp}\psi \tag{3.179}$$

and

$$\lim_{n\to\infty}\lim_{T\to\infty} \frac{1}{T}\int_0^T \mathrm{e}^{\mathrm{i}tA} (1-K_n) \mathrm{e}^{-\mathrm{i}tA}\psi \mathrm{d}t = P_c\psi. \tag{3.180}$$

4 Spectral Theory of Self-Adjoint Operators

We will discuss the (approximate) stability of the spectrum of a self-adjoint operator A, $D(A)$ under "small" perturbations. We will first introduce the new notions of discrete and essential spectrum that are well adapted to this. We will then see in examples that the spectral types ac, pp, sc introduced in the previous section are not stable in the same way. Then, we will consider the stability of σ_{ac} in more detail, in the context of scattering theory.

Definition 4.1. Let A, $D(A)$ be self-adjoint. The *discrete spectrum* of A is

$$\sigma_{\mathrm{disc}}(A) := \{\lambda \in \sigma(A) | \exists \varepsilon > 0 : \dim \operatorname{ran}(P_A(\lambda - \varepsilon, \lambda + \varepsilon)) < \infty\}. \tag{4.1}$$

The *essential spectrum* of A is $\sigma_{\mathrm{ess}}(A) = \sigma(A) \setminus \sigma_{\mathrm{disc}}(A)$.

The set σ_{disc} is the set of isolated eigenvalues of finite multiplicity (Exercise).

4.1 The Essential Spectrum

Examples 4.2.

a) If A is compact then $\sigma_{\mathrm{ess}}(A) \subset \{0\}$. If the resolvent of A is compact, then $\sigma(A) = \sigma_{\mathrm{disc}}(A)$.

b) If $V \in L^\infty(\mathbb{R}, \mathbb{R})$ is an operator of multiplication on $L^2(\mathbb{R})$ then (compare Exercise 02)

$$\sigma(V) = \sigma_{\mathrm{ess}}(V) = \operatorname{essran}(V). \tag{4.2}$$

Note that the spectrum as a set, or any of its components, cannot be exactly stable under addition of bounded operators, since adding a multiple of the identity to A applies a shift to the spectrum. We thus have to either reduce the class of perturbations, or consider the weaker notion of approximate stability.

Proposition 4.3 (Weyl's Criterion for the Essential Spectrum)**.** *A point $\lambda \in \mathbb{R}$ is an element of $\sigma_{\mathrm{ess}}(A)$ if and only if it has a singular Weyl sequence, that is there exist normalised $(\psi_n)_n$ such that $w-\lim_{n\to\infty} \psi_n = 0$ and $\|(A - \lambda)\psi_n\| = 0$. If such a sequence exists, the vectors ψ_n can be chosen to be orthonormal.*

Proof. If there exists a Weyl sequence at λ, then $\lambda \in \sigma(A)$ by Exercise 11. Now assume there exists a singular Weyl sequence for $\lambda \in \sigma_{\mathrm{disc}}$. Let ε be such that $\dim \operatorname{ran}(P_A(\lambda -$

$\varepsilon, \lambda+\varepsilon)) < \infty$ and denote this spectral projection by P_ε. Then $\tilde{\psi}_n := P_\varepsilon \psi_n$ is a sequence in a finite dimensional space that converges weakly, and thus also in norm, to zero. But

$$\begin{aligned}\left\|\psi_n - \tilde{\psi}_n\right\|^2 &= \|(1-P_\varepsilon)\psi_n\|^2 \\ &= \int_{\mathbb{R}\setminus(\lambda-\varepsilon,\lambda+\varepsilon)} \mu_{\psi_n}(\mathrm{d}t) \\ &\le \varepsilon^{-2} \int_{\mathbb{R}\setminus(\lambda-\varepsilon,\lambda+\varepsilon)} (t-\lambda)^2 \mu_{\psi_n}(\mathrm{d}t) \\ &= \varepsilon^{-2} \|(A-\lambda)\psi_n\|^2 \overset{n\to\infty}{\to} 0,\end{aligned}$$

and thus $\left\|\tilde{\psi}_n\right\| \to 1$, a contradiction.

Conversely, if $\lambda \in \sigma_{\mathrm{ess}}(A)$, then for every $\varepsilon > 0$

$$\dim \operatorname{ran} P_A((\lambda-\varepsilon, \lambda+\varepsilon)) = \infty. \tag{4.3}$$

Let P_n be this projection with $\varepsilon = 1/n$. We then obtain an orthonormal singular Weyl sequence by taking $\psi_n \in \operatorname{ran} P_n$ to orthogonal to $\{\psi_1, \dots, \psi_{n-1}\}$ (in $P_1\mathscr{H}$ – note that the projection P_n is orthogonal to the projection onto $P_{n-1}\mathscr{H} \setminus P_n\mathscr{H}$). □

Proposition 4.4. *Let A, $D(A)$ be self-adjoint. The essential spectrum of A is invariant under addition of self-adjoint compact operators, and it exactly characterised by this property, that is*

$$\sigma_{\mathrm{ess}}(A) = \bigcap_{K=K^* \text{ compact}} \sigma(A+K). \tag{4.4}$$

Proof. Since K is bounded, it is also A-bounded with relative bound zero, so $A+K$ is self-adjoint on $D(A)$ by Kato-Rellich. Now let $\lambda \in \sigma_{\mathrm{ess}}(A)$ and let $(\psi_n)_{\mathbb{N}}$ be a singular Weyl-sequence for λ. Then, since ψ_n converges weakly to zero, $K\psi_n$ converges to zero in norm and thus

$$\|(A+K-\lambda)\psi_n\| \le \|(A-\lambda)\psi_n\| + \|K\psi_n\| \to 0. \tag{4.5}$$

Hence $(\psi_n)_{\mathbb{N}}$ is also a singular Weyl sequence for $A+K$ and $\lambda \in \sigma_{\mathrm{ess}}(A+K)$. Reversing the roles of A and $A+K$ shows that $\sigma_{\mathrm{ess}}(A) = \sigma_{\mathrm{ess}}(A+K)$ for every compact K.

It remains to prove that

$$\bigcap_{K=K^* \text{ compact}} \sigma_{\mathrm{disc}}(A+K) = \varnothing. \tag{4.6}$$

For this, let $\lambda \in \sigma_{\mathrm{disc}}(A)$ (i.e. for $K=0$).Then $P_A(\{\lambda\})$ has finite and nonzero rank, and we denote this projection by P. Then

$$A = PAP + (1-P)A(1-P) = \lambda P + (1-P)A(1-P). \tag{4.7}$$

Hence $A+P$ is a compact perturbation of A, and

$$\lambda \in \rho((\lambda+1)P) \cap \rho((1-P)A(1-P)) = \rho(A+P). \tag{4.8}$$

□

Theorem 4.5 (Weyl)**.** *Let A, $D(A)$ and B, $D(B)$ be self-adjoint. If $R_z(A) - R_z(B)$ is compact for some $z \in \rho(A) \cap \rho(B)$, then*

$$\sigma_{\mathrm{ess}}(A) = \sigma_{\mathrm{ess}}(B). \tag{4.9}$$

Proof. Let $\lambda \in \sigma_{\mathrm{ess}}(A)$ and let $(\psi_n)_{\mathbb{N}}$ be a singular Weyl-sequence for λ. Then

$$\left(R_z(A) - (\lambda - z)^{-1}\right) \psi_n = \frac{R_z(A)}{\lambda - z}(A - \lambda)\psi_n, \tag{4.10}$$

so $\|\left(R_z(A) - (\lambda - z)^{-1}\right) \psi_n\| \to 0$. Since the difference of the resolvents is compact and ψ_n tends weakly to zero, then also $\|\left(R_z(B) - (\lambda - z)^{-1}\right) \psi_n\| \to 0$. Consequently for $\varphi_n = R_z(B)\psi_n$

$$\|(B - \lambda)\varphi_n\| = |z - \lambda| \left\|\left(R_z(B) - (\lambda - z)^{-1}\right) \psi_n\right\| \to 0, \tag{4.11}$$

and

$$\|\varphi_n\| = \|R_z(B)\psi_n\| \overset{n\to\infty}{\to} |\lambda - z|^{-1} \neq 0. \tag{4.12}$$

Hence by normalising the sequence $(\varphi_n)_{\mathbb{N}}$ we obtain a singular Weyl sequence for B and $\lambda \in \sigma_{\mathrm{ess}}(B)$. Reversing the roles of A and B yields the claim. □

Example 4.6. Let $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ with $\lim_{|x|\to\infty} V(x) = 0$ then V is $-\Delta$-compact (this was shown in Exercise 09 for continuous V and follows for general V by approximation), so by the second resolvent formula

$$R_{\mathrm{i}}(-\Delta) - R_{\mathrm{i}}(-\Delta + V) = R_{\mathrm{i}}(-\Delta + V)VR_{\mathrm{i}}(-\Delta) \tag{4.13}$$

is compact. Hence for all such V, we have

$$\sigma_{\mathrm{ess}}(-\Delta + V) = [0, \infty). \tag{4.14}$$

The spectrum of such an operator thus always looks similar, with the same essential spectrum and possibly some negative eigenvalues of finite multiplicity, as for the Hydrogen atom.

Corollary 4.7. *Let A, $D(A)$ be symmetric with equal finite deficiency indices. Then all self-adjoint extensions of A have the same essential spectrum.*

Proof. Let A_1, A_2 be two self-adjoint extensions. Then for $\psi = (A + \mathrm{i})\varphi \in \operatorname{ran}(A + \mathrm{i})$, $R_{\mathrm{i}}(A_1)\psi = R_{\mathrm{i}}(A_2)\psi = \varphi$, since both extend A. Thus, the difference of resolvents is nonzero only on $\operatorname{ran}(A + \mathrm{i})^\perp = \ker(A^* - \mathrm{i})$, which has finite dimension, and thus the difference of resolvents has finite rank. The statement now follows from Weyl's Theorem. □

4.2 The Discrete Spectrum

We already know that the discrete spectrum consists of eigenvalues of finite multiplicity. We will now prove a variational characterisation of these eigenvalues in the case of operators that are bounded from below. After, we will prove approximate stability of such eigenvalues under perturbations.

Theorem 4.8 (Courant-Fischer). *Let A, $D(A)$ be self-adjoint and bounded from below. Denote*

$$\Sigma(A) := \min \sigma_{\mathrm{ess}}(A).$$

Define a sequence μ_n, $n \geq 1$ of real numbers by the min-max values

$$\mu_n(A) := \inf_{\substack{V \subset D(A) \\ \dim(V)=n}} \max_{\substack{\psi \in V \\ \|\psi\|_{\mathscr{H}}=1}} \langle \psi, A\psi \rangle = \inf_{\substack{V \subset Q(A) \\ \dim(V)=n}} \max_{\substack{\psi \in V \\ \|\psi\|_{\mathscr{H}}=1}} q_A(\psi,\psi). \tag{4.15}$$

Then for every $n \geq 1$ we have $\mu_n(A) \leq \Sigma(A)$, and if $\mu_n(A) < \Sigma(A)$ then A has hat least n eigenvalues (counted with multiplicity) below $\Sigma(A)$ and $\mu_n(A)$ is the n-nth smallest eigenvalue of A.

The min-max values are equal to the max-min values

$$\mu_n(A) = \sup_{\substack{W \subset D(A) \\ \dim(W^\perp)=n-1}} \inf_{\substack{\psi \in W \\ \|\psi\|_{\mathscr{H}}=1}} \langle \psi, A\psi \rangle. \tag{4.16}$$

Proof. The two expressions on the right of (4.15) are equal since $D(A)$ is dense in $Q(A)$.

To see that $\mu_n(A) \leq \Sigma(A)$, we argue by contradiction: Assume that for some $n \geq 1$, $\mu_n(A) - \Sigma(A) = \delta > 0$. Then, by definition of the essential spectrum, $P_A((\Sigma(A), \Sigma(A) + \delta/2)$ has infinite rank, and so $\mu_k(A) - \Sigma(A) < \delta/2$ for all $k \geq 1$, by taking a k-dimensional subspace of the range of P_A.

Denote by λ_n, $n = 1, \dots, N_{\max}$ the eigenvalues of A below $\Sigma(A)$, ordered and counted with multiplicity, and ψ_n a corresponding sequence of orthonormal eigenvectors (where $N_{\max} = \infty$ is allowed). Set $V_n = \operatorname{span}\{\psi_k : k \leq n\}$. Then for $\psi \in V_n$

$$\langle \psi, A\psi \rangle = \sum_{k=1}^{n} \lambda_k |\langle \psi, \psi_k \rangle|^2 \leq \lambda_n \|\psi\|^2, \tag{4.17}$$

and thus $\mu_n(A) \leq \lambda_n$.

For the reverse inequality, and existence of the eigenvalues, we argue recursively. Starting with $n = 1$, we have $\mu_1(A) \in \sigma(A)$ by Exercise 12. Assuming that $\mu_1(A) < \Sigma(A)$ we then have that $\mu_1(A) \in \sigma_{\mathrm{disc}}(A)$, and thus $\mu_1(A) = \lambda_1$ is an isolated eigenvalue. Now assume we have $\mu_k(A) = \lambda_k$ for all $k \leq n$ and $\mu_{n+1}(A) < \Sigma(A)$. Denote by $P_n^\perp$ the projection to the orthogonal complement of V_n (defined above). Then for any subspace $V \subset D(A)$ of dimension at least $n+1$, $P_n^\perp V \neq \{0\}$. Let ψ_V be a maximiser of $\langle \psi, A\psi \rangle / \|\psi\|^2$ in V. Then, since $\mu_{k+1} \geq \lambda_k$ we may assume that $P_n^\perp \psi_V \neq 0$ and we have

$$\max_{\substack{\psi \in V \\ \|\psi\|_{\mathscr{H}}=1}} \langle \psi, A\psi \rangle = \max_{\substack{\psi \in \tilde{V} \\ \|\psi\|_{\mathscr{H}}=1}} \langle \psi, A\psi \rangle. \tag{4.18}$$

with $\tilde{V} = V_n \oplus \operatorname{span}(\psi_V)$. Now $P_n^\perp \psi_V = \psi_V - P_n\psi_V \in \tilde{V}$, so

$$\max_{\substack{\psi\in\tilde{V} \\ \|\psi\|_{\mathscr{H}}=1}} \langle \psi, A\psi\rangle \geq \sigma(P_n^\perp A P_n^\perp). \tag{4.19}$$

Consequently

$$\mu_{n+1}(A) \geq \min \sigma(P_n^\perp A P_n^\perp) \geq \lambda_{n+1}, \tag{4.20}$$

so $\mu_{n+1} = \lambda_{n+1}$ and μ_{n+1} is an eigenvalue of $P_n^\perp A P_n^\perp$ by the same argument as for $n = 1$.

The proof of the max-min formulation is an exercise. □

Corollary 4.9. *Let A, $D(A)$ and B, $D(B)$ be self adjoint and bounded from below with $Q(B) \subset Q(A)$ and*

$$q_A(\psi,\psi) \leq q_B(\psi,\psi) \tag{4.21}$$

for all $\psi \in Q(B)$. Then $\Sigma(A) \leq \Sigma(B)$ and for all $n \geq 1$ we have $\mu_n(A) \leq \mu_n(B)$.

Example 4.10. Let $\Omega \subset \mathbb{R}$ be open, bounded with C^1-boundary. Then the quadratic form of the Dirichlet Laplacian $-\Delta_D$ is defined on $H_0^1(\Omega)$ and the form of the Neumann-Laplacian $-\Delta_N$ on $H^1(\Omega) \supset H_0^1(\Omega)$, and both are given by the expression

$$\int_\Omega |\nabla\psi(x)|^2 \mathrm{d}x. \tag{4.22}$$

Both operators have compact resolvent (this is where the regularity condition on the boundary plays a role). By the Corollary, we have $\lambda_n(-\Delta_N) \leq \lambda_n(-\Delta_D)$.

4.3 Approximate Stability of Isolated Spectrum

While the spectrum as a set is not stable under perturbations, in applications one often wants to know how a certain part of the spectrum, for example an isolated eigenvalue, changes precisely. In this section we will establish that isolated parts of the spectrum stay isolated if the perturbation is sufficiently small. In particular, isolated eigenvalues stay isolated eigenvalues and their dependence on a small perturbation can be calculated.

An important tool for this is an integral formula for the spectral projection that generalises Chauchy's integral formula. Let $E \subset \sigma(A)$ be a connected component and compact. Then there exists some contour γ in the complex plane such that $\gamma \subset \rho(A)$ and $\sigma(A) \cap \operatorname{int}(\gamma) = E$. We will show that

$$P_A(E) = \frac{\mathrm{i}}{2\pi}\int_\gamma R_z(A)\mathrm{d}z. \tag{4.23}$$

Of course, we need to define the operator-valued integral first. Since $z \mapsto R_z(A)$ is a continuous function on γ we could define it as a Riemann integral. However, for simplicity we will stick to the weak integral and define it by the identity

$$\Big\langle \varphi, \frac{\mathrm{i}}{2\pi}\int_\gamma R_z(A)\mathrm{d}z\psi \Big\rangle = \frac{\mathrm{i}}{2\pi}\int_\gamma \langle\varphi, R_z(A)\psi\rangle \mathrm{d}z, \tag{4.24}$$

for any $\varphi, \psi \in \mathscr{H}$.

The following proposition shows that the integral formula defines a projection also if A is just closed, in which case the spectral projection is not defined.

Proposition 4.11. *Let A, $D(A)$ be a closed operator and assume that there exist $\lambda \in \mathbb{R}$, $r > 0$ such that $\gamma := \{z \in \mathbb{C} : |z - \lambda| = r\} \subset \rho(A)$. Then the operator defined by (4.24) is a projection. If A is self-adjoint, then this projection is orthogonal.*

Proof. Denote the operator in question by P_γ. We first note that P_γ is bounded, since

$$|\langle \varphi, P_\gamma \psi \rangle| \leq r \, \|\varphi\| \, \|\psi\| \sup_{z \in \gamma} \|R_z(A)\| \,, \tag{4.25}$$

and the supremum is in fact a maximum because $z \to R_z(A)$ is continuous on $\rho(A)$ and γ is compact.

Let γ' be defined like γ but with a larger radius $r' < r$. Since $\rho(A)$ is open we can choose r' so that $\gamma' \subset \rho(A)$. Then $\langle \varphi, R_z(A)\psi \rangle$ is a holomorphic function on the annulus between γ and γ', so $P_\gamma = P_{\gamma'}$ by the Cauchy integral theorem. We can thus prove that P_γ is a projection by showing that $P_{\gamma'} P_\gamma = P_\gamma$. Inserting the definition and using the resolvent formula, we have

$$\begin{aligned}
\langle \varphi, P_{\gamma'} P_\gamma \psi \rangle &= \frac{\mathrm{i}}{2\pi} \int_{\gamma'} \langle \varphi, R_z(A) P_\gamma \psi \rangle \mathrm{d}z \\
&= \left(\frac{\mathrm{i}}{2\pi}\right)^2 \int_\gamma \int_{\gamma'} \langle \varphi, R_z(A) R_w(A) \psi \rangle \mathrm{d}z \mathrm{d}w \\
&= \left(\frac{\mathrm{i}}{2\pi}\right)^2 \int_\gamma \int_{\gamma'} \frac{1}{z - w} \langle \varphi, (R_z(A) - R_w(A)) \psi \rangle \mathrm{d}z \mathrm{d}w.
\end{aligned}$$

Now $w \mapsto (z - w)^{-1}$ is a holomorphic function on the disc bounded by γ, since $|z - \lambda| = r' > r$, and thus $\int_\gamma \frac{\mathrm{d}w}{z-w} = 0$. This gives with Cauchy's formula

$$\begin{aligned}
\langle \varphi, P_{\gamma'} P_\gamma \psi \rangle &= \left(\frac{\mathrm{i}}{2\pi}\right)^2 \int_\gamma \int_{\gamma'} \frac{1}{w - z} \langle \varphi, R_w(A) \psi \rangle \mathrm{d}z \mathrm{d}w \\
&= \frac{\mathrm{i}}{2\pi} \int_\gamma \langle \varphi, R_w(A) \psi \rangle \mathrm{d}w = \langle \varphi, P_\gamma \psi \rangle.
\end{aligned}$$

If A is self-adjoint, one easily checks that $\langle \psi, P_\gamma \psi \rangle$ is real, since the map $z \mapsto \overline{z}$ reverses the orientation of γ. □

Theorem 4.12. *Let A, $D(A)$ be self-adjoint and assume that there exist $\lambda \in \mathbb{R}$, $r > 0$ such that $\gamma = \{\mu \in \mathbb{R} : |\lambda - \mu| = r\} \subset \rho(A)$. Then*

$$P_A((\lambda - r, \lambda + r)) = \frac{\mathrm{i}}{2\pi} \int_\gamma R_z(A) \mathrm{d}z. \tag{4.26}$$

Proof. Let γ, P_γ be the same objects as in the previous proposition. Fix an arbitrary $\psi \in \mathscr{H}$. Since $R_z(A)$ leaves the space $\mathscr{H}_\psi$ (the A-cyclic space generated by ψ) invariant, we have $\langle \varphi, P_\gamma \psi\rangle = 0$ for $\varphi \in \mathscr{H}_\psi^\perp$. It is thus sufficient to consider $\varphi = f(A)\psi$ with $f \in C_\infty(\mathbb{R})$, since the set of these vectors is dense in $\mathscr{H}_\psi$ and P_γ is continuous. For such a φ, we have

$$\langle \varphi, P_\gamma \psi\rangle = \frac{\mathrm{i}}{2\pi}\int_\gamma \langle f(A)\psi, R_z(A)\psi\rangle = \frac{\mathrm{i}}{2\pi}\int_\gamma\int_{\mathbb{R}} \frac{\overline{f(x)}}{x-z}\mu_\psi(\mathrm{d}x)\mathrm{d}z. \tag{4.27}$$

Since

$$\frac{\mathrm{i}}{2\pi}\int_\gamma \frac{1}{x-z}\mathrm{d}z = \begin{cases} 1 & x \in B_r(\lambda) \\ 0 & x \notin B_r(\lambda) \end{cases} \tag{4.28}$$

this equals

$$\int_{\mathbb{R}} \overline{f(x)}\frac{\mathrm{i}}{2\pi}\int_\gamma \frac{1}{x-z}\mathrm{d}z\mu_\psi(\mathrm{d}x) = \int_{\mathbb{R}} \chi_{B_r(\lambda)}(x)\overline{f(x)}\mu_\psi(\mathrm{d}x) = \langle \varphi, P_A((\lambda - r, \lambda + r))\psi\rangle, \tag{4.29}$$

by Fubini's theorem. □

Theorem 4.13 (Analytic Perturbation Theory). *Let A, $D(A)$ be self-adjoint, B, $D(B)$ symmetric and A-bounded. If there exist $\lambda \in \mathbb{R}$, $r > 0$ such that $\gamma = \{\mu \in \mathbb{R} : |\lambda - \mu| = r\} \subset \rho(A)$, there is $\varepsilon_0 > 0$ such that for $\varepsilon < \varepsilon_0$*

$$\{\mu \in \mathbb{R} : |\lambda - \mu| = r\} \subset \rho(A + \varepsilon B). \tag{4.30}$$

The spectral projection

$$P_\varepsilon := P_{A+\varepsilon B}((\lambda - r, \lambda + r)) \tag{4.31}$$

is an analytic $\mathrm{B}(\mathscr{H})$-valued function of $\varepsilon < \varepsilon_0$. In particular, the rank of P_ε is constant.

Proof. For ε small enough, $A+\varepsilon B$ is self-adjoint by the Kato-Rellich Theorem. Moreover, the resolvent can be written as

$$R_z(A + \varepsilon B) = R_z(A)(1 + \varepsilon B R_z(A))^{-1} = R_z(A)\sum_{k=0}^{\infty} (-\varepsilon B R_z(A))^k\,, \tag{4.32}$$

for $\varepsilon < \|BR_z(A)\|$. We deduce that $\{\mu \in \mathbb{R} : |\lambda - \mu| = r\} \subset \rho(A + \varepsilon B)$ for ε small enough, and that $R_z(A + \varepsilon B)$ is an analytic function of ε in a neighbourhood of γ (with the notation as above). Analyticity of the spectral projection now follows from Theorem 4.12. If the rank of P_ε is finite for some $\varepsilon < \varepsilon_0$, then $\mathrm{rk}(P_\varepsilon) = \mathrm{tr}(P_\varepsilon)$ is a continuous function taking integer values, and thus constant. □

Corollary 4.14. *Let A, B satisfy the hypothesis of Theorem 4.13 and assume that A has an isolated simple eigenvalue λ_0. Then for $\varepsilon < \varepsilon_0$, $A + \varepsilon B$ has an isolated simple eigenvalue λ_ε, and λ_ε is an analytic function of $\varepsilon < \varepsilon_0$.*

Proof. Let ψ_0 be a normalised element of $\ker(A-\lambda_0)$. By Theorem 4.13, P_ε is a rank-one projection for $\varepsilon < \varepsilon_0$. By continuity of P_ε, $P_\varepsilon\psi_0 \neq 0$ for ε sufficiently small, and thus the range of P_ε is spanned by $P_\varepsilon\psi_0$. Since P_ε is a spectral projection of $A+\varepsilon B$,

$$(A+\varepsilon B)P_\varepsilon\psi_0 = \lambda_\varepsilon P_\varepsilon\psi_0, \tag{4.33}$$

and

$$\lambda_\varepsilon = \frac{\langle P_\varepsilon\psi_0, (A+\varepsilon B)P_\varepsilon\psi_0\rangle}{\|P_\varepsilon\psi_0\|^2}. \tag{4.34}$$

Since BP_ε is bounded and $P_\varepsilon\psi_0 \neq 0$, λ_ε is analytic. □

4.4 Stability and Instability of σ_{pp}, σ_{sc}, σ_{ac}

We will know discuss the instability of σ_{pp} and σ_{sc} in the simple example of rank-one perturbations. We will then show that σ_{ac} is stable under such perturbations and discuss the *ac*-spectrum in more detail in the context of scattering theory.

4.4.1 Rank-one Perturbations

We start by discussing in some detail rank-one perturbations, which provide a family of models that can be solved more or less exactly.

Let A, $D(A)$ be a self-adjoint operator on $\mathscr{H}$ and $\psi \in \mathscr{H}$. If P denotes the orthogonal projection to $\operatorname{span}\{\psi\}$, then

$$T_\alpha := A + \alpha P \tag{4.35}$$

with domain $D(T_\alpha) = D(A)$ defines a one-parameter familiy of self adjoint operators.

These have have following properties (cf. Exercise 29)

Proposition 4.15. *With the notation above we have*

a) The A-cyclic subspace $\mathscr{H}_\psi$ is T_α-invariant for all $\alpha \in \mathbb{R}$ and $T_\alpha|_{\mathscr{H}_\psi^\perp} = A|_{\mathscr{H}_\psi^\perp}$.

b) The resolvent of T_α can be expressed as

$$R_z(T_\alpha)\varphi = R_z(T_\beta)\varphi + R_z(T_\beta)\psi\frac{(\beta-\alpha)\langle\psi, R_z(T_\beta)\varphi\rangle}{1+(\alpha-\beta)\Phi_\beta(z)} \tag{4.36}$$

for $z \in \mathbb{C}\setminus\mathbb{R}$ and $\beta \neq \alpha$, where

$$\Phi_\beta(z) = \langle\psi, R_z(T_\beta)\psi\rangle = \int_{\mathbb{R}} \frac{\mu^\beta(\mathrm{d}t)}{t-z} \tag{4.37}$$

is the Borel transform of the spectral measure $\mu^\beta = \mu_\psi^\beta$ of ψ with respect to T_β.

By point a) it is not really a restriction to assume that ψ is A-cyclic, since on the orthogonal complement of $\mathscr{H}_\psi$ nothing interesting happens. By b), the spectrum of T_α is completely encoded by the functions $\Phi_\beta(z)$ for any $\beta \neq \alpha$. We will now study these in some more detail.

Remark 4.16. The function Φ_α is a Herglotz (or Nevanlinna) function, meaning that it is holomorphic on the upper (lower) complex half-plane and maps this to itself. It clearly satisfies $|\Phi_\alpha(z)| \leq C|\mathrm{Im}(z)|^{-1}$.

Theorem 4.17. *Let F be a Herglotz function on the upper complex half plane satisfying*

$$|F(z)| \leq \frac{C}{\mathrm{Im}(z)} \tag{4.38}$$

for some $C > 0$. Then there exists a unique finite Borel measure μ so that F is the Borel transform of μ.

Proof (sketch). Fix $z = x + \mathrm{i}y$ with $y > \varepsilon > 0$. By Cauchy's formula we can write

$$F(z) = \frac{1}{2\pi\mathrm{i}} \int_\gamma \left(\frac{1}{\zeta - z} - \frac{1}{\zeta - \overline{z} - 2\mathrm{i}\varepsilon} \right) F(\zeta) \mathrm{d}\zeta, \tag{4.39}$$

where γ is the contour

$$\gamma = (x + \mathrm{i}\varepsilon + [-R, R]) \cup \{x + \mathrm{i}\varepsilon + R\mathrm{e}^{\mathrm{i}\varphi} : \varphi \in [0, \pi]\} \tag{4.40}$$

(note that $\overline{z} - 2\mathrm{i}\varepsilon$ lies outside the contour). Due to the bound on F, the integrand over the semi-circle decays like R^{-2}, so letting $R \to \infty$ we have

$$F(z) = \frac{1}{\pi} \int_{\mathbb{R}} \frac{y - \varepsilon}{t^2 + (y - \varepsilon)^2} F(t + \mathrm{i}\varepsilon + x) \mathrm{d}t. \tag{4.41}$$

Let $V(z) := \mathrm{Im}F(z)$, which is positive, then

$$V(z) = \frac{1}{\pi} \int_{\mathbb{R}} \frac{y - \varepsilon}{t^2 + (y - \varepsilon)^2} V(t + \mathrm{i}\varepsilon + x) \mathrm{d}t. \tag{4.42}$$

We have for all $\varepsilon > 0$ by Fatou

$$C \geq \liminf_{y \to \infty} yV(x + \mathrm{i}y) = \frac{1}{\pi} \int_{\mathbb{R}} V(t + \mathrm{i}\varepsilon + x) \mathrm{d}t. \tag{4.43}$$

Consequently, the measures $\mu_\varepsilon := \pi^{-1} V(t + \mathrm{i}\varepsilon + x)\mathrm{d}t$ for $\varepsilon > 0$ form a bounded set in the dual of $C_\infty(\mathbb{R})$. They thus have an accumulation point μ (by Banach-Alaoglu) which (by Riesz-Markov) is a Borel measure. Then

$$V(z) = \lim_{\varepsilon \to 0} \int_{\mathbb{R}} \frac{y - \varepsilon}{t^2 + (y - \varepsilon)^2} \mu_\varepsilon(\mathrm{d}t) = \int_{\mathbb{R}} \frac{y}{t^2 + (y - \varepsilon)^2} \mu(\mathrm{d}t) = \mathrm{Im} \left(\int \frac{1}{t - z} \mu(\mathrm{d}t) \right). \tag{4.44}$$

Hence $F(z)$ and the Borel transform of μ have the same imaginary parts, and as holomorphic functions they must be equal up to a real constant. Since both tend to zero as $\mathrm{Im}z \to \infty$ this constant must be zero.

Uniqueness of μ follows from the formula

$$\frac{1}{2} \left(\mu((\lambda_1, \lambda_2)) + \mu([\lambda_1, \lambda_2]) \right) = \lim_{\varepsilon \to 0} \frac{1}{\pi} \int_{\lambda_1}^{\lambda_2} \mathrm{Im}F(t + \mathrm{i}\varepsilon) \mathrm{d}t, \tag{4.45}$$

see [Te, Thm 3.21] and Exercise 25. □

Since we are interested in the (in-)stability of the singular and absolutely continuous spectrum we want to recover these from the Borel transform.

Lemma 4.18. *Let μ be a finite Borel measure and Φ its Borel transform. Denote by $I_\varepsilon(x)$ the interval $(x-\varepsilon, x+\varepsilon)$ and define the lower and upper Radon-Nikodym derivatives of μ as*

$$\begin{aligned}\underline{D}\mu(x) &:= \liminf_{\varepsilon\to 0} \frac{\mu(I_\varepsilon)}{2\varepsilon}\\ \overline{D}\mu(x) &:= \limsup_{\varepsilon\to 0} \frac{\mu(I_\varepsilon)}{2\varepsilon}.\end{aligned}$$

Then

$$\underline{D}\mu(x) \leq \liminf_{\varepsilon\to 0} \frac{1}{\pi}\mathrm{Im}\Phi(x+\mathrm{i}\varepsilon) \leq \limsup_{\varepsilon\to 0} \frac{1}{\pi}\mathrm{Im}\Phi(x+\mathrm{i}\varepsilon) \leq \overline{D}\mu(x). \tag{4.46}$$

In particular, if $\underline{D}\mu(x) = \overline{D}\mu(x)$ then $\lim_{\varepsilon\to 0}\frac{1}{\pi}\mathrm{Im}\Phi(x+\mathrm{i}\varepsilon)$ exists and equals the Radon-Nikodym derivative of μ.

Proof. See [Te, Thm 3.22]. □

Theorem 4.19. *Let μ be a finite Borel measure and Φ its Borel transform. Then*

$$\lim_{\varepsilon\to 0} \frac{1}{\pi}\mathrm{Im}\Phi(x+\mathrm{i}\varepsilon) \tag{4.47}$$

exists Lebesgue a.e.. Moreover, the sets

$$M_{ac} := \{x\in\mathbb{R} : \lim_{\varepsilon\to 0}\mathrm{Im}\Phi(x+\mathrm{i}\varepsilon) \text{ exists and is finite}\} \tag{4.48}$$

and

$$M_s := \{x\in\mathbb{R} : \liminf_{\varepsilon\to 0}\mathrm{Im}\Phi(x+\mathrm{i}\varepsilon) = \infty\} \tag{4.49}$$

are supports for μ_{ac} and μ_s, respectively.

Proof (sketch). Consider the Lebesgue decomposition $\mu = \mu_{ac} + \mu_s$, where the singular part μ_s is supported on some set of Lebesgue measure zero. Since μ_{ac} is absolutely continuous, its Radon-Nikodym derivative exists a.e. in M_{ac} (w.r.t. to the Lebesgue measure and μ_{ac}). By Lemma 4.18 we thus have convergence of $\mathrm{Im}\Phi(x+\mathrm{i}\varepsilon)$ a.e., and the set where this holds is a support for μ_{ac}. To prove the statement on the singular part, one proves that the restriction of μ to the set

$$\{x\in\mathbb{R} : \underline{D}\mu(x) < \infty\} \tag{4.50}$$

is absolutely continuous (see [Te, Thm A.38]), so μ_s is supported on the complement. □

Corollary 4.20. *Let μ be a finite Borel measure and Φ its Borel transform. For Lebesgue-almost every $x\in\mathbb{R}$, $\Phi(x+\mathrm{i}\varepsilon)$ has a limit as $\varepsilon\to 0$.*

Proof. For the imaginary part this was already shown in Theorem 4.19. We will reduce the convergence of the real part to this result. For this, note that $\sqrt{\Phi}$ is a Herglotz function with positive real part, so $\mathrm{i}\sqrt{\Phi}$ is also a Herglotz function. By Theorems 4.17[1] and 4.19 the limit of

$$\sqrt{\Phi(x+\mathrm{i}\varepsilon)} = \mathrm{Im}\sqrt{\Phi(x+\mathrm{i}\varepsilon)} + \mathrm{Im}\left(\mathrm{i}\sqrt{\Phi(x+\mathrm{i}\varepsilon)}\right) \tag{4.51}$$

exists a.e., and then so does the limit of its square. □

In Exercise 32 we have seen that a real number λ can be an eigenvalue of T_α for at most one $\alpha \in \mathbb{R}$. This shows that the pure-point parts μ^β_{pp}, μ^α_{pp} are mutually sigular for $\alpha \neq \beta$. We will now show this for the entire singular parts, and discuss some examples (following [Don]).

Proposition 4.21 (Instability of the singular spectrum)**.** *Let T_α, $\alpha \in \mathbb{R}$ be the family of self-adjoint operators defined above and suppose that ψ is an A-cyclic vector. Then for $\alpha \neq \beta$ the measures μ^α_s and μ^β_s are mutually singular.*

Proof. Using the formula (compare Exercise 29)

$$\Phi_\alpha(z) = \frac{\Phi_\beta(z)}{1+(\alpha-\beta)\Phi_\beta(z)}, \tag{4.52}$$

we take the imaginary part, writing $\Phi_\alpha(z) = U_\alpha(z) + \mathrm{i}V_\alpha(z)$ and obtain

$$\begin{aligned} V_\alpha(z) &= \frac{\mathrm{Im}\left(\Phi_\beta(z)\left(1+(\alpha-\beta)\overline{\Phi}_\beta(z)\right)\right)}{(1+(\alpha-\beta)U_\beta(z))^2 + (\alpha-\beta)^2 V_\beta(z)^2} \\ &= \frac{V_\beta(z)}{(1+(\alpha-\beta)U_\beta(z))^2 + (\alpha-\beta)^2 V_\beta(z)^2}. \end{aligned} \tag{4.53}$$

If $x \in M^\beta_s$ (defined as above with $\Phi = \Phi_\beta$), then this implies that

$$\lim_{\varepsilon\to 0} V_\alpha(x+\mathrm{i}\varepsilon) = 0, \tag{4.54}$$

so $x \notin M^\alpha_s$. Hence μ^α_s and μ^β_s have disjoint supports and are mutually singular □

Example 4.22 (Disappearing singular spectrum)**.** Let $\rho \in L^1(\mathbb{R})$ be a continuous and strictly positive function and let ν be a finite measure singular with respect to Lebesgue measure (for example $\nu = \delta_0$). We set μ to be the normalised sum of the two measures,

$$\mu = \frac{\rho \mathrm{d}x + \nu}{\|\rho\|_{L^1} + \nu(\mathbb{R})}, \tag{4.55}$$

[1] Actually, we cannot apply this theorem as such, since it requires the growth estimate $|F(z)| \leq M\mathrm{Im}(z)^{-1}$. There is a more general representation theorem without this assumption, see [Te2, Thm.3.20] (second edition)

and let $A = T_0$ be multiplciation by x on $L^2(\mathbb{R}, \mu)$. Then

$$\sigma_s(T_0) = \operatorname{supp}(\nu)$$
$$\sigma_{ac}(T_0) = \mathbb{R}.$$

Now let $\psi \equiv 1$ be the natural cyclic vector for A and consider the corresponding family T_α. Since Φ has positive imaginary part, we see from Exercise 33 that for all $\lambda \in \mathbb{R}$

$$\liminf_{\varepsilon \to 0} \operatorname{Im}\Phi_0(\lambda + \mathrm{i}\varepsilon) \geq \rho(\lambda) > 0. \tag{4.56}$$

In view of (4.53) this implies that for all $\alpha \neq 0$

$$\limsup_{\varepsilon \to 0} \operatorname{Im}\Phi_\alpha(\lambda + \mathrm{i}\varepsilon) \leq \frac{1}{\alpha\rho(\lambda)}, \tag{4.57}$$

and thus $M_s^\alpha = \varnothing$. The operators T_α have only absolutely continuous spectrum.

If we do not assume that ρ is positive everywhere, then the reasoning still holds wherever $\rho > 0$, but T_α can have sigular sepctrum where ρ vanishes.

Example 4.23 (Dense point spectrum and singular continuous spectrum)**.** We start by constructing a pure-point measure on $[0, 1]$. Let $(a_n)_\mathbb{N} \in \ell^2$ be a square-summable sequence of positive numbers that is not summable. Set

$$\lambda_k = \left(\sum_{j=1}^{k} a_j\right) \bmod 1. \tag{4.58}$$

Then the sequence $(\lambda_n)_N$ is dense in the unit interval, since the sequence a_n tends to zero but is not summable. Define a measure μ on the unit interval as

$$\mu|_{[0,1]} = \sum_{k=1}^{\infty} a_k^2 \delta_{\lambda_k}, \tag{4.59}$$

and on $\mathbb{R}$ by translation and normalising $\mu|_{[n-1,n]} = n^{-2}$. Now clearly $A = M_\lambda$ on $L^2(\mathbb{R}, \mu)$ has a dense set of eigenvalues in $\mathbb{R}$ given by $\{\lambda_k + n : n, k \in \mathbb{N}\}$. Let $\psi \equiv 1 \in L^2(\mathbb{R}, \mu)$ and consider the corresponding family of operators T_α. From Exercise 32 we know that the eigenvalues above are not eigenvalues of T_α for $\alpha \neq 0$ and by the proposition the spectral measure μ_ψ^α is supported on the compement of this set. Now any $\lambda \in [0, 1]$ in this complement satisfies

$$\lambda_{k_{n-1}} < \lambda < \lambda_{k_n} \tag{4.60}$$

for an infinite sequence of integers $(k_n)_\mathbb{N}$. Then

$$\int_\mathbb{R} \frac{1}{(t-\lambda)^2} \mu_\psi^0(\mathrm{d}t) \geq \sum_{k=1}^{\infty} \frac{a_k^2}{(\lambda_k - \lambda)^2} \geq \sum_{n=1}^{\infty} \frac{a_{k_n}^2}{(\lambda_{k_n} - \lambda_{k_{n-1}})^2} = \sum_{n=1}^{\infty} 1 = \infty. \tag{4.61}$$

Hence, in view of Exercise 32, T_α has no eigenvalues in $[0, 1]$, and by the same argument anywhere. The spectrum of T_α for $\alpha \neq 0$ is purely singular continuous, by the next Proposition.

Proposition 4.24 (Stability of the absolutely continuous spectrum)**.** *Let T_α, $\alpha \in \mathbb{R}$ be the family of self-adjoint operators of Proposition 4.15 and suppose that ψ is an A-cyclic vector. Then for $\alpha \neq \beta$ the measures μ_{ac}^α and μ_{ac}^β are mutually absolutely continuous, and $P_{ac}(T_\alpha)T_\alpha$ is unitarily equivalent to $P_{ac}(T_\beta)T_\beta$.*

Proof. By Theorem 4.19 and Corollary 4.20, the set

$$S_\alpha := \{x \in \mathbb{R} : \lim_{\varepsilon\to 0} \Phi(x + \mathrm{i}\varepsilon) \text{ exists and has non-zero imaginary part}\} \tag{4.62}$$

is a support for μ_{ac}^α. On S_β, we have

$$\lim_{\varepsilon\to 0} V_\alpha(x+\mathrm{i}\varepsilon) = \lim_{\varepsilon\to 0} \frac{V_\beta(x+\mathrm{i}\varepsilon)}{(1+(\alpha-\beta)U_\beta(x+\mathrm{i}\varepsilon))^2 + (\alpha-\beta)^2 V_\beta(x+\mathrm{i}\varepsilon)^2}, \tag{4.63}$$

which is non-zero, and by the corresponding formula for the real parts, $S_\alpha = S_\beta$. By Lemma 4.18, the a density of μ_{ac}^α w.r.t. the Lebesgue measure is given (a.e.) by setting

$$\rho_\alpha(x) = \tfrac{1}{\pi} \lim_{\varepsilon\to 0} V_\alpha(x+\mathrm{i}\varepsilon), \tag{4.64}$$

for $x \in S_\alpha$. We then find the density of μ_{ac}^β with respect to μ_{ac}^α as

$$\frac{\mathrm{d}\mu_{ac}^\alpha}{\mathrm{d}\mu_{ac}^\beta} = \lim_{\varepsilon\to 0} \frac{1}{|1+(\alpha-\beta)\Phi_\beta(x+\mathrm{i}\varepsilon)|^2}, \tag{4.65}$$

and the unitary equivalence is given, e.g., by

$$\begin{aligned} U : L^2(\mathbb{R}, \mu_{ac}^\alpha) &\to L^2(\mathbb{R}, \mu_{ac}^\beta) \\ f &\mapsto \lim_{\varepsilon\to 0} \frac{f(\cdot)}{1+(\alpha-\beta)\Phi_\beta(\cdot+\mathrm{i}\varepsilon)}. \end{aligned}$$

□

4.4.2 Instability of spectral types under Hilbert Schmidt perturbations

We have shown that the singular spectrum is unstable under rank one perturbations, while the absolutely continuous part is stable. When taking sums of rank-one perturbations, the situation depends on the norm in which the sum converges.

Definition 4.25. Let $\mathscr{H}$ be a separable Hilbert space, $K \in \mathrm{B}(\mathscr{H})$ compact operator and $\kappa = (\kappa_n)_\mathbb{N}$ be the sequence of its singular values (c.f. [FA1, Thm.5.37]; these are the eigenvalues in case K is symmetric). The operator K is an element of the p-th *Schatten class* $\mathfrak{S}_p(\mathscr{H})$ if $\kappa \in \ell^p$. We call $\mathfrak{S}_1(\mathscr{H})$ the *trace class* and $\mathfrak{S}_2(\mathscr{H})$ the *Hilbert-Schmidt* class.

Proposition 4.26. *The space $\mathfrak{S}_p(\mathscr{H})$, $1 \le p < \infty$ is a Banach space with the norm*

$$\|K\|_{\mathfrak{S}_p} = \mathrm{tr}\left((K^*K)^{p/2}\right)^{1/p} = \|\kappa\|_{\ell^p}$$

where the trace is defined by

$$\operatorname{tr}(K) = \sum_{j=1}^{\infty} \langle \psi_j, K\psi_j \rangle, \tag{4.66}$$

for any complete orthonormal set $(\psi_n)_{\mathbb{N}}$ *and* $K \geq 0$. *The Hilbert Schmidt operators,* $p = 2$*, form a Hilbert space, and the Hölder-type inequality*

$$\|K_1 K_2\|_{\mathfrak{S}_1} \leq \|K_1\|_{\mathfrak{S}_p} \|K_2\|_{\mathfrak{S}_q} \tag{4.67}$$

holds for $K_1 \in \mathfrak{S}_p, K_2 \in \mathfrak{S}_q$, $p^{-1} + q^{-1} = 1$.

Proof. The case $p = 2$ follows by checking that $\operatorname{tr}(A^*B)$ defines a scalar product on finite-rank operators. The case $p = 1$ is an exercise. For the general case see [Te, Lem.6.12]. □

We will now prove the following result on instability of the spectral type under perturbations of Hilbert-Schmidt class. Later we will also prove that the absolutely continuous part is stable under perturbations of trace-class.

Theorem 4.27 (Weyl-von Neumann)**.** *Let* A*,* $D(A)$ *be self-adjoint on the separable Hilbert space* $\mathscr{H}$*. For every* $\varepsilon > 0$ *there exists a self-adjoint Hilbert-Schmidt operator* K *with norm* $\|K\|_{\mathfrak{S}_2} < \varepsilon$ *so that* $A + K$ *has pure point spectrum.*

Remark 4.28. The theorem means in particular that if A has absolutely continuous spectrum $\mathscr{H}_{ac}(A) = \mathscr{H}$, there exists a small operator K as above such that $\mathscr{H}_{ac}(A + K) = \{0\}$. The same holds for singular continuous spectrum. Of course, the absolutely continuous spectrum is part of the essential spectrum, so *as a set* this remains stable under the compact perturbation K.

On the other hand, we have already shown that there are operators A with pure point spectrum such that $A + \alpha P$ has no eigenvalues, for a rank-one projection P and α arbitrarily small 4.23. This shows that the spectral types are generally unstable.

For the proof of Theorem 4.27 we need:

Lemma 4.29. *Let* A*,* $D(A)$ *be self-adjoint on* $\mathscr{H}$*, and* $\psi \in \mathscr{H}$*. For any* $\delta > 0$ *there exists a projection* P *of finite rank and a self-adjoint* $K \in \mathfrak{S}_2(\mathscr{H})$ *such that* $\|(1 - P)\psi\| < \delta$*,* $\|K\|_{\mathfrak{S}_2} < \delta$ *and the range of* P *is invariant under* $A + P$*.*

Proof. Given $\delta > 0$ we may choose L large enough so that

$$\left\|(1 - \chi_{[(-L/2, L/2]}(A))\psi\right\| < \delta. \tag{4.68}$$

Let $n \in \mathbb{N}$ to be chosen later, and set for $k = 1, \dots, n$

$$P_k := P_A\Big((-L/2 + (k-1)L/n, -L/2 + kL/n]\Big) = \chi_{(-L/2+(k-1)L/n, -L/2+kL/n]}(A). \tag{4.69}$$

Set $\varphi_k = 0$ if $P_k\psi = 0$ and otherwise $\varphi_k := P_k\psi / \|P_k\psi\|$. Then the set $\{\varphi_k, k = 1, \dots n\}$ is orthonormal by the basic properties of the PVM. Let P be the orthogonal projection onto the span of this set. Then P has rank at most n, and

$$P\psi = \sum_{k=1}^{n} \varphi_k \langle \varphi_k, \psi \rangle = \sum_{k \in \{1,\dots,n:\varphi_k \neq 0\}} P_k\psi \frac{\langle \psi, P_k\psi \rangle}{\|P_k\psi\|^2} = \chi_{[(-L/2,L/2]}(A))\psi, \tag{4.70}$$

so $\|(1-P)\psi\| < \delta$.

Now set $K = -PA(1-P) - (1-P)AP$. This operator is well-defined since $\operatorname{ran}(P) \subset D(A)$ (even $\|AP\| \leq L/2$), symmetric, and has rank $r \leq n$. We have

$$A + K = PAP + (1-P)A(1-P), \tag{4.71}$$

and this leaves the range of P invariant.

It remains to prove the bound on the Hilbert-Schmidt norm of K, by choosing n. First, we clearly have $A\varphi_k \in \operatorname{ran} P_k$, and thus also $PA\varphi_k \in \operatorname{ran} P_k$ and $(1-P)\varphi_k \in \operatorname{ran} P_k$. Consequently,

$$\begin{aligned} \|(1-P)AP\|^2 &= \sup_{\|\varphi\|=1} \sum_{j,k=1}^{n} \langle \varphi, \varphi_j \rangle \langle \varphi_k, \varphi \rangle \langle (1-P)A\varphi_j, (1-P)A\varphi_k \rangle \\ &= \sup_{\|\varphi\|=1} \sum_{k=1}^{n} |\langle \varphi_k, \varphi \rangle|^2 \, \|(1-P)A\varphi_k\|^2 \\ &\leq \max_{k \in \{1,\dots,n\}} \|(1-P)A\varphi_k\|^2 \end{aligned}$$

We estimate this, using that $(1-P)P = 0$ and setting $\lambda_k = -L/2 + kL/n$, by

$$\|(1-P)A\varphi_k\| = \|(1-P)(A-\lambda_k)\varphi_k\| \leq \|(A-\lambda_k)\varphi_k\| \leq L/n. \tag{4.72}$$

Let η_j, $j = 1, \dots, r \leq n$ be an orthonormal basis of $\operatorname{ran} K (= \operatorname{ran} K^*)$, then

$$\|K\|_{\mathfrak{S}_2}^2 = \sum_{j=1}^{r} \langle \eta_j, K^* K \eta_j \rangle \leq r \, \|K\|^2 \leq n(2L/n)^2. \tag{4.73}$$

The claim now follows by choosing n large enough. $\square$

Proof of Theorem 4.27. Let $(\psi_n)_N$ be a dense subset of $\mathscr{H}$. we will prove the Theorem by applying Lemma 4.29 recursively. Start with $\psi = \psi_1$, $\delta = \varepsilon/2$, and denote by P_1, K_1 the resulting projection and Hilbert Schmidt operator. In the second step, apply the Lemma to $(1-P_1)(A+K_1)(1-P_1)$ with $\psi = (1-P_1)\psi_2$ and $\delta = \varepsilon/2^2$, and extend the resulting P_2, K_2 to the whole space $\mathscr{H}$ by zero. Then $A + K_1 + K_2$ leaves the ranges of both P_1 and P_2 invariant, since

$$\begin{aligned} &(A + K_1 + K_2)P_1 = (A + K_1)P_1 = P_1(A + K_1)P_1, \\ &(A + K_1 + K_2)P_2 = ((1-P_1)(A + K_1)((1-P_1) + K_2)P_2 = P_2(A + K_1 + K_2)P_2. \end{aligned}$$

Continuing this procedure, we obtain a sequence of finite-dimensional projections P_j, $j = 1, \dots$ with $P_j P_\ell = 0$ and self-adjoint operators K_j with $\|K_j\|_{\mathfrak{S}_2} < \varepsilon 2^{-j}$. The sum $\sum_{j=1}^n K_j$ converges in $\mathfrak{S}_2$ to an operator K with $\|K\|_{\mathfrak{S}_2} < \varepsilon$. For the projection, note that

$$\|(1 - P_1 - \cdots - P_n)\psi_n\| = \|(1 - P_1 - \cdots - P_{n-1})\psi_n - P_n(1 - P_1 - \cdots - P_{n-1})\psi_n\| < \varepsilon 2^{-n},$$

and thus for $N > n$,

$$\left\| \sum_{j=n+1}^{N} P_j \psi_n \right\| = \left\| \sum_{j=n+1}^{N} P_j (1 - P_1 - \cdots - P_n)\psi_n \right\| \leq \varepsilon 2^{-n}$$

This implies that $\sum_{j=1}^\infty P_j = 1$ (with convergence in the strong operator topology), because the set $(\psi_n)_{\mathbb{N}}$ is dense (note that after removal of $\psi - 1, \dots, \psi_{n-1}$ the set is still dense, so we may choose n large).

To prove the Theorem we show now that $A + K$ has pure point spectrum. Since the ranges of the projections P_n are finite dimensional and span $\mathscr{H}$ it is sufficient to prove that each of these is invariant under $A + K$, since $P_n(A + K)P_n$ has finite rank and thus pure point spectrum. By construction, $P_n\mathscr{H}$ is a subspace of $(1 - P_1 - \cdots - P_{n-1})\mathscr{H}$ and K_j, $j > n$ vanishes on $\operatorname{ran} P_n$, so

$$\begin{aligned}
(A + K)P_n &= (A + K_1 + \cdots + K_n)P_n + \underbrace{\sum_{j=n+1}^{\infty} K_j P_n}_{=0} \\
&= P_n(A + K_1 + \cdots + K_n)P_n \\
&= P_n(A + K)P_n.
\end{aligned}$$

This completes the proof. □

We remark that the above proof works similarly with $K \in \mathfrak{S}_p$, $p > 1$. For $p = 1$ it is not possible to choose n in (4.73) large to make the norm of K small. We will see below that the *ac*-spectrum is actually stable under trace-class perturbations.

4.4.3 Perturbation of absolutely continuous spectrum: Scattering theory

We will now investigate in greater generality the stability of the a.c. spectrum that we found in the example of rank-one perturbations. We will take a different point of view that emphasizes the dynamics. This is best illustrated in the example of the Schrödinger operator $H = -\Delta + V$ with a bounded and decaying potential V (e.g. of compact support). Consider the behaviour of $\mathrm{e}^{-\mathrm{i}Ht}\psi$ for $\psi \in \mathscr{H}_{ac}$. We know from the RAGE theorem (or more precisely Proposition 3.65) that $\mathrm{e}^{-\mathrm{i}Ht}\psi$ tends to zero locally, in particular on the support of V, and

$$\lim_{t \to \infty} \left\| V \mathrm{e}^{-\mathrm{i}Ht}\psi \right\| = 0. \tag{4.74}$$

Hence after a long time the influence of V becomes negligible and we expect that $e^{-iHt}\psi$ behaves like a solution to the equation with $V = 0$ for large t, i.e. that there exists $\psi_+ \in \mathscr{H}$ so that

$$\lim_{t\to\infty} \left\| e^{-iHt}\psi - e^{i\Delta t}\psi_+ \right\| = 0. \tag{4.75}$$

Using the unitarity of the groups, this is equivalent to

$$\psi = \lim_{t\to\infty} e^{iHt} e^{i\Delta t}\psi_+. \tag{4.76}$$

The same argument would hold for $t \to -\infty$ and some ψ_-.

Definition 4.30. Let A, $D(A)$ and B, $D(B)$ be self-adjoint operators on $\mathscr{H}$. We define the *wave-operators* by

$$\Omega_\pm(A,B) = s - \lim_{t\to\pm\infty} e^{itA} e^{-itB}$$

on the domains

$$D(\Omega_\pm(A,B)) = \{\psi \in \mathscr{H}_{ac}(B) : \exists \lim_{t\to\pm\infty} e^{itA} e^{-itB}\psi\}. \tag{4.77}$$

The elements of $D(\Omega_\pm(A,B))$ correspond to the asymptotic outgoing/incoming states $\psi_\pm$, and the range of $\Omega_\pm$ correspond to the elements $\psi \in \mathscr{H}$ for which such states exist.

Proposition 4.31. *The sets $D(\Omega_\pm(A,B))$ and $\operatorname{ran}\Omega_\pm$ are closed in $\mathscr{H}$, and*

$$\Omega_\pm(A,B) : D(\Omega_\pm(A,B)) \to \operatorname{ran}\Omega_\pm(A,B) \tag{4.78}$$

is unitary.

Proof. If the strong limit $\Omega_\pm$ of a uniformly bounded sequence exists on some set, it also exists on the closure, so $D(\Omega_\pm)$ are closed. We have

$$\|\Omega_\pm\psi\| = \lim_{t\to\pm\infty} \left\| e^{itA} e^{-itB}\psi \right\| = \|\psi\|, \tag{4.79}$$

so $\Omega_\pm$ are isometric, and thus unitary to their range by Exercise 01.

Since $\operatorname{ran}\Omega_\pm$ are isometric to $D(\Omega_\pm)$, they are complete and thus closed in $\mathscr{H}$. other □

Theorem 4.32. *The subspaces $D(\Omega_\pm(A,B))$ are B-invariant and $\operatorname{ran}\Omega_\pm(A,B)$ are A-invariant. Moreover*

$$\operatorname{ran}\Omega_\pm(A,B) \subset \mathscr{H}_{ac}(A), \tag{4.80}$$

$\Omega_\pm(A,B)\,(D(B) \cap D(\Omega_\pm)) \subset D(A)$ *and we have the intertwining property*

$$\Omega_\pm(A,B)B = A\Omega_\pm(A,B) \tag{4.81}$$

on $D(B) \cap D(\Omega_\pm)$.

Proof. First observe that for $s \in \mathbb{R}$

$$\Omega_\pm(A,B)\mathrm{e}^{-\mathrm{i}sB}\psi = \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tA}\mathrm{e}^{-\mathrm{i}(t+s)B}\psi = \lim_{\tau\to\pm\infty} \mathrm{e}^{-\mathrm{i}sA}\mathrm{e}^{\mathrm{i}\tau A}\mathrm{e}^{-\mathrm{i}\tau B}\psi = \mathrm{e}^{-\mathrm{i}sA}\Omega_\pm(A,B)\psi, \tag{4.82}$$

so $\psi \in D(\Omega_\pm)$ iff $\mathrm{e}^{-\mathrm{i}sB}\psi \in D(\Omega_\pm)$ and $D(\Omega_\pm)$ is B-invariant. The equation also shows that if $\varphi = \Omega_\pm\psi \in \operatorname{ran}\Omega_\pm$, then $\mathrm{e}^{-\mathrm{i}sA}\varphi = \Omega_\pm \mathrm{e}^{-\mathrm{i}sB}\psi \in \operatorname{ran}\Omega_\pm$, and $\operatorname{ran}\Omega_\pm$ is A-invariant.

Equation (4.82) can be differentiated w.r.t. s iff $\psi \in D(B)$, which is thereby equivalent to $\Omega_\pm\psi \in D(A)$ (see Theorem 3.49). The derivative then yields the intertwining property.

This property together with the unitarity of $\Omega_\pm$ means that the restriction of B to $D(\Omega_\pm)$ is unitarily equivalent to the restriction of A to $\operatorname{ran}\Omega_\pm$. Since $D(\Omega_\pm) \subset \mathscr{H}_{ac}(B)$ by definition this yields that $\operatorname{ran}\Omega_\pm \subset \mathscr{H}_{ac}(A)$. □

Of course, we have not yet shown that $D(\Omega_\pm(A,B))$ really is non-trivial.

Definition 4.33. Let $A, D(A)$ and $B, D(B)$ be as above. We say that

- the *wave operators exist* if $D(\Omega_\pm(A,B)) = \mathscr{H}_{ac}(B)$,
- the *wave operators are complete* if $\operatorname{ran}\Omega_\pm(A,B) = \mathscr{H}_{ac}(A)$,
- the wave operators are *asymptotically complete* if they exist, are complete and $\mathscr{H}_{sc}(B) = \{0\} = \mathscr{H}_{sc}(A)$.

Existence means that any $\psi_\pm \in \mathscr{H}_{ac}(B)$ is an asymptotic incomming/outgoing state. Completeness means that the dynamics for any $\psi \in \mathscr{H}_{ac}(A)$ can be described in terms of asymptotic states. If the wave operators exist and are complete, then the *ac*-parts of A and B are unitarily equivalent. Asymptotic completeness then means that the dynamics $\mathrm{e}^{-\mathrm{i}At}$ decompose into periodic parts, acting on $\mathscr{H}_{pp}(A)$ and a part with an asymptotic description in terms of B, acting on $\mathscr{H}_{ac}(B)$. If the wave operators exist and are complete, then the *scattering operator*

$$S := \Omega_+(A,B)^{-1}\Omega_-(A,B) \tag{4.83}$$

is unitary on $\mathscr{H}_{ac}(B)$.

Lemma 4.34 (Cook's Criterion)**.** *Suppose $D(A) \subset D(B)$. If for $\psi \in D(B) \cap \mathscr{H}_{ac}(B)$ and some $T \in \mathbb{R}$ we have*

$$\int_T^\infty \left\| (B-A)\mathrm{e}^{\mp\mathrm{i}tB}\psi \right\| \mathrm{d}t < \infty, \tag{4.84}$$

then $\psi \in D(\Omega_\pm(A,B))$, respectively. In particular, if this condition is fulfilled for all $\psi \in D(B) \cap \mathscr{H}_{ac}(B)$ then the wave operators exist.

Proof. For $\psi \in D(B)$ we have

$$\mathrm{e}^{\mathrm{i}tA}\mathrm{e}^{-\mathrm{i}tB}\psi = \mathrm{e}^{\mathrm{i}TA}\mathrm{e}^{-\mathrm{i}TB}\psi + \mathrm{i}\int_T^t \mathrm{e}^{\mathrm{i}sA}(A-B)\mathrm{e}^{-\mathrm{i}sB}\psi \mathrm{d}s \tag{4.85}$$

by the fundamental theorem of calculus. The integrability condition then implies that the left hand side is Cauchy, so its limit as $t \to \pm\infty$ exists. The final statement follows from the fact that $D(\Omega_\pm)$ are closed. □

This criterion allows for a simple proof of existence of the wave operators for $-\Delta + V$ if V decays sufficiently (here in $d = 3$).

Proposition 4.35. *Let $V \in L^2(\mathbb{R}^3, \mathbb{R})$ and set $H = -\Delta + V$, $H_0 = -\Delta$ with $D(H) = D(H_0) = H^2(\mathbb{R}^d) \subset L^2(\mathbb{R}^d)$. Then the wave operators $\Omega_\pm(H, H_0)$ exist.*

Proof. We use the explicit form of the unitary group for H_0:

$$\left(\mathrm{e}^{\mathrm{i}t\Delta}\psi\right)(x) = \frac{1}{(4\pi \mathrm{i}t)^{d/2}} \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\frac{|x-y|^2}{4t}}\psi(y)\mathrm{d}y. \tag{4.86}$$

For $\psi \in L^1(\mathbb{R}^3)$ this implies

$$\left\|\mathrm{e}^{\mathrm{i}t\Delta}\psi\right\|_{L^\infty} \leq \frac{\|\psi\|_{L^1}}{(4\pi|t|)^{3/2}}, \tag{4.87}$$

so we have

$$\int_1^\infty \left\|V\mathrm{e}^{\pm\mathrm{i}t\Delta}\psi\right\|_{L^2} \mathrm{d}t \leq \frac{\|V\|_{L^2}}{(4\pi)^{3/2}} \int_1^\infty |t|^{-3/2}\mathrm{d}t < \infty. \tag{4.88}$$

Thus, by Cook's Criterion, we have $D(H_0) \cap L^1(\mathbb{R}^3) \subset D(\Omega_\pm)$. Since this set is dense in $\mathscr{H}$ this shows that the wave operators exist, $D(\Omega_\pm) = \mathscr{H} = \mathscr{H}_{ac}(H_0)$. □

Lemma 4.36. *Let $A, D(A)$ be self-adjoint, $\psi \in \mathscr{H}$ be A-cyclic, P the projection to* span$\{\psi\}$*, and $T_\alpha = A + \alpha P$ be the family of rank-one perturbations of Section 4.4.1. Assume additionally that $(\mu_\psi)_{ac} = \rho(x)\mathrm{d}x$ with $\rho \in \mathscr{S}(\mathbb{R})$, where μ_ψ is the spectral measure of ψ w.r.t. A. Then for all $\alpha \in \mathbb{R}$ the wave operators $\Omega_\pm(T_\alpha, A)$ exist.*

Proof. Let $\varphi \in \mathscr{H}_{ac}(A)$, and assume additionally that $\varphi = f(A)\psi$ with $f \in \mathscr{S}(\mathbb{R})$ (the set of such φ is dense). We have

$$\mathrm{e}^{\mathrm{i}tT_\alpha}(T_\alpha - A)\mathrm{e}^{-\mathrm{i}tA}\varphi = \alpha\mathrm{e}^{\mathrm{i}tT_\alpha}\psi\langle\psi, \mathrm{e}^{-\mathrm{i}tA}\varphi\rangle. \tag{4.89}$$

Now $\left\|\mathrm{e}^{\mathrm{i}tT_\alpha}\psi\right\| = \|\psi\|$, and

$$\langle\psi, \mathrm{e}^{-\mathrm{i}tA}\varphi\rangle = \langle P_{ac}(A)\psi, \mathrm{e}^{-\mathrm{i}tA}\varphi\rangle = \int \mathrm{e}^{-\mathrm{i}tx}\rho(x)f(x)\mathrm{d}x. \tag{4.90}$$

Since $\rho, f \in \mathscr{S}$, the Fourier transform $\widehat{\rho f}(t) \in \mathscr{S}$. In particular, it is integrable in t, so the wave operators exist. □

In the following, we will sometimes need the subspace $\mathscr{M}(A) \subset \mathscr{H}_{ac}(A)$ given by

$$\mathscr{M}(A) := \{\varphi \in \mathscr{H}_{ac}(A) : \mu_\varphi(\mathrm{d}x) = \rho_\varphi(x)\mathrm{d}x,\ \rho_\varphi \in L^\infty(\mathbb{R})\}. \tag{4.91}$$

This is a Banach space with the norm

$$\|\varphi\|_{\mathscr{M}(A)} := \|\rho_\varphi\|_{L^\infty}^{1/2}, \tag{4.92}$$

and a dense subspace of $\mathscr{H}_{ac}(A)$ (Exercise; the only property we will need is density).

The main use of this concept is the following:

Lemma 4.37. *Let A, $D(A)$ be self-adjoint. For all $\psi \in \mathscr{H}$ and $\varphi \in \mathscr{M}(A)$ we have*

$$\int_{\mathbb{R}} |\langle \psi, \mathrm{e}^{-\mathrm{i}tA}\varphi\rangle|^2 \mathrm{d}t \le 2\pi \|\psi\|_{\mathscr{H}}^2 \|\varphi\|_{\mathscr{M}(A)}^2. \tag{4.93}$$

Proof. Let $U_\varphi : \mathscr{H} \to L^2(\mathbb{R}, \mu_\varphi)$ be the partial isometry given by composition of the projection to $\mathscr{H}_\varphi$ and the unitary to $L^2(\mathbb{R}, \mu_\varphi)$ used in the spectral theorem. Then

$$\langle \psi, \mathrm{e}^{-\mathrm{i}tA}\varphi\rangle = \int \mathrm{e}^{-\mathrm{i}tx}(U_\varphi\psi)(x)\mu_\varphi(\mathrm{d}x), \tag{4.94}$$

so by Plancherel's Theorem

$$\int |\langle \psi, \mathrm{e}^{-\mathrm{i}tA}\varphi\rangle|^2 \mathrm{d}t \le 2\pi \int \rho_\varphi^2(x)|U_\varphi\psi|^2(x)\mathrm{d}x \le 2\pi \|\rho_\varphi\|_{L^\infty} \|U_\varphi\psi\|_{L^2(\mu_\varphi)}^2 \le 2\pi \|\varphi\|_{\mathscr{M}}^2 \|\psi\|^2. \tag{4.95}$$

□

Lemma 4.38. *Assume the hypothesis of Lemma 4.36 and let $\varphi \in \mathscr{M}(A)$, then*

$$\|(\Omega_\pm(T_\alpha, A) - 1)\varphi\| \le \sqrt{4\pi|\alpha|}\, \|\varphi\|_{\mathscr{M}(A)} \|\psi\|. \tag{4.96}$$

Proof. Using the formula (4.85) for $t = \infty$ and $T = 0$, we find

$$\begin{aligned}
\|(\Omega_\pm - 1)\varphi\|^2 &= 2\|\varphi\|^2 - 2\mathrm{Re}\langle \Omega_\pm\varphi, \varphi\rangle = 2\mathrm{Re}\left(\langle \Omega_\pm\varphi, (\Omega_\pm\varphi - 1)\varphi\rangle\right) \\
&= -2\alpha \mathrm{Im} \int_0^\infty \langle \Omega_\pm\varphi, \mathrm{e}^{\mathrm{i}tT_\alpha}\psi\rangle\langle \psi, \mathrm{e}^{-\mathrm{i}tA}\psi\rangle \mathrm{d}t \\
&\le 2|\alpha| \left(\int_0^\infty |\langle \Omega_\pm\varphi, \mathrm{e}^{\mathrm{i}tT_\alpha}\psi\rangle|^2 \mathrm{d}t\right)^{1/2} \left(\int_0^\infty |\langle \varphi, \mathrm{e}^{-\mathrm{i}tA}\psi\rangle|^2 \mathrm{d}t\right)^{1/2}.
\end{aligned} \tag{4.97}$$

By Lemma 4.37 we have

$$\left(\int_0^\infty |\langle \varphi, \mathrm{e}^{-\mathrm{i}tA}\psi\rangle|^2 \mathrm{d}t\right)^{1/2} \le \sqrt{2\pi}\, \|\psi\| \|\varphi\|_{\mathscr{M}}. \tag{4.98}$$

For the term with $\Omega_\pm$ we additionally use the intertwining property to obtain

$$\begin{aligned}
\left(\int_0^\infty |\langle \Omega_\pm\varphi, \mathrm{e}^{\mathrm{i}tT_\alpha}\psi\rangle|^2 \mathrm{d}t\right)^{1/2} &= \left(\int_0^\infty |\langle \varphi, \mathrm{e}^{\mathrm{i}tA}\Omega_\pm^* P_{ac}(T_\alpha)\psi\rangle|^2 \mathrm{d}t\right)^{1/2} \\
&\le \sqrt{2\pi}\, \|\varphi\|_{\mathscr{M}} \|\Omega_\pm^* P_{ac}(T_\alpha)\psi\| \le \sqrt{2\pi}\, \|\varphi\|_{\mathscr{M}} \|\psi\|.
\end{aligned}$$

Together these yield the claim. □

Theorem 4.39. *Let $T_\alpha = A+\alpha P$ be the family of rank-one perturbations of Section 4.4.1 and ψ A-cyclic. For all α, β the wave operators $\Omega_\pm(T_\alpha, T_\beta)$ exist and are complete.*

Proof. Completeness of $\Omega_\pm(T_\alpha, T_\beta)$ follows from existence of $\Omega_\pm(T_\beta, T_\alpha)$ (Exercise), so it is sufficient to prove the latter for arbitrary α, β. We follow a similar reasoning as for Cook's Criterion. Set

$$W(t) := \mathrm{e}^{\mathrm{i}tT_\alpha}\mathrm{e}^{-\mathrm{i}tT_\beta}. \tag{4.99}$$

Assume first that ψ satisfies the conditions of Lemma 4.36 for $A = T_\beta$ and that $\varphi \in \mathscr{M}(T_\beta)$. Then the wave operators $\Omega_\pm(T_\alpha, T_\beta)$ exist and by the reasoning of (4.97) satisfy

$$\|(\Omega_\pm - W(s))\varphi\| \le \sqrt{2|\alpha-\beta|\sqrt{2\pi}\,\|\varphi\|_{\mathscr{M}}\,\|\psi\|}\left(\int_s^\infty |\langle\varphi, \mathrm{e}^{-\mathrm{i}tT_\beta}\psi\rangle|^2 \mathrm{d}t\right)^{1/4}. \tag{4.100}$$

Using this twice together with the triangle inequality gives

$$\|(W(t) - W(s))\varphi\| \le 2\sqrt{2|\alpha-\beta|\sqrt{2\pi}\,\|\varphi\|_{\mathscr{M}}\,\|\psi\|}\left(\int_{\min\{s,t\}}^\infty |\langle\varphi, \mathrm{e}^{-\mathrm{i}tT_\beta}\psi\rangle|^2 \mathrm{d}t\right)^{1/4}. \tag{4.101}$$

Note that this inequality is again independent of $\Omega_\pm$ with both sides depending continuously on $\psi \in \mathscr{H}$ (for fixed s, t). The set of $\psi \in \mathscr{H}_{ac}(T_\beta)$ with $\rho_\psi \in \mathscr{S}$ is dense[2] in $\mathscr{H}_{ac}(T_\beta)$, so the inequality above holds for arbitrary $\psi \in \mathscr{H}$ by approximation. By Lemma 4.37 the right hand side converges to zero as $\min\{s,t\} \to \infty$, so the sequence $W(t)\varphi$ is Cauchy and $\varphi \in D(\Omega_\pm)$. Since $\mathscr{M}(T_\beta)$ is dense this shows that $\Omega_\pm$ exists. □

Corollary 4.40. *Let A, $D(A)$ be self-adjoint and $K = K^*$ an operator of finite rank. Then the wave operators $\Omega_\pm(A+K, A)$ exist and are complete.*

Proof. The operator K can be written as a finite sum of rank-one operators

$$K = \sum_{j=1}^N \alpha_j P_j. \tag{4.102}$$

Denote for $n \le N$, $A_n = A + \sum_{j=1}^n \alpha_j P_j$. Then $A_{n+1} = A_n + \alpha_j P_j$ and by Theorem 4.39 the wave operators $\Omega_\pm(A_{n+1}, A_n)$ exist and are complete. By the chain rule for the wave operators (Exercise 39), we then have existence of the wave operators

$$\Omega_\pm(A+K, A) = \Omega_\pm(A_N, A_{N-1}) \cdot \ldots \Omega_\pm(A_1, A_0). \tag{4.103}$$

Completeness follows from considering $\tilde{A} = A + K$, $\tilde{K} = -K$ and Exercise (?). □

We can also compare the wave operators $\Omega_\pm$ with the unitary $U : L^2(\mathbb{R}, \mu_{ac}^\beta) \to L^2(\mathbb{R}, \mu_{ac}^\alpha)$ found in Proposition 4.24. By the following proposition we have $U^* = U_\psi^\alpha \Omega_+(T_\alpha, T_\beta)$

[2] $\mathscr{H}_\psi$ is isomorphic to $L^2(\mathbb{R}, \rho_\psi \mathrm{d}x)$ and in the latter space the set of functions $g = f\rho_\psi^{-1}$ with $f \in \mathscr{S}$ is dense. The spectral measure of $g(T_\beta)\psi$ has density $|f|^2 \in \mathscr{S}$. Density in $\mathscr{H}_{ac}(T_\beta)$ of such vectors follows by decomposing into cyclic subspaces.

Proposition 4.41. *Let T_α, ψ be as in Theorem 4.39, assuming additionally that $\mu^\beta = \mu^\beta_{ac}(\mathrm{d}x) = \rho(x)\mathrm{d}x$ with $\rho \in C^{0,r}$, $r > 0$. Denote by U^α_ψ the unitary $U^\alpha_\psi : \mathscr{H}_{ac}(T_\alpha) \to L^2(\mathbb{R}, \mu^\alpha_{ac})$. Then*

$$\left(U^\alpha_\psi \Omega_\pm(T_\alpha, T_\beta)\psi\right)(x) = \lim_{\varepsilon\to 0} \frac{1}{1 + (\beta - \alpha)\Phi_\alpha(x \pm \mathrm{i}\varepsilon)}. \tag{4.104}$$

Proof. Let $f \in L^2(\mathbb{R}, \mu^\alpha_{ac})$, $\varphi = (U^\alpha_\psi)^* f$, then we can calculate

$$\begin{aligned}\langle f, U^\alpha_\psi(\Omega_\pm(T_\alpha, T_\beta) - 1)\psi\rangle &= \mathrm{i}(\alpha - \beta)\int_0^{\pm\infty} \langle \varphi, \mathrm{e}^{\mathrm{i}tT_\alpha}\psi\rangle\langle\psi, \mathrm{e}^{-\mathrm{i}tT_\beta}\psi\rangle \mathrm{d}t \\ &= \mathrm{i}(\alpha - \beta)\int_0^{\pm\infty}\int_{\mathbb{R}} \overline{f(x)}\mathrm{e}^{\mathrm{i}tx}\langle\psi, \mathrm{e}^{-\mathrm{i}tT_\beta}\psi\rangle \mu^\alpha_{ac}(\mathrm{d}x)\mathrm{d}t.\end{aligned}$$

Using Exercise T26 this equals

$$\langle\varphi, (\Omega_\pm - 1)\psi\rangle = \lim_{\varepsilon\to 0}\int_0^{\pm\infty}\int_{\mathbb{R}} \overline{f(x)}\langle\psi, \mathrm{e}^{-\mathrm{i}t(T_\beta - x \mp \mathrm{i}\varepsilon)}\psi\rangle\mu^\alpha_{ac}(\mathrm{d}x)\mathrm{d}t. \tag{4.105}$$

The dt-integral yields

$$\mathrm{i}\int_0^{\pm\infty}\langle\psi, \mathrm{e}^{-\mathrm{i}t(T_\beta - x\mp\mathrm{i}\varepsilon)}\psi\rangle\mathrm{d}t = \left\langle\psi, \frac{1}{T_\beta - x \mp \mathrm{i}\varepsilon}\psi\right\rangle = \int\frac{\rho(y)\mathrm{d}y}{y - x\mp\mathrm{i}\varepsilon}. \tag{4.106}$$

Thus

$$\langle\varphi, (\Omega_\pm - 1)\psi\rangle = (\alpha - \beta)\lim_{\varepsilon\to 0}\int\overline{f(x)}\int\frac{\rho(y)\mathrm{d}y}{y - x\mp\mathrm{i}\varepsilon}\mu^\alpha_{ac}(\mathrm{d}x). \tag{4.107}$$

In the limit, we have
We thus find

$$\begin{aligned}\langle f, U^\alpha_\psi\Omega_\pm\psi\rangle &= \lim_{\varepsilon\to 0}\int\overline{f(x)}(1 + (\beta - \alpha)\Phi_\beta(x \pm \mathrm{i}\varepsilon))\mu^\alpha_{ac}(\mathrm{d}x) \\ &= \lim_{\varepsilon\to 0}\langle f, (1 + (\beta - \alpha)\Phi_\beta(\cdot \pm \mathrm{i}\varepsilon))\rangle_{L^2(\mathbb{R}, \mu^\alpha_{ac})}\end{aligned}$$

Using Hölder continuity of ρ we can pass the limit under the integral (compare Exercise 30) and obtain

$$\begin{aligned}\left(U^\alpha_\psi\Omega_\pm\psi\right)(x) &= \lim_{\varepsilon\to 0}(1 + (\beta - \alpha)\Phi_\beta(x \pm \mathrm{i}\varepsilon)) \\ &= \lim_{\varepsilon\to 0}\frac{1}{1 + (\alpha - \beta)\Phi_\alpha(x \pm \mathrm{i}\varepsilon)}.\end{aligned}$$

□

Remark 4.42. Supposing additionally that $\rho = f^2$ for $f \in C^{0,r}$, $r > 1/2$ (say for $\beta = 0$) we can show that $\mathscr{H}_{sc}(T_\alpha) = \{0\}$ for $\alpha \neq \beta$, so assuming that $\mathscr{H}_{sc}(A) = \{0\}$ we have asymptotic completeness. With what we have proved, we can at least see that every element of M^α_s is an eigenvalue: If $\lambda \in M^\alpha_s$ then necessarily $\rho(\lambda) = 0$ and

$\lim_{\varepsilon\to 0}\Phi_0(\lambda \pm \mathrm{i}\varepsilon) = -\alpha^{-1}$, since otherwise $\mathrm{Im}\Phi_\alpha$ has a finite limit. Then, using that $r > 1/2$,

$$\int_{\mathbb{R}} \frac{f^2}{(x-\lambda)^2}\mathrm{d}x < \infty. \tag{4.108}$$

This implies that λ is an eigenvalue of T_α by Exercise 32. Showing that λ cannot also be part of the singular continuous spectrum requires additional tools.

In general, one does not have asymptotic completeness, since a dense set of eigenvalues of A may turn into *sc*-spectrum of T_α, as we have seen in Example 4.23.

We will now generalise our results on existence and completeness of wave operators to perturbations of trace-class and relative trace-class. For this, we will use a more general notion of wave operator. Let $\mathscr{H}_1$, $\mathscr{H}_2$ be Hilbert spaces, A, $D(A)$ self-adjoint on $\mathscr{H}_1$, B, $D(B)$ self-adjoint on $\mathscr{H}_2$, and $J : \mathscr{H}_1 \to \mathscr{H}_2$ a bounded operator. Then the generalised wave operator is defined by

$$\begin{aligned}\Omega_\pm(A,B,J) &= s - \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tA} J \mathrm{e}^{-\mathrm{i}tB},\\ D(\Omega_\pm(A,B,J)) &= \{\psi \in P_{ac}(B)\mathscr{H}_1 : \exists \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tA} J \mathrm{e}^{-\mathrm{i}tB}\psi\}.\end{aligned} \tag{4.109}$$

We will use these as a technical tool, but such operators are also relevant in many-body scattering. For example, a system with three particles may have asymptotic states that consist of *two* freely moving particles, one of which is a bound system of two of the original particles, like an atom or molecule.

Theorem 4.43 (Pearson)**.** *Let $\mathscr{H}_1 = \mathscr{H}_2$ and $J \in \mathrm{B}(\mathscr{H})$. If there exists $C \in \mathfrak{S}_1(\mathscr{H})$ such that for all $\varphi \in D(A)$, $\psi \in D(B)$*

$$\langle A\varphi, J\psi\rangle - \langle J^*\varphi, B\psi\rangle = \langle \varphi, C\psi\rangle, \tag{4.110}$$

then $D(\Omega_\pm(A,B,J)) = P_{ac}(B)\mathscr{H}$.

Proof. The condition means that $AJ - JB = C$ in the sense of quadratic forms. For simplicity we assume additionally that J maps $D(B)$ to $D(A)$, so we may treat this as an equality of operators. Let

$$W_J(t) := \mathrm{e}^{\mathrm{i}tA} J \mathrm{e}^{-\mathrm{i}tB}, \tag{4.111}$$

then it suffices to prove that

$$\|(W_J(t) - W_J(s))\eta\|^2 = \langle \eta, W_J^*(t)((W_J(t)-W_J(s))\eta\rangle - \langle \eta, W_J^*(s)((W_J(t)-W_J(s))\eta\rangle \tag{4.112}$$

tends to zero as $s,t \to \pm\infty$ for all η in some dense set $D \subset \mathscr{H}_{ac}(B)$. Let us consider the case $s,t\to+\infty$. We can express the difference as

$$W_J(t) - W_J(s) = \mathrm{i}\int_s^t \mathrm{e}^{\mathrm{i}\tau A}\underbrace{(AJ - JB)}_{=C}\mathrm{e}^{-\mathrm{i}\tau B}\mathrm{d}\tau. \tag{4.113}$$

This operator is compact since C is compact and the integrand is uniformly bounded (take a bounded sequence $(\psi_n)_{\mathbb{N}}$ converging weakly to zero and use dominated convergence to see that $(W_J(t) - W_J(s))\psi_n$ converges to zero in norm). By Proposition 3.65 we thus have for all $\eta \in \mathscr{H}_{ac}(B)$

$$\lim_{\rho\to\infty} (W_J(t) - W_J(s))\mathrm{e}^{-\mathrm{i}\rho B}\eta = 0. \tag{4.114}$$

This implies that

$$\begin{aligned}&\langle \eta, W_J^*(t)((W_J(t) - W_J(s))\eta\rangle \\ &= \lim_{\rho\to\infty} \langle \eta, W_J^*(t)((W_J(t) - W_J(s))\eta\rangle - \langle \eta, \mathrm{e}^{\mathrm{i}B\rho} W_J^*(t)((W_J(t) - W_J(s))\mathrm{e}^{-\mathrm{i}B\rho}\eta\rangle.\end{aligned}$$

Now assuming that $\eta \in D(B)$

$$\begin{aligned}&\langle \eta, W_J^*(s)W_J(t)\eta\rangle - \langle \eta, \mathrm{e}^{\mathrm{i}B\rho} W_J^*(s)W_J(t)\mathrm{e}^{-\mathrm{i}B\rho}\eta\rangle \\ &= -\mathrm{i}\int_0^\rho \langle \eta, \mathrm{e}^{\mathrm{i}\tau B}[B, W_J^*(s)W_J(t)]\mathrm{e}^{-\mathrm{i}\tau B}\eta\rangle \mathrm{d}\tau.\end{aligned}$$

We have, since $JB = -C + AJ$,

$$\begin{aligned}[B, W_J^*(s)W_J(t)] &= \mathrm{e}^{\mathrm{i}sB} B J^* \mathrm{e}^{\mathrm{i}(t-s)A} J \mathrm{e}^{-\mathrm{i}tB} - \mathrm{e}^{\mathrm{i}sB} J^* \mathrm{e}^{\mathrm{i}(t-s)A} J B \mathrm{e}^{-\mathrm{i}tB} \\ &= -\mathrm{e}^{\mathrm{i}sB} C^* \mathrm{e}^{\mathrm{i}(t-s)A} J \mathrm{e}^{-\mathrm{i}tB} + \mathrm{e}^{\mathrm{i}sB} J^* \mathrm{e}^{\mathrm{i}(t-s)A} C \mathrm{e}^{-\mathrm{i}tB}.\end{aligned}$$

Inserting this into the equation before, we obtain

$$\mathrm{i}\int_0^\rho \langle \mathrm{e}^{-\mathrm{i}(\tau+s)B}\eta, \left(C^* \mathrm{e}^{\mathrm{i}(t-s)A} J - J^* \mathrm{e}^{\mathrm{i}(t-s)A} C\right) \mathrm{e}^{-\mathrm{i}(\tau+t)B}\eta\rangle \mathrm{d}\tau. \tag{4.115}$$

An upper bound of, e.g., the second term is given by expanding $C = \sum c_n \varphi_n \langle \psi_n, \cdot\rangle$ with $(\varphi_n)_{\mathbb{N}}$, $(\psi_n)_{\mathbb{N}}$ orthonormal and using the Cauchy-Schwarz inequality

$$\begin{aligned}&\left|\sum_{n=1}^\infty \int_0^\rho c_n \langle \mathrm{e}^{-\mathrm{i}(\tau+s)B}\eta, J^* \mathrm{e}^{\mathrm{i}(t-s)A}\varphi_n\rangle \langle \psi_n, \mathrm{e}^{-\mathrm{i}(\tau+t)B}\eta\rangle \mathrm{d}\tau\right| \\ &\le \left(\sum_{n=1}^\infty \int_s^\infty |c_n| |\langle \mathrm{e}^{-\mathrm{i}\tau B}\eta, J^* \mathrm{e}^{\mathrm{i}(t-s)A}\varphi_n\rangle|^2 \mathrm{d}\tau\right)^{1/2} \left(\sum_{n=1}^\infty \int_t^\infty |c_n| |\langle \psi_n, \mathrm{e}^{-\mathrm{i}\tau B}\eta\rangle|^2 \mathrm{d}\tau\right)^{1/2}\end{aligned} \tag{4.116}$$

Assume that $\eta \in \mathscr{M}(B)$. Then by Lemma 4.37

$$\int_0^\infty |\langle \psi_n, \mathrm{e}^{-\mathrm{i}\tau B}\eta\rangle|^2 \mathrm{d}\tau \le 2\pi \left\|\psi_n\right\|_{\mathscr{H}}^2 \left\|\eta\right\|_{\mathscr{M}}^2, \tag{4.117}$$

and

$$\int_0^\infty |\langle \mathrm{e}^{-\mathrm{i}\tau B}\eta, J^* \mathrm{e}^{\mathrm{i}(t-s)A}\varphi_n\rangle|^2 \mathrm{d}\tau \le 2\pi \left\|\varphi_n\right\|_{\mathscr{H}}^2 \left\|J\right\|^2 \left\|\eta\right\|_{\mathscr{M}}^2. \tag{4.118}$$

Collecting all the terms (there are four, which all satisfy a similar estimate), we obtain the upper bound

$$|\langle \eta, W_J^*(t)((W_J(t) - W_J(s))\eta\rangle| \\ \leq 4\sqrt{2\pi \|C\|_{\mathfrak{S}_1}} \|\eta\|_{\mathscr{M}} \|J\| \left(\sum_{n=1}^{\infty} \int_{\min\{s,t\}}^{\infty} |c_n| |\langle \psi_n, \mathrm{e}^{-\mathrm{i}\tau B}\eta\rangle|^2 \mathrm{d}\tau \right)^{1/2}, \tag{4.119}$$

and the right hand side tends to zero as $s, t \to \infty$. This shows that $\eta \in D(\Omega_+(A, B, J))$ and, since $\mathscr{M}(B) \cap D(B)$ is dense in $\mathscr{H}_{ac}(B)$, that $D(\Omega_+(A, B, J)) = \mathscr{H}_{ac}(B)$. □

Corollary 4.44. *Assume the hypothesis of Theorem 4.43 and let $\varphi \in \mathscr{M}(B)$. Then*

$$\|(\Omega_\pm(A, B, J) - J)\,\varphi\|^2 \leq 16\pi \|C\|_{\mathfrak{S}_1} \|J\| \|\varphi\|^2_{\mathscr{M}(B)} \tag{4.120}$$

Proof. Set $s = 0$ in (4.119) and let $t \to \infty$. □

Corollary 4.45 (Kato-Rosenblum)**.** *Let A, $D(A)$ and B, $D(B) = D(A)$ be self-adjoint on $\mathscr{H}$ and suppose that $A - B \in \mathfrak{S}_1(\mathscr{H})$. Then $\Omega_\pm(A, B)$ exist and are complete.*

Proof. In the previous theorem take $J = 1$. This condition is now symmetric, so $\Omega_\pm(B, A)$ also exist, and this gives completeness by Exercise 40. □

Theorem 4.46 (Kuroda-Birman)**.** *Let A, $D(A)$ and B, $D(B)$ be self-adjoint on $\mathscr{H}$ and suppose that*

$$R_\mathrm{i}(A) - R_\mathrm{i}(B) \in \mathfrak{S}_1(\mathscr{H}). \tag{4.121}$$

Then $\Omega_\pm(A, B)$ exist and are complete.

Proof. Take $J = R_\mathrm{i}(A)R_\mathrm{i}(B)$, then

$$\langle A\varphi, J\psi\rangle - \langle J^*\varphi, B\psi\rangle = \langle (A + \mathrm{i})\varphi, J\psi\rangle - \langle J^*\varphi, (B - \mathrm{i})\psi\rangle = \langle \varphi, (R_\mathrm{i}(A) - R_\mathrm{i}(B))\,\psi\rangle. \tag{4.122}$$

By Theorem 4.43, the limit

$$\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tA} R_\mathrm{i}(A)R_\mathrm{i}(B)\mathrm{e}^{-\mathrm{i}tB}\psi \tag{4.123}$$

exists for all $\psi \in \mathscr{H}_{ac}(B)$. Since $R_\mathrm{i}(A) - R_\mathrm{i}(B)$ is compact,

$$\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tA}\,(R_\mathrm{i}(A) - R_\mathrm{i}(B))\,R_\mathrm{i}(B)\mathrm{e}^{-\mathrm{i}tB}\psi = 0, \tag{4.124}$$

for all $\psi \in \mathscr{H}_{ac}(B)$ and the limit

$$\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tA} R_\mathrm{i}(B)^2 \mathrm{e}^{-\mathrm{i}tB}\psi \tag{4.125}$$

exists. In particular, we may choose $\psi = (B - \mathrm{i})^2\varphi$ with some $\varphi \in D(B^2)$, and conclude that

$$\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tA}\mathrm{e}^{-\mathrm{i}tB}\varphi \tag{4.126}$$

exists. By density of $D(B^2)$ in $\mathscr{H}$, we find that $\Omega_\pm(A, B)$ exists, and by symmetry of the conditions that $\Omega_\pm(B, A)$ exists and is complete. □

The trace-class condition for the difference of resolvents is much more useful than the simple trace condition, since it can be applied to $-\Delta + V$.

Corollary 4.47. *Let $d \leq 3$ and $V \in L^1(\mathbb{R}^d, \mathbb{R}) \cap L^2(\mathbb{R}^d)$ and set $H = -\Delta + V$, $H_0 = -\Delta$ with $D(H) = D(H_0) = H^2(\mathbb{R}^d) \subset L^2(\mathbb{R}^d)$. Then the wave operators $\Omega_\pm(H, H_0)$ exist and are complete.*

Proof. We have to show that $R_{\mathrm{i}}(H) - R_{\mathrm{i}}(H_0) \in \mathfrak{S}_1(L^2(\mathbb{R}^d))$. We have

$$R_{\mathrm{i}}(H) - R_{\mathrm{i}}(H_0) = -R_{\mathrm{i}}(H) V R_{\mathrm{i}}(H_0) = \underbrace{R_{\mathrm{i}}(H)(H_0 - \mathrm{i})}_{\in \mathrm{B}(\mathscr{H})} R_{\mathrm{i}}(H_0) V R_{\mathrm{i}}(H_0). \tag{4.127}$$

By the boundedness of the pre-factor (which follows from Kato-Rellich, since $V \in L^2$) it is sufficient to show that $R_{\mathrm{i}}(H_0) V R_{\mathrm{i}}(H_0)$ is trace-class. This can be achieved by proving that $R_{\mathrm{i}}(H_0) V R_{\mathrm{i}}(H_0) = T^* S$ with $S, T \in \mathfrak{S}_2$. We choose

$$\begin{aligned} T &= |V|^{1/2} R_{-\mathrm{i}}(H_0) \\ S &= \operatorname{sgn}(V) |V|^{1/2} R_{\mathrm{i}}(H_0), \end{aligned}$$

which clearly yields the right result for $T^* S$. Both T and S have the form $f \mathscr{F}^{-1} g \mathscr{F}$, where $|f| = |V|^{1/2} \in L^2$ if $V \in L^1$ and $g(k) = (k^2 \mp \mathrm{i})$, which is an element of $L^2(\mathbb{R}^d)$ for $d \leq 3$. It thus follows from Exercise 42 that $S, T \in \mathfrak{S}_2$. $\square$

For $d = 3$ we can apply both this Corollary and the earlier Proposition. The Corollary needs the additional assumption that $V \in L^1$, but it also gives completeness of the wave operators!

Theorem 4.48. *Let A, $D(A)$ and B, $D(B)$ be self-adjoint on $\mathscr{H}$ and suppose that for some integer $m \geq 1$ and all $z \in \mathbb{C} \setminus \mathbb{R}$*

$$R_z(A)^m - R_z(B)^m \in \mathfrak{S}_1(\mathscr{H}). \tag{4.128}$$

Then $\Omega_\pm(A, B)$ exist and are complete.

Proof. We use the same strategy as for the Kuroda-Birman Theorem. Let

$$J = \sum_{\ell=0}^{m-1} R_{\mathrm{i}}(A)^{m+\ell} R_{\mathrm{i}}(B)^{m-\ell}. \tag{4.129}$$

Then

$$\begin{aligned} (A - \mathrm{i})J - J(B - \mathrm{i}) &= R_{\mathrm{i}}(A)^{m-1} \sum_{\ell=0}^{m-1} \left(R_{\mathrm{i}}(A)^{\ell} R_{\mathrm{i}}(B)^{m-\ell} - R_{\mathrm{i}}(A)^{\ell+1} R_{\mathrm{i}}(B)^{m-\ell-1} \right) \\ &= -R_{\mathrm{i}}(A)^{m-1} \left(R_{\mathrm{i}}(A)^m - R_{\mathrm{i}}(B)^m \right) \in \mathfrak{S}_1. \end{aligned}$$

This gives existence of $\Omega_\pm(A,B,J)$. Now

$$\begin{aligned} J - mR_{\mathrm{i}}(B)^{2m} &= \sum_{\ell=0}^{m-1} R_{\mathrm{i}}(A)^{m+\ell} R_{\mathrm{i}}(B)^{m-\ell} - R_{\mathrm{i}}(B)^{2m} \\ &= \sum_{\ell=0}^{m-1} \left(R_{\mathrm{i}}(A)^{m+\ell} - R_{\mathrm{i}}(B)^{m+\ell} \right) R_{\mathrm{i}}(B)^{m-\ell}. \end{aligned}$$

The summand for $\ell = 0$ is compact, and this also holds for $\ell > 0$, since

$$R_z(A)^{m+\ell} = \frac{(-1)^\ell (\ell-1)!}{(m+\ell-1)!} \frac{\mathrm{d}^\ell}{\mathrm{d}z^\ell} R_z(A)^m, \tag{4.130}$$

so $R_{\mathrm{i}}(A)^{m+\ell} - R_{\mathrm{i}}(B)^{m+\ell}$ can be approximated in norm by compact operators by writing out the difference quotients. We conclude that for $\psi = (B-\mathrm{i})^{2m}\varphi$, $\varphi \in D(B^{2m})$, the limits

$$\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tA} R_{\mathrm{i}}(B)^{2m} \mathrm{e}^{-\mathrm{i}tB}\psi = \lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tA}\mathrm{e}^{-\mathrm{i}tB}\varphi \tag{4.131}$$

exist. By density of $D(B^{2m})$ this gives existence of $\Omega_\pm(A,B)$, and by symmetry of the conditions completeness. $\square$

Theorem 4.49. *Let $V \in L^1(\mathbb{R}^d,\mathbb{R}) \cap H^{2m}(\mathbb{R}^d)$ with $m = \min\{n \in \mathbb{N} : n > d/2 - 1\}$ and set $H = -\Delta + V$, $H_0 = -\Delta$ with $D(H) = D(H_0) = H^2(\mathbb{R}^d) \subset L^2(\mathbb{R}^d)$. Then the wave operators $\Omega_\pm(H,H_0)$ exist and are complete.*

Proof (sketch). We want to apply the previous theorem for the given m. We have

$$\begin{aligned} R_z(H)^m - R_z(H_0)^m &= \sum_{\ell=0}^{m-1} R_z(H)^\ell \left(R_z(H) - R_z(H_0)\right) R_z(H_0)^{m-\ell-1} \\ &= -\sum_{\ell=0}^{m-1} R_z(H)^{\ell+1} V R_z(H_0)^{m-\ell}, \end{aligned}$$

so it is sufficient to prove that $R_z(H)^{\ell+1} V R_z(H_0)^{m-\ell} \in \mathfrak{S}_1(L^2(\mathbb{R}^d))$ for every $\ell \le m-1$. Using that $V \in H^{2m}(\mathbb{R}^d)$ one can show that $H_0^k R_z(H)^k$ is bounded for all $k \le m$, so we may replace $R_z(H)$ by $R_z(H_0)$ for this purpose. We now use the inequality $\|KL\|_{\mathfrak{S}_1} \le \|K\|_{\mathfrak{S}_p} \|L\|_{\mathfrak{S}_q}$, with $p^{-1} + q^{-1} = 1$, splitting the operator as

$$\begin{aligned} K &= R_z(H_0)^{\ell+1} \operatorname{sgn}(V)|V|^{1/p} \\ L &= |V|^{1/q} R_z(H_0)^{m-\ell}. \end{aligned}$$

To prove the $\mathfrak{S}_p$-bounds with the appropriate p,q, we use the Kato-Seiler-Simon inequality

$$\|M_f \mathscr{F}^* M_g \mathscr{F}\|_{\mathfrak{S}_p} \le C_p \|f\|_{L^p} \|g\|_{L^p} \tag{4.132}$$

(we have proved this for $p = \infty$, in Exercise 09, and for $p = 2$, Exercise 42; the inequality for general p follows from an interpolation argument). Under the condition that $m+1 >$

$d/2$, we can choose $p > \frac{d}{2(\ell+1)}$ and $q > \frac{d}{2(m-\ell)}$, $p^{-1} + q^{-1} = 1$, which give the necessary L^p-bounds.

The claim now follows from Theorem 4.48. $\square$

Symbol	**Explanation**	**Page**
X	Usually a complex Banach space	
$\mathrm{B}(X,Y)$	Banach space of bounded linear operators from X to Y	
$\mathrm{B}(X)$	Banach space of bounded linear operators from X to X	
X'	Space of continuous linear functionals on X (=$\mathrm{B}(X,\mathbb{C})$)	
$\mathscr{H}$	Complex Hilbert space	
$A, D(A)$	Densely defined linear operator	
$\mathscr{G}(A)$	Graph of A	3
$\overline{A}$	Closure of $(A, D(A))$	3
$\lVert\cdot\rVert_{D(A)}$	Graph norm on $D(A)$	3
A^*	(Hilbert-) adjoint of $(A, D(A))$	5
$\ker(A)$	Kernel of A	
$\mathrm{ran}(A)$	Range of A	
$\rho(A)$	Resolvent set of A	4
$R_z(A)$	Resolvent of A in $z \in \rho(A)$	4
$\sigma(A)$	Spectrum of A	4
ℓ^p	Banach space of p-summable sequences $\mathbb{N} \to \mathbb{C}$	
c_0	Banach space of sequences converging to zero	
c_{00}	Space of sequences that are eventually zero	
$C^k(\Omega)$	Space of k-times differentiable functions $\Omega \to \mathbb{C}$	
$C_0^k(\Omega)$	Space of k-times differentiable functions $\Omega \to \mathbb{C}$ with compact support, $\operatorname{supp} f \Subset \Omega$	
$H^k(\Omega)$	Sobolev space of functions in $L^2(\Omega)$ with k weak derivatives in L^2	13
$H_0^k(\Omega)$	Closure of $C_0^k(\Omega)$ in $H^k(\Omega)$	15
$\mathfrak{S}_p$	p-th Schatten class	71

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