Lecture notes: *Spectral Theory of selfadjoint operators*

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1 Unbounded operators on a (separable) Hilbert space

1.1 Unbounded operators and their domains

Notation 1. $\mathcal{H}$ is a separable Hilbert space, and the scalar product on $\mathcal{H}$ will be anti-linear w.r.t. the first argument: $\langle \alpha u, \beta v \rangle = \overline{\alpha \beta} \langle u, v \rangle$. When there is no ambiguity on the Hilbert space we are dealing with, the norm $\|u\|$ will denote the Hilbert norm of a state $u \in \mathcal{H}$, while $\|A\|$ denotes the operator norm of a bounded operator $A : \mathcal{H} \to \mathcal{H}$.

An bounded linear op. $A : \mathcal{H} \to \mathcal{H}$ is defined for all $u \in \mathcal{H}$, and satisfies

$$\forall u \in \mathcal{H}, \quad \|Au\| \leq C\|u\|,$$

the infimum of all possible $C$ defining the norm $\|A\|$. On the opposite, an unbounded operator on $\mathcal{H}$ is a priori not defined on all of $\mathcal{H}$, but only on a proper subspace called its domain $D(A) \subset \mathcal{H}$, so to define an operator one should include its domain and write $(A, D(A))$. We will always assume that $D(A)$ is dense in $\mathcal{H}$. Being unbounded means that

$$\sup_{0 \neq u \in D(A)} \frac{\|Au\|}{\|u\|} = \infty,$$

implying that $A$ cannot be extended to a continuous operator on all of $\mathcal{H}$.

An operator $A$ can be defined by its graph

$$\text{gr}(A) = \{(u, Au), \ u \in D(A)\}, \quad \text{a linear subspace of } \mathcal{H} \times \mathcal{H}.$$ 

In practice, we will often be interested in differential operators\(^1\) $P = \sum_{|\alpha| \leq m} a_\alpha(x) D_x^\alpha$ acting on the Hilbert space $L^2(X, |dx|)$, with $X = \mathbb{R}^d$, $X = \Omega \subset \mathbb{R}^d$, $X$ a Riemannian manifold and $|dx|$ the volume measure. Such operators are well-defined on $C^\infty_c(X)$; we would like to extend $P$ to a “more natural” subspace of $L^2$, that is define a “natural” extension $\tilde{P}$ of $P$, with $D(P) \subset D(\tilde{P})$. To denote such an extension we will write $P \subset \tilde{P}$.

Are there many ways to do so?

One nice property of an operator on $\mathcal{H}$ is closedness: $(A, D(A))$ is closed iff $\text{gr}(A)$ is a closed subspace of $\mathcal{H} \times \mathcal{H}$. Equivalently, it means that its domain $D(A)$ is a complete vector space for the

**graph norm**

$$\|u\|_A \overset{\text{def}}{=} \|u\| + \|Au\|.$$ 

Example 2. Any bounded operator is closed (closed graph theorem).

On the opposite, a differential operator $P$ with domain $D(P) = C^\infty_c(X)$ is not closed on $L^2(X)$.

An operator $A$ is closable if the closure of its graph, $\overline{\text{gr}(A)}$, is still the graph of an operator, which we call $\bar{A}$ the closure of $A$:

$$\overline{\text{gr}(A)} = \{(u, \bar{A}u), \ u \in D(\bar{A})\}.$$ 

\(^1\) $\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{N}^d$ is a multi-index, $|\alpha| = \sum \alpha_i$, and the operator $D_x = -i \partial_x$. 

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Not all operators are closable, but differential operators are closable on $L^2(X)$. Indeed, we know that for any $u \in \mathcal{H}$, $Pu$ makes sense in the space of distributions $\mathcal{D}'(X)$. One then has
\[
\overline{\text{gr} P} \subset \text{gr}(P_{\text{max}}) = \{(u, Pu), u, Pu \in L^2(X)\},
\]
showing that $\overline{\text{gr} P}$ is still a graph, hence that $P$ is closable. If $X$ has a boundary, in general $P_{\text{max}}$ is a proper extension of $\bar{P}$.

**Example 3.** $P = D_x$ on $X = \mathbb{R}$, with domain $C_0^\infty(\mathbb{R})$, admits as closure $\bar{P}$ with domain $H^1(\mathbb{R})$ the Sobolev space of degree 1. The Laplacian $P = -\Delta$ on $C^\infty_c(\mathbb{R}^d)$ can be extended to the operator $\bar{P}$ defined on $H^2(\mathbb{R}^d)$.

**Remark 4.** A counterexample to closability: for some $v_0 \in \mathcal{H}$ and $x_0 \in X$, the operator $Au = u(x_0)v_0$ defined on $D(A) = C^0(X)$, is not closable.

### 1.2 Adjoint of an unbounded operator

If $A : \mathcal{H} \to \mathcal{H}$ is bounded, then its adjoint is defined by duality: for any given $u \in \mathcal{H}$, the map $v \mapsto \langle u, Av \rangle$ is a bounded linear form $\ell_u$ on $\mathcal{H}$, so by Riesz’s representation theorem there is a unique $w \in \mathcal{H}$ s.t. this linear form is equal to $\ell_u(v) = \langle w, v \rangle$. Obviously, the dependence $u \mapsto w$ defines a bounded linear operator, which we call the adjoint $A^*$ of $A$.

Things become more tricky when $A$ is unbounded, since questions of domains pop up. The scalar product $v \mapsto \langle u, Av \rangle$ only defines a linear form on the space $D(A)$. If $\ell_u$ can be extended continuously to all $v \in \mathcal{H}$, then we may write $\ell_u(v) = \langle w, v \rangle$, an define the operator $A^*$ by stating that $u \in D(A^*)$ and $w = A^*u$. $(A^*, D(A^*))$ is called the adjoint of $(A, D(A))$.

$A^*$ can be alternatively defined through its graph: $\text{gr}(A^*) = J(\text{gr}(A)^\perp)$, where we use the “rotation” $J(u_1, u_2) = (u_2, -u_1)$ on $\mathcal{H} \times \mathcal{H}$. This representation shows that $A^*$ is **automatically closed**. Taking the adjoint automatically constructs a closed op. If $A$ is closable, then $D(A^*)$ is dense and $(A^*)^* = A$.

**Example 5.** Case of a diff. operator $P = \sum_{|α| \leq m} a_m(x)D^α$. By integration by parts (for $X \subset \mathbb{R}^d$), the adjoint $P^*$ acts, on functions $u \in C_0^\infty$, as the differential operator $\sum_{|α| \leq m} D^αa_m$. What is its domain?

If $P_0 = D_x$ with $D(P_0) = C^\infty_c(\mathbb{R})$, we find by integration by parts that $P_0^* = D_x$, and has the domain $D(P_0^*) = H^1(\mathbb{R})$. If we take the double adjoint, we get $(P_0^*)^* = \bar{P}_0 = P_0^*$.

If $P_1 = D_x$ on $L^2([0,1])$, $D(P_1) = C^\infty_c([0,1])$, we also find $P_1^* = D_x$, and its domain is $D(P_1^*) = H^1([0,1])$. But $D((P_1^*)^*) = H^1_0([0,1]) = \{u \in H^1([0,1]), u(0) = u(1) = 0\}$, the completion of $C^\infty_c([0,1])$ in $H^1(([0,1])$. Hence $D(\bar{P}_1) = H^1_0([0,1])$.

**Definition 6.** $(A, D(A))$ is symmetric if $\forall u, v \in D(A)$, $\langle u, Av \rangle = \langle Au, v \rangle$, equivalently if $A \subset A^*$. In particular, $A$ is then closable. This property is in general easy to check (e.g. by integration b.p.).

A more constraining, but very fundamental notion in spectral theory, is self-adjointness.

$(A, D(A))$ is selfadjoint if $A = A^*$ (also in terms of their domains). It is often not easy to check, due to a strong constraint on domains.

An intermediate notion: $(A, D(A))$ is essentially selfadjoint if $\bar{A} = A^*$. 

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Example 7. Let us re-examine the above example: \( P_1 = D_x \) with \( D(P) = C^\infty_c(\mathbb{R}) \), resp. \( D(P) = C^\infty_c([0,1]) \), are both symmetric. \( P_0^* \) is selfadjoint, and equal to \( \tilde{P}_0 \), showing that \( P_0 \) is essentially selfadjoint. On the opposite, \( P_1^* \) is not symmetric, since its domain is larger than the domain of \( (P_1^*)^* \); this shows that \( P_1 \) is not essentially selfadjoint.

Proposition 8. Two equivalent characterizations of essential selfadjointness, assuming \((A, D(A))\) is symmetric:

i) \( \{(A, D(A))\} \) is closed and \( \ker(A^* + i) = \ker(A^* - i) = \{0\} \)

ii) \( \text{Ran}(A + i), \text{Ran}(A - i) \) are dense in \( \mathcal{H} \) (are equal to \( \mathcal{H} \)).

Why will we be interested in selfadjointness?
— selfadjoint operators form the basis of quantum mechanics
— for \( A \) selfadjoint, we will be able to construct construct operators of the form \( f(A) \), where \( f : \mathbb{R} \rightarrow \mathbb{C} \) measurable function. This construction is called a functional calculus.
— the spectrum of \( A \) is real. The spectral theorem shows that \( A \) is equivalent to a multiplication operator by a real-valued function on some \( L^2(\mu) \) space. This fact will allow to analyze its spectrum in great detail, and write down \( A \) as a projection-valued measure.

1.3 Constructing semibounded selfadjoint operators using quadratic forms

1.3.1 Closed quadratic forms

Let us consider another example of differential operator, namely the (positive) Laplacian \( P = -\Delta \) on \( \Omega \subset \mathbb{R}^d \), where \( \Omega \) is a bounded open domain with smooth boundaries. Let us start with the standard \( D(P) = C^\infty_c(\Omega) \), where \( P \) is obviously symmetric. The maximal extension of \( P \) is on the domain \( D(P_{\text{max}}) = \{ u \in H^2(\Omega) \} \), which is obviously closed. However, \( P_{\text{max}} \) is not symmetric, hence not selfadjoint. All extensions of \( P \) will be contained in \( P_{\text{max}} \). The most famous ones are two selfadjoint operators:

1. the Dirichlet Laplacian \( P_D \) of domain \( D(P_D) = \{ u \in H^2(\Omega) \cap H^1_0(\Omega) \} \).
2. the Neumann Laplacian \( P_N \), of domain \( D(P_N) = \{ u \in H^2(\Omega) \}, \partial_n u|_{\partial \Omega} = 0 \} \), where \( \partial_n u(x) \) is derivative of \( u \) along the vector \( n(x) \) normal to \( \partial \Omega \) at the point \( x \). Note that for \( u \in H^2(\Omega) \), the derivatives of \( u \) are not well-defined everywhere, so the above conditions should be understood in a weak sense: it means that for any \( v \in H^1(\Omega) \), the Dirichlet form \( \int_{\Omega} \nabla v \nabla u = -\int_{\Omega} \bar{v} \Delta u \) (with the absence of boundary term \( \int_{\partial \Omega} \bar{v} \partial_n u \)).

These two extensions \( P_D, P_N \) are both selfadjoint. Is there a “natural way” to obtain these extensions? Notice that neither of the two is an extension of the other one.

YES, using quadratic forms to construct these operators. This is possible due to the fact that \( P \) is a positive operator: for all \( u \in D(P) \), \( \langle u, Pu \rangle \geq 0 \).

Definition 9. A sesquilinear form \( \langle q(u, v) \rangle \), with domain \( D(q) \subset \mathcal{H} \), is bounded if \( |\langle q(u, v) \rangle| \leq C\|u\|\|v\| \) for all \( u, v \in D(q) \). It is then elliptic (or coercive) if \( |\langle q(u, u) \rangle| \geq c\|u\|^2 \) for some \( c > 0 \). It is semibounded below if \( \langle q(u, u) \rangle \geq \alpha\|u\|^2 \) for some \( \alpha \in \mathbb{R} \) (this property implies that it is symmetric).
By Riesz duality, a bounded form $q$ generates a unique bounded operator $A_q$: $q(u, v) = \langle u, A_q v \rangle$. If $q$ is elliptic, $A$ is invertible (implicitly, this means that $A^{-1} : \mathcal{H} \to \mathcal{H}$ extends to a bounded operator).

On the other hand, a form $q$ can be unbounded, and be defined only on a domain $D(q) \subseteq \mathcal{H}$ (as above we assume that $D(q)$ is dense).

**Definition 10.** The form $q$ is said to be **closed** if it is semibounded below, and $D(q)$ is a complete Hilbert space w.r.t. the norm $\|u\|^2_q = q(u, u) + (|\alpha| + 1)\|u\|^2$.

How to associate an operator $A_q$ to such a closed form? Similarly as for the construction of the adjoint, we say that $v \in D(A_q)$ iff the antilinear form $u \mapsto q(u, v)$, initially defined for $u \in D(q)$, extends as a continuous form on $u \in \mathcal{H}$. This form can then be written as $\langle u, w \rangle$ for some state $w \in \mathcal{H}$, and we take $w \overset{\text{def}}{=} A_q v$. Notice that $D(A_q) \subseteq D(q)$.

**Theorem 11.** If $q$ is closed, then the induced operator $A_q : D(A_q) \to \mathcal{H}$ is automatically selfadjoint. The domain $D(A_q)$ is dense in $\mathcal{H}$, and also in $D(q)$ equipped with $\|\cdot\|_q$. $D(q)$ is called the **form domain** of the operator $A_q$.

If $(q, D(q))$ is not closed, it could be closable, meaning that $D(\bar{q})$ is the completion of $D(q)$ for the norm $\|\cdot\|_q$.

**Example 12.** The Dirichlet form on $\mathbb{R}^d$, $q(u, v) = \int_{\mathbb{R}^d} \nabla u \nabla v$, initially defined for $D(q) = C_c^\infty(\mathbb{R})$, can be closed by taking $D(q) = H^1(\mathbb{R}^d)$ (indeed, the norm $\|\cdot\|_q \equiv \|\cdot\|_{H^1}$). The associated operator $A_q = -\Delta$, with $D(A_q) = H^2(\mathbb{R}^d)$.

The construction becomes more interesting on bounded domains.

**Example 13.** The Dirichlet form $q$ on $D(q) = C_c^\infty(\Omega)$ can be closed by taking the completion of $C_c^\infty(\Omega)$ for the form norm $\|\cdot\|_{H^1}$, which gives the domain $D(q) = H^1(\Omega)$. Let us call this form $q_D$. One then obtains as associated operator the Dirichlet Laplacian $P_D$.

On the other hand, if we consider the extension of $q$ to the full space $H^1(\Omega)$, we get another closed form $q_N$, which is an extension of $q_D$. The operator associated with $q_1$ is the Neumann Laplacian $P_N$ on $\Omega$.

### 1.3.2 Symmetric operator → quadratic form → selfadjoint extension

If we start from $A$ symmetric and semibounded below operator, we may induce a quadratic form $q_A(u, v) \overset{\text{def}}{=} \langle u, A v \rangle$, with $D(q_A) \overset{\text{def}}{=} D(A)$. In general $q_A$ is not closed, but it is **closable**, namely it can be extended to a closed form $\bar{q}_A$. The selfadjoint operator $A_F \overset{\text{def}}{=} A_{q_A}$ induced by $\bar{q}_A$ is called the **Friedrich extension** of $A$. One has then the inclusions $D(A) = D(q_A) \subset D(A_F) \subset D(\bar{q}_A)$.

For the example of the two extensions of the Dirichlet forms, we have $D(q_D) \subset D(q_N)$, while this is not true for $D(P_D)$ and $D(P_N)$. Besides, the form domains seem (at least to me) “more natural” than those of the operators.

**Example 14.** The differential operator $P = -\Delta + V$, with $V \geq 0, V \in L^2_{\text{loc}}(\mathbb{R}^d)$, of initial domain $C_c^\infty(\mathbb{R}^d)$, generates the quadratic form $q_P(u, v) = \int \nabla u \nabla v + \int V uv$, which extends to the closed form $\bar{q}_P$ of domain $H^1_0 \overset{\text{def}}{=} \{ u \in H^1(\mathbb{R}^d), u \sqrt{V} \in L^2 \}$. The selfadjoint operator $P_F$ induced from $\bar{q}_P$ is the Schrödinger operator. The condition that $V$ is bounded below can be relaxed modulo some conditions.
2. Spectrum of unbounded operators

2.1 Definition and standard properties of the spectrum

Definition 15. The resolvent set of an operator \( (A, D(A)) \) is the set of points \( z \in \mathbb{C} \) s.t. \( (z - A) : D(A) \to \mathcal{H} \) is bijective, of bounded inverse \( (z - A)^{-1} \).

Remark 16. The existent of a point \( z_0 \in \text{Res}(A) \) implies that \( A \) is closed operator.

\( z_0 \in \text{Res}(A) \iff \ker(z_0 - A) = \{0\} \text{ AND} \text{ Ran}(z_0 - A) = \mathcal{H}. \)

\( \text{Res}(A) \) is an open subset of \( \mathbb{C} \), and the resolvent operator \( (z - A)^{-1} \) depends analytically of \( z \) inside \( \text{Res}(A) \) (analytic operator-valued function).

The \textbf{resolvent identity} allows to control the difference between nearby resolvent operators:

\[ \forall z_0, z_1 \in \text{Res}(A), \quad (z_1 - A)^{-1} - (z_0 - A)^{-1} = (z_0 - z_1)(z_1 - A)^{-1}(z_0 - A)^{-1}. \]

Definition 17. The \textbf{spectrum} of \( A \), \( \text{Spec}(A) \equiv \mathbb{C} \setminus \text{Res}(A) \). It is hence a closed subset of \( \mathbb{C} \). The \textbf{point spectrum} \( \text{Spec}_p(A) = \{z \in \mathbb{C}, z \text{ eigenvalue of } A\} \). The \textbf{discrete spectrum} is the set of isolated eigenvalues of finite (algebraic) multiplicity, that is such that \( \dim \ker(z - A)^n = m_z \) for \( n \) large enough. The \textbf{essential spectrum} \( \text{Spec}_{\text{ess}}(A) = \text{Spec}(A) \setminus \text{Spec}_{\text{dis}}(A) \).

Example 18. Let \( M_f \) be the multiplication operator by \( f \in L^\infty_{\text{loc}}(X, d\mu) \) for some locally finite measure \( \mu \). Then

\[ \text{Spec}(M_f) = \text{ess-ran}_\mu(f) = \{z \in \mathbb{C}, \forall \epsilon > 0, \mu \left( f^{-1}(D(z, \epsilon)) \right) > 0 \}. \]  

Example 19. On \( L^2([0, 1]) \), consider the various realizations of \( P = D_x \). For instance, \( P_0 \) defined on \( D(P_0) = \{u \in H^1, u(0) = 0\} \) has empty spectrum: \( \text{Spec}(P_0) = \emptyset \). On the opposite, its extension \( P_1 \) with \( D(P_1) = H^1([0, 1]) \) satisfies \( \text{Spec}(P_1) = \mathbb{C} \).

Proposition 20. Assume \( (A, D(A)) \) is selfadjoint. Then \( \text{Spec}(A) \) is a \textbf{nonempty subset of} \( \mathbb{R} \). Furthermore, we have the following resolvent estimate:

\[ \forall z \in \mathbb{C} \setminus \mathbb{R}, \quad \|z - A\|^{-1} \leq |\Re z|^{-1}. \]  

\textbf{Proof.} For the estimate we use a form of Pythagoras’s Lemma:

\[ \langle u, (z - A)u \rangle = \Re \|u\|^2 - \langle u, Au \rangle + i\Im \|u\|^2 \]

\[ \implies |\langle u, (z - A)u \rangle|^2 = (\Re \|u\|^2 - \langle u, Au \rangle)^2 + |\Im \|u\|^2|^4 \]

\[ \implies \|u\|\|(z - A)u\| \geq |\langle u, (z - A)u \rangle| \geq |\Im \|u\|^2| \]

\[ \square \]

Proposition 21. (Variational principle, 1)

If \( A \) is bounded and selfadjoint, then \( \text{Spec}(A) \) contains the points

\[ m = \inf_{0 \neq u \in \mathcal{H}} \frac{\langle u, Au \rangle}{\|u\|^2} \text{ and } M = \sup_{0 \neq u \in \mathcal{H}} \frac{\langle u, Au \rangle}{\|u\|^2}. \]  

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2.2 Unbounded operators with discrete spectrum: compact resolvent method

In Quantum Chaos one is often interested in differential operators with discrete spectra. The main example is the (Dirichlet or Neumann) Laplacian $P = -\Delta$ on a bounded open domain $\Omega \subset \mathbb{R}^d$ with smooth enough boundaries. One wants to prove that its spectrum consists in a sequence $\{\lambda_n\}_{n \in \mathbb{N}}^\ast$ of non-negative eigenvalues of finite multiplicities, such that $\lambda_n \to^{\infty} \infty$.

The main trick is to show that its resolvent $(z - P)^{-1}$, for some $z \in \mathbb{C} \setminus \mathbb{R}_+$, is a compact operator.

**Definition 22.** A bounded operator $A$ is compact if it maps the unit ball into a precompact set of $H$. That is, for any sequence $(u_n \in B(0, 1))_{n \in \mathbb{N}}$, one can extract a converging subsequence from $(Au_n)_{n}$.  

**Proposition 23.** A bounded operator $A$ is compact iff

1. it is the norm limit of a sequence of finite rank operators
2. for any weakly convergent (hence bounded) sequence $u_n \rightharpoonup u$, $Au_n \to u$ strongly.
3. for any infinite orthonormal system $(e_n)$, $Ae_n \to 0$.

**Theorem 24.** [Fredholm alternative] If $A$ is a compact operator, for any $z_0 \neq 0$,

1. either $(z_0 - A)^{-1}$ exists and is a bijection $\mathcal{H} \to \mathcal{H},$
2. or $z_0$ is an eigenvalue of finite algebraic multiplicity, meaning that the residue of $z \mapsto (z - A)^{-1}$ at $z_0$ has finite rank.

**Corollary 25.** If $A$ is compact, $\text{Spec}(A) = \text{Spec}_{\text{dis}}(A) \cup \{0\}$, with the discrete spectrum being composed of finitely or countably many eigenvalues of finite multiplicities, accumulating only at $z = 0$.

In the case $A$ is also selfadjoint, we have more informations:

**Theorem 26.** If $A$ is compact and selfadjoint, then it admits an orthonormal eigenbasis $(u_n, \lambda_n)$ with $\lambda_n \to 0$.

This generalizes to compact normal operators (that is, s.t. $[A, A^*] = 0$): they admit an o.n. eigenbasis $(u_n, z_n)$ with $z_n \to 0$.

We will use this property to identify unbounded operators $A$ with discrete spectra:

**Proposition 27.** If for some $z_0 \in \text{Res}(A)$, the resolvent $(z_0 - A)^{-1}$ is a compact operator, then $A$ has a purely discrete spectrum $(z_n)_{n \geq 1}$, with $|z_n| \to \infty$.

**Proof.** Let us give the proof in the case $A$ is selfadjoint. Call $(\mu_n, u_n)$ the spectrum of $(z_0 - A)^{-1}$. A resolvent operator has a trivial kernel, hence all $\mu_n \neq 0$. We have the identities

$$(z_0 - A)^{-1}u_n = \mu_n u \iff (1 - \mu_n z_0)u_n = -\mu_n Au.$$ 

$$\mu_n z_0 - 1 \mu_n^{-1} u_n = Au_n,$$

so the spectrum of $A$ is made of eigenvalues $\lambda_n = \frac{\mu_n z_0 - 1}{\mu_n}$ of finite multiplicities. We know that $\lambda_n \in \mathbb{R}$, and $(u_n)$ forms an orthonormal basis. □
Let us consider the special case where \( A \) is a semibounded selfadjoint operator, associated with a quadratic form \( q \). Up to an additive constant, we may assume that \( q \geq 1 \), so that \( \| u \|_q = q(u, u)^{1/2} \) defines the Hilbert norm on \( D(q) \). Then \( A^{-1} : \mathcal{H} \to D(q) \) is a bounded operator, with \( \text{Ran}(A) = D(A) \subset D(q) \).

**Corollary 28.** Assume \( A = A_q \) for a closed form \( q \geq 1 \). If the injection \( D(q) \hookrightarrow \mathcal{H} \) is compact, then \( A^{-1} : \mathcal{H} \to \mathcal{H} \) is compact, hence \( A \) has discrete positive spectrum.

**Example 29.** Let us consider the Dirichlet/Neumann Laplacian \( A = P_{D/N} + 1 \) on a bounded domain \( \Omega \subset \mathbb{R}^d \). In that case \( D(q) = H^1_0(\Omega) \), resp. \( H^1(\Omega) \). So proving the compactness of \( A^{-1} = (P + 1)^{-1} \) amounts to proving that the injection \( H^1_0(\Omega) \hookrightarrow L^2(\Omega) \) is compact. For this fact we may use the Riesz-Fréchet-Kolmogorov criterion of compactness in \( L^p(\Omega) \).

**Theorem 30.** [Riesz-Fréchet-Kolmogorov-Tamarkin] For \( \Omega \subset \mathbb{R}^d \) open, a subset \( \mathcal{F} \subset L^p(\Omega) \) is compact iff

1) the elements of \( \mathcal{S} \) are uniformly bounded: \( \forall u \in \mathcal{S}, \| u \|_{L^p} \leq C \)

2) the elements of \( \mathcal{F} \) are essentially supported in a bounded part of \( \Omega \): \( \lim_{r \to \infty} \| u \|_{L^p(\Omega)} = 0 \) uniformly for \( u \in \mathcal{F} \).

3) the elements of \( \mathcal{F} \) do not oscillate too much: for any \( \omega \Subset \Omega \), \( \lim_{h \to 0} \| \nabla u - u \|_{L^p(\omega)} = 0 \) uniformly for \( u \in \mathcal{F} \).

**Example 31.** One easily checks that \( H^1_0(\Omega) \) satisfies this criterion if \( \Omega \) is bounded (only the last statement needs some computations).

We may replace the boundedness of \( \Omega \) by a confining potential:

**Example 32.** Let us consider the Schrödinger operator \( P = -\Delta + V \) such that the potential \( V \in L^2_{\text{loc}}(\mathbb{R}^d) \) is bounded below (say by \( V \geq 1 \)) and is confining \( (V(x) \to \infty \text{ as } |x| \to \infty) \). Then it is easy to show that its form domain \( D(q_V) = \left\{ u \in H^1(\mathbb{R}^d), u\sqrt{V} \in L^2 \right\} \) also satisfies the RFKT criterion.

# 3 Spectral Theorem of selfadjoint operators and functional calculus

Aim of this section: prove that a general selfadjoint op. \( A : \mathcal{H} \to \mathcal{H} \) is unitarily equivalent with a multiplication operator (by the identity function \( f(\lambda) = \lambda \)) on a space of the form \( \bigoplus_{n=1}^N L^2(\mathbb{R}, \mu_n) \), where each \( \mu_n \) is a finite measure on \( \mathbb{R} \). Here the number of copies \( N \) may be finite or countable.

Once this will be done, many properties of self-adjoint ops can be inferred directly from those of multiplication operators. For instance, we will be able to construct a functional calculus \( f \mapsto f(A) \) for bounded measurable functions \( f \) on \( \mathbb{R} \), in particular \( f = 1_{\Omega} \) for \( \Omega \subset \mathbb{R} \) any Borel set: this provides the construction of spectral projectors \( \Pi_\Omega = 1_{\Omega}(A) \), as well as their properties.
3.1 Construction of the unitary equivalence

The strategy of this construction goes as follows:

1. We start by constructing a functional calculus for smooth functions \( f \in C_c^\infty(\mathbb{R}) \). For unbounded operators \( A \), this can be done by using a Cauchy formula and an almost analytic extension \( \tilde{f} \in C_c^\infty(\mathbb{C}) \) of \( f \). The Stokes formula implies that, for any \( g \in C_c^\infty(\mathbb{C}) \), one has

\[
\forall w \in \mathbb{C}, \quad g(w) = \frac{1}{\pi} \int_{\mathbb{C}} \frac{1}{w - z} \partial_z g(z) \, dz.
\]

We want to express \( f(A) \), for some function \( f \in C_c^\infty(\mathbb{R}) \). For this aim, let us extend \( f \) to a function \( \tilde{f} \in C_c^\infty(\mathbb{C}) \), and consider the integral

\[
f(A) \overset{\text{def}}{=} \frac{1}{\pi} \int_{\mathbb{C}} (A - z)^{-1} \partial_z \tilde{f}(z) \, dz.
\]  

The resolvent \( (A - z)^{-1} \) explodes when \( z \to \text{Spec}(A) \subset \mathbb{R} \), so to make the integral convergent we need \( \partial_z \tilde{f}(z) \) to go to zero fast enough as \( \Im z \to 0 \). This is the case if we choose the extension \( \tilde{f} \) of \( f \) to be almost analytic (up to order \( n \geq 3 \)) namely to satisfy

\[
\partial_z \tilde{f}(z) = O((\Im z)^n) \quad \text{as } \Im z \to 0.
\]

This can be done, for instance, by taking

\[
\tilde{f}(x + iy) \overset{\text{def}}{=} \sum_{j=0}^{n} f^{(j)}(x) \frac{(iy)^j}{j!} \chi(x + iy),
\]

with \( \chi \in C_c^\infty(\mathbb{C}) \) equal to unity near \( \text{supp} f \). The integral (4) then converges to a bounded operator, which we call \( f(A) \), since it can be shown to be independent of the choice of almost analytic extension \( \tilde{f} \). One can show that the map \( f \in C_c^\infty(\mathbb{R}) \mapsto f(A) \) is a \(*\)-algebra homomorphism, with

\[
\|f(A)\| \leq \|f\|_{L^\infty}.
\]  

Besides, for any \( w \in \mathbb{C} \setminus \mathbb{R} \), the function \( f_w(z) \overset{\text{def}}{=} (z - w)^{-1} \) indeed leads to the resolvent \( (A - w)^{-1} \), showing the consistency of the construction.

2. The closure of \( C_c^\infty(\mathbb{R}) \) for the norm \( \|\cdot\|_{L^\infty} \) is the space \( C^0_0(\mathbb{R}) \) of continuous functions vanishing at infinity. Hence, using the bound (5) one easily extends this functional calculus to functions \( f \in C^0_0(\mathbb{R}) \).

3. We cleverly choose a normalized state \( \psi_1 \in \mathcal{H} \), and the \(*\)-homomorphism of the “quantization” \( f \mapsto f(A) \) induces the existence of define the spectral measure \( \mu_{\psi_1} \), such that

\[
\forall f, g \in C^0_0(\mathbb{R}), \quad \langle f(A)\psi_1, g(A)\psi_1 \rangle_{\mathcal{H}} = \int \tilde{f} g \, d\mu_{\psi_1} = \langle f, g \rangle_{L^2(\mathbb{R}, \mu_{\psi_1})}.
\]

\( \mu_{\psi_1} \) is a probability measure on \( \mathbb{R} \). This equality provides an isometry between \( C^0_0(\mathbb{R}) \subset L^2(\mu_{\psi_1}) \), and the subspace span \( \{f(A)\psi_1, f \in C^0_0(\mathbb{R})\} \) of \( \mathcal{H} \). Taking the Hilbert space closures on the two sides, produces a unitary equivalence \( U_1 \) between the closed subspace \( \mathcal{H}_1 \overset{\text{def}}{=} \overline{\text{span} \{f(A)\psi_1, f \in C^0_0(\mathbb{R})\}} \) and \( L^2(\mathbb{R}, \mu_{\psi_1}) \):

\[
U_1 f(A)\psi_1 = f \in L^2(\mathbb{R}, \mu_{\psi_1}).
\]
4. If we are lucky (namely, if the state $\psi_1$ is cyclic), one has $\mathcal{H}_1 = \mathcal{H}$, and we have constructed a unitary equivalence $\mathcal{U}_1 \mathcal{H} = L^2(\mathbb{R}, \mu_{\psi_1})$. For instance, if $\text{Spec}(A)$ is composed of simple eigenvalues $(\lambda_n, u_n)$, then any state of the form $\psi_1 = \sum_n c_n u_n$, with all $c_n \neq 0$, is cyclic. On the opposite, if some eigenvalues are multiple, there is no cyclic vector.

5. If $\mathcal{H}_1 \subsetneq \mathcal{H}$, we start again with a state $\psi_2 \in \mathcal{H}_1^\perp$, construct its spectral measure $\mu_{\psi_2}$, the closed subspace $\mathcal{H}_2 \perp \mathcal{H}_1$ spanned by $\{f(A)\psi_2\}$, and obtain a unitary equivalence $\mathcal{U}_2 \mathcal{H}_2 = L^2(\mathbb{R}, \mu_{\psi_2})$. After at most countably many steps, we obtain the full space $\mathcal{H} = \bigoplus_{n=1}^{\infty} \mathcal{H}_n$, mapped unitarily through $\mathcal{U} = \bigoplus_{n=1}^{\infty} \mathcal{U}_n$ onto the space $\bigoplus_{n=1}^{\infty} L^2(\mathbb{R}, \mu_n)$ def \( L^2(\mathbb{R}^N, \mu_\psi) \). The latter is composed of $N$-vectors $\varphi = (\varphi_1, \ldots, \varphi_N)$, where each $\varphi_n \in L^2(\mathbb{R}, \mu_n)$. We can renormalize the $\psi_n$, so that the full measure $\mu_\psi = \sum_n \mu_{\psi_n}$ on $\mathbb{n}R$ is normalized.

6. Any bounded Borel function $f \in B_\infty(\mathbb{R})$ acts on $L^2(\mathbb{R}, \mu)$ by simultaneous multiplication on all the copies of $\mathbb{R}$:

$$ \varphi = (\varphi_1, \ldots, \varphi_N) \in L^2(\mathbb{R}^N, \mu) \mapsto M_f \varphi = (f\varphi_1, \ldots, f\varphi_N), $$

forming a bounded operator on $L^2(\mathbb{R}^N, \mu_\psi)$. The unitary conjugate of this operator defines the quantization $f(A)$ on $\mathcal{H}$: $f(A) = U^{-1} M_f U$. If $f \in B_\infty(\mathbb{R})$ is approached pointwise by functions $f_j \in C^0_0(\mathbb{R})$, then the operators $f_j(A)$ defined above, converge strongly to $f(A)$.

7. We may relax the boundedness condition. If $f$ is a locally bounded Borel function, then the operator $M_f$ is well-defined on the domain $D(M_f) = \{ \varphi \in L^2(\mathbb{R}, \mu_\psi), \ f\varphi \in L^2(\mathbb{R}, \mu_\psi) \}$. The conjugation by $\mathcal{U}$ then maps $M_f$ to an operator $f(A)$ acting on $D(f(A)) = \mathcal{U}^{-1} D(M_f)$.

8. For example, the multiplication by the identity function $f(\lambda) = \lambda$, well-defined on the domain $D(M_\lambda) = \{ \varphi \in L^2(\mathbb{R}, \mu_\psi), \ \lambda \varphi \in L^2(\mathbb{R}, \mu_\psi) \}$, is exactly conjugate with the action of $A$ on $D(A) \subset \mathcal{H}$.

9. If a family of functions $f_n \in B_\infty(\mathbb{R})$ uniformly bounded, converge pointwise to $f$, then $f_n(A)$ converge to $f(A)$ in the strong operator topology: $\forall u \in \mathcal{H}, f_n(A) u \to f(A) u$.

This achieves the construction of the functional calculus for locally bounded Borel functions, together with the spectral theorem relating $(A, D(A))$ with $(M_\lambda, D(M_\lambda))$.

4 Consequences of the Spectral theorem

Remark 33. The construction of the conjugacy to $L^2(\mathbb{R}, \mu_\psi)$ is not unique (since it depends on the choice of the $\psi_n$), and is not very explicit. In general the measures $\mu_{\psi_n}$ cannot be computed explicitly, even the number $N$ of copies of $\mathbb{R}$ is not easy to compute. In the case of a discrete spectrum, $N$ is at least equal to the maximum of all multiplicities.

For some operators, an “obvious” unitary transformation leads to represent $A$ as a multiplication operator. This is the case of translation-invariant differential operators on $\mathbb{R}^d$, which are conjugate, through the Fourier transform, to multiplication operators on $L^2(\mathbb{R}, |d\xi|)$:

$$ F^{-1} \sum_{\alpha} a_\alpha D^\alpha \xi F = M_{\sum_n a_n \xi^n}. $$
Even if the construction of $\mu$ is “noncanonical”, the unitary conjugacy allows us to deduce properties of the operator $A$ directly from properties of the multiplication operator $\tilde{M}_\lambda$ on $L^2(\mathbb{R}, \mu)$. For instance, the spectrum of multiplication operators, described in (1), leads to:

**Proposition 34.** $\text{Spec}(A) = \bigcup_n \text{supp} \mu_n$.

More generally, for $f$ locally bounded Borel function on $\mathbb{R}$, $\text{Spec}(f(A)) = \bigcup_n \text{ess-ran} \mu_n(f)$.

Another application is on norm estimates of bounded operators obtained as functions of $A$:

**Proposition 35.** For $f$ bounded, $\|f(A)\| = \text{ess-sup}_\mu |f(\lambda)|$.

In particular we get the resolvent estimate

$$\|(A - z)^{-1}\| = \text{dist}(z, \text{Spec}(A))^{-1},$$

which improves (2).

### 4.1 Decomposition of the spectral measure into pp, ac and sc parts

Let us assume that $\psi_0$ is cyclic, call $\mu_{\psi_0} = \mu$, such that $\mathcal{H}$ is conjugated with $L^2(\mathbb{R}, d\mu)$. $\mu$ is a Borel probability measure on $\mathbb{R}$, so it can be split into 3 mutually singular components:

1. a pure point component $\mu_{pp} = \sum_i c_i \delta_{\lambda_i}$
2. an absolutely continuous component $\mu_{ac} = \rho(\lambda) d\lambda$, with density $\rho \in L^1(\mathbb{R}, d\lambda)$
3. a singular continuous component $\mu_{sc}$ (which pops up only for very special differential operators).

To the decomposition $\mu = \mu_{pp} + \mu_{ac} + \mu_{sc}$ corresponds the splitting

$$L^2(\mathbb{R}, \mu) = L^2(\mathbb{R}, \mu_{pp}) \oplus L^2(\mathbb{R}, \mu_{ac}) \oplus L^2(\mathbb{R}, \mu_{sc}).$$

A state $\varphi \in L^2(\mathbb{R}, \mu)$ belongs to a single subspace $L^2(\mathbb{R}, \mu_\ast)$ iff the measure $\mu_\varphi$ it generates is of type $\ast$, due to the relation $\int f d\mu_\varphi = \int |f|^2 d\mu$.

We may bring back the decomposition (6) to $\mathcal{H}$ through $U^{-1}$: $\mathcal{H}_\ast = U^{-1}L^2(\mathbb{R}, \mu_\ast)$. We have $\psi \in \mathcal{H}_\ast$ iff $\mu_\psi$ is of type $\ast$.

These 3 subspaces $\mathcal{H}_\ast$ are closed and invariant through $A$, so it makes sense to consider $A|_{\mathcal{H}_\ast}$. We had defined $\text{Spec}_{pp}(A) = \{\lambda \text{ eigenvalue of } A\}$, which is not necessarily a closed set. In general we have $\text{Spec}(A|_{\mathcal{H}_{pp}}) = \overline{\text{Spec}_{pp}(A)}$. We $\text{Spec}_{ac}(A) \overset{\text{def}}{=} \text{Spec}(A|_{\mathcal{H}_{ac}}) = \text{supp} \mu_{ac}$, and similarly for $\text{Spec}_{sc}(A)$.

We finally have $\text{Spec}(A) = \overline{\text{Spec}_{pp}(A)} \cup \text{Spec}_{ac}(A) \cup \text{Spec}_{sc}(A)$, with possible overlaps between the 3 parts.

### 4.2 Spectral projectors

One reason to construct a functional calculus applicable to Borel functions is to be able to deal with characteristic functions $1_\Omega$ associated with Borel sets $\Omega \subset \mathbb{R}$. The quantization of these functions provide the spectral projectors of $A$: 
Definition 36. Let $A$ be self-adjoint. For any Borel set $\Omega \subset \mathbb{R}$, the operator

$$E_\Omega = E_\Omega(A) \overset{\text{def}}{=} \mathbb{1}_\Omega(A)$$

is called the spectral projector of $A$ on $\Omega$.

Proposition 37. The family $(E_\Omega)_{\Omega}$ satisfies the following properties:

1) for any Borel set $\Omega$, $E_\Omega$ is an orthogonal projector (which commutes with $A$).
2) $E_{\Omega_1 \cap \Omega_2} = E_{\Omega_1} \cap E_{\Omega_2}$.
3) $E_{\emptyset} = 0$, while $E_{\mathbb{R}} = \text{Id}$.

The properties 1, 5, 6, 7 imply that the family $(E_\Omega)_{\Omega}$ forms a **projection-valued measure** (PVM). This means that for any $\psi \in \mathcal{H}$, the function $\Omega \mapsto \langle \psi, E_\Omega \psi \rangle \overset{\text{def}}{=} \mu_\psi(\Omega)$ defines a probability measure on $\mathbb{R}$ (which is the spectral measure generated by $\psi$).

This PVM allows to represent the operators $f(A)$ as an integral:

$$f(A) = \int_{\mathbb{R}} f(\lambda) \, dE_\lambda.$$

This operator admits for domain $D(f(A)) = \{ \varphi \in \mathcal{H}, \int |f(\lambda)|^2 d\langle \varphi, E_\lambda \varphi \rangle < \infty \}$. This exactly corresponds with the domain of $f(A)$ characterized through the conjugacy with multiplication operators.

Theorem 38. There is a 1-to-1 correspondence between selfadjoint operators $A$ and PVM $(E_\Omega)_{\Omega}$.

The functional calculus on bounded Borel functions shows that certain spectral projectors can be obtained directly from the resolvent operators:

$$E((\lambda_0)) = -i \lim_{\varepsilon \searrow 0} \frac{\varepsilon}{(A - \lambda_0 - i\varepsilon)}$$

$$\frac{1}{2} \left( E_{[a,b]} + E_{(a,b)} \right) = \frac{1}{\pi} \lim_{\varepsilon \searrow 0} \int_a^b \Im(A - \lambda - i\varepsilon)^{-1} d\lambda \quad \text{(Stones’s formula)}$$

(in both cases, the limit is to be understood in the strong operator topology).

If a closed curve $\gamma$ circles once around an interval $(a,b)$ such that $\gamma \cap \text{Spec}(A) = \emptyset$, we have Cauchy’s formula

$$E_{(a,b)} = \frac{1}{2\pi i} \oint_{\gamma} (z - A)^{-1} dz.$$

Proposition 39. We may characterize the various spectra of $A$ in terms of these projectors:

1) $\lambda \in \text{Spec}(A) \iff \forall \varepsilon > 0$, dim $\text{Ran} \, E_{(\lambda - \varepsilon, \lambda + \varepsilon)} > 0$
2) $\lambda \in \text{Spec}_p(A) \iff E_{(\lambda)} \neq 0$ (since $\text{Ran} \, E_{(\lambda)} = \ker(A - \lambda)$)
3) $\lambda \in \text{Spec}_{\text{dis}}(A) \iff \lambda \in \text{Spec}(A)$ and $\exists \varepsilon > 0$, dim $\text{Ran} \, E_{(\lambda - \varepsilon, \lambda + \varepsilon)} < \infty$
4) $\lambda \in \text{Spec}_{\text{ess}}(A) \iff \forall \varepsilon$, dim $\text{Ran} \, E_{(\lambda - \varepsilon, \lambda + \varepsilon)} = \infty$
4.3 Construction of the Schrödinger propagator

The propagator of the (non-semiclassical) Schrödinger equation is formally written \( U(t) = e^{-it\hat{A}} \), where \( \hat{A} \) is the quantum Hamiltonian, which is usually an unbounded selfadjoint operator. Since the function \( e_t : \lambda \mapsto e^{-it\lambda} \) is Borel and bounded, we can apply the functional calculus to construct \( U(t) = e_t(A) \). Direct applications of the spectral theorem show that

1) \( U(t) \) is unitary, and forms a 1-parameter abelian group

2) \( s - \lim t \to 0 U(t) = \text{Id} \), showing that this group is strongly continuous.

3) \( u \in D(A) \iff \lim t \to 0 \frac{U(t) - \text{Id}}{t} = -iAu \), showing that \( A \) is the infinitesimal generator of this group.

4.4 Perturbation theory: stability of the essential spectrum

4.4.1 Weyl criterion for the essential spectrum

The spectrum of \( A \) can be characterized by the existence of arbitrarily precise quasimodes:

\[ \lambda \in \text{Spec}(A) \text{ iff there exists a family } (u_n)_{n \geq 1} \text{ of normalized states, such that } \| (A - \lambda) u_n \| \to 0. \]

When \( A \) is selfadjoint, the essential spectrum can be characterized by adding one condition on the family \( (u_n) : \lambda \in \text{Spec}_{ess}(A) \text{ iff the quasimodes } u_n \text{ can be chosen such that they weakly converge to zero: } u_n \rightharpoonup 0 \). In some sense, this means that the space generated by these quasimodes has infinite dimension.

Another equivalent condition for \( \lambda \) to be in the essential spectrum is that the \( (u_n) \) can be chosen to form an orthonormal sequence.

The states \( (u_n) \) are called quasimodes of \( A \), of quasi-eigenvalue \( \lambda \). A sequence \( (u_n) \) with \( u_n \rightharpoonup 0 \) is called a Weyl singular sequence.

In some situations, e.g. when \( A = P \) is a differential operator on \( L^2(X) \), these quasimodes can be constructed by truncating or smoothing a well-identified generalized eigenstate \( u_\lambda \notin L^2 \) which satisfies \( (P - \lambda)u_\lambda = 0 \) in the sense of distributions.

Example 40. Take \( P = -\Delta \) on \( L^2(\mathbb{R}^d, dx) \). For any \( \xi \in \mathbb{R}^d \), the plane wave \( u_\xi(x) = e^{i\xi \cdot x} \) satisfies the equation \( (P - |\xi|^2)u_\xi = 0 \), but obviously \( u_\xi \notin L^2(\mathbb{R}^2) \). Choose some cutoff function \( \chi \in C_c^\infty(\mathbb{R}^d, [0, 1]) \) such that \( \| \chi \|_{L^2} = 1 \), dilate it by \( n \in \mathbb{N}^* \) to \( \chi_n(x) = n^{-d/2}\chi(\frac{x}{n}) \), and use \( \chi_n \) to form the truncated (and normalized) functions \( u_n \overset{\text{def}}{=} \chi_n(x) u_\xi \). A simple computation shows that \( \| (P - |\xi|^2)u_n \|_{L^2} \leq C/n \), and one can also check that \( u_n \rightharpoonup 0 \) (this is the already case for the functions \( \chi_n \)). Hence \( (u_n) \) forms a singular Weyl sequence, showing that \( \lambda = |\xi|^2 \) lies in the essential spectrum of \( P \).

Singular sequences can be easily constructed in the case of multiplication operators by continuous functions.

Example 41. Take \( f \in C^0(\mathbb{R}^d) \), possibly unbounded, and consider \( \lambda \in \text{Ran}(f) \). Assume \( x_0 \in \mathbb{R}^d \) is such that \( f(x_0) = \lambda \). The delta distribution \( \delta_{x_0} \) satisfies \( M_f \delta_{x_0} = \lambda \delta_{x_0} \) in the sense of distributions. Fix as above \( \chi \in C^0(\mathbb{R}^d, [0, 1]) \) such that \( \| \chi \|_{L^2} = 1 \), and consider the
rescaled functions $\chi_{1/n}(x) = n^{d/2} \chi(nx)$. The squares of these functions weakly converge to $\delta_0$, so we shift them to take the normalized functions $u_n(x) \overset{\text{def}}{=} \chi_{1/n}(x-x_0)$. Due to the continuity of $f$ at the point $x_0$, one easily checks that $\| (M_f - \lambda) u_n \| \to 0$ as $n \to \infty$. Besides, the functions $u_n \to 0$.

4.4.2 Stability of the essential spectrum

The essential spectrum looks “more fuzzy” than the point spectrum, since it does not necessarily correspond to true eigenfunctions, but rather generalized eigenfunctions or quasi-modes. However, because it is associated with spectral projectors of infinite rank (see Prop.(39)), the essential spectrum enjoys an interesting stability property with respect to (mild enough) perturbations of the operator.

**Theorem 42.** Assume $A, B$ are self-adjoint, and that there exists $z \in \text{Res}(A) \cap \text{Res}(B)$ such that $K(z) \overset{\text{def}}{=} (A-z)^{-1} - (B-z)^{-1} : \mathcal{H} \to \mathcal{H}$ is a compact operator. Then $\text{Spec}_{\text{ess}}(A) = \text{Spec}_{\text{ess}}(B)$.

**Proof.** The idea is to start from a Weyl singular basis $(u_n)$ associated with $\lambda \in \text{Spec}_{\text{ess}}(A)$, and construct from it, using the resolvent identity, a Weyl sequence $(v_n)$ for $B$ and the same value $\lambda$. \hfill $\square$

One application of this result consists in perturbing an operator $A$ with an $A$-compact perturbation.

**Definition 43.** Assume $A$ is selfadjoint, $B$ is closable, $D(A) \subset D(B)$. $B$ is said to be $A$-compact iff there exists $z \in \text{Res}(A)$ s.t. $B(A-z)^{-1}$ is compact.

**Corollary 44.** Assume $A$ is selfadjoint, $B$ is symmetric and $A$-compact. Then $(A + B, D(A))$ is self-adjoint, and $\text{Spec}_{\text{ess}}(A+B) = \text{Spec}_{\text{ess}}(A)$.

**Example 45.** This corollary is very important in scattering theory. Let us start from the operator $P_0 = -\Delta$ on $L^2(\mathbb{R}^3)$, with $\text{Spec}_{\text{ess}}(P_0) = \mathbb{R}_+$. As explained in A.Hassell’s lectures on scattering theory, we may perturb it with a potential $V \in C^\infty_c(\mathbb{R}^3)$; it is easy to show that the multiplication operator $M_V$ is not only bounded, but also $P_0$-compact, hence $\text{Spec}_{\text{ess}}(-\Delta + V) = \mathbb{R}_+$. This property extends to more general potentials, for instance to potentials in the so-called Kato class: potentials such that, for any $\epsilon > 0$, $V$ can be decomposed as $V = V_{1,\epsilon} + V_{2,\epsilon}$ with $\|V_{1,\epsilon}\|_{L^\infty} \leq \epsilon$ and $V_{1,\epsilon} \in L^2$. Such potentials are also $\Delta$-compact, hence satisfy $\text{Spec}_{\text{ess}}(-\Delta + V) = \mathbb{R}_+$. The Kato class contains potentials with singularities. One famous example is the Coulomb potential $V(x) = \alpha|x|^{-1}$ (for some constant $\alpha \in \mathbb{R} \setminus 0$). In the case $\alpha < 0$, it gives the Hamiltonian of the Hydrogen atom, with essential spectrum corresponding to the ionization of the atom (the electron escaping to infinity).

4.5 Variational methods for semibounded selfadjoint operators

We have already seen in (3) that the self-adjointness of a bounded operator allows to obtain the extrema of its spectrum from a variational formula, namely by minimizing or maximizing the Rayleigh quotient $\frac{\langle u, Au \rangle}{\|u\|^2}$ over all $u \in \mathcal{H}$. If $A$ is selfadjoint, the bottom of $\text{Spec}(A)$ can be obtained by a similar formula:
**Proposition 46.** Assume $A$ is selfadjoint. Then

$$\inf \text{Spec}(A) = \inf_{0 \neq v \in D(A)} \frac{\langle v, Av \rangle}{\|v\|^2}.$$  

Noticing that $\langle v, Av \rangle = q_A(v,v)$ for all $v \in D(A)$, we can extend the Rayleigh quotient to all $v \in D(q_A)$, replacing it by $\frac{q_A(v,v)}{\|v\|^2}$. Hence, the bottom of $\text{Spec}(A)$ is also given by

$$\inf \text{Spec}(A) = \inf_{0 \neq v \in D(q_A)} \frac{q_A(v,v)}{\|v\|^2}. \quad (7)$$

These formulae are interesting in the case where $A$ is bounded below, which we will assume from now on. In situations where the bottom of the spectrum is made of eigenvalues of finite multiplicities, this variational expression gives the lowest eigenvalue $\lambda_1$. How about the next eigenvalues?

**Notation 47.** Let us order the eigenvalues counting multiplicities: if $\lambda_1 < \lambda_2 < \lambda_3 < \cdots$ denote the distinct eigenvalues of $A$, of finite multiplicities $m_1, m_2, \ldots$, let us call $\mu_1 = \cdots = \mu_{m_1} = \lambda_1$, $\mu_{m_1+1} = \cdots = \mu_{m_1+m_2} = \lambda_2$ etc. If there are only $N$ discrete eigenvalues (counted with multiplicities) below the essential spectrum, then call $\mu_{N+1} = \mu_{N+2} = \cdots = \inf \text{Spec}_{\text{ess}}(A)$.

**Theorem 48.** [Max-Min principle] Assume $A$ is selfadjoint and bounded below. The values $(\mu_n)$ admit the following variation expressions:

$$\forall n \geq 1, \quad \mu_n = \sup_{(u_1, \ldots, u_{n-1})} \left\{ \inf_{u \in D(A)} \frac{\langle v, Av \rangle}{\|v\|^2}, \; u \perp \text{Span}(u_1, \ldots, u_{n-1}) \right\}$$

$$= \sup_{\mathcal{H}_{n-1}} \inf_{u \in D(A)} \left\{ \frac{\langle v, Av \rangle}{\|v\|^2}, \; u \perp \mathcal{H}_{n-1} \right\}, \quad (8)$$

where $\mathcal{H}_{n-1}$ is any subspace of $\mathcal{H}$ of dimension $n-1$.

In the above expressions we may replace $\langle v, Av \rangle$ by $q_A(v,v)$, respectively $u \in D(A)$ by $u \in D(q_A)$, as in (7).

The values $\mu_n$ could be called the **variational eigenvalues** of $A$, remembering that the upper ones may not be true eigenvalues.

**Proof.** The proof consists in computing the ranks of spectral projectors $E(a) = E_{[-\infty,a]}$ depending on $a$. If we call $\tilde{\mu}_n$ the RHS in (8), then one shows that if $a < \tilde{\mu}_n$, then rank $E(a) < n$, while if $a > \tilde{\mu}_n$, then rank $E(a) \geq n$. If rank $E(\tilde{\mu}_n + \epsilon) = \infty$ for any $\epsilon > 0$, then $\mu_n \in \text{Spec}_{\text{ess}}(A)$; on the other hand rank $E(\tilde{\mu}_n - \epsilon) < \infty$, so $\tilde{\mu}_n$ must be the bottom of $\text{Spec}_{\text{ess}}(A)$. Otherwise, since the function $a \mapsto \text{rank} E(a)$ is increasing and takes values in $\mathbb{N} \cup \{\infty\}$, we deduce that $\tilde{\mu}_n$ is an eigenvalue, or is the bottom of $\text{Spec}_{\text{ess}}(A)$. \(\square\)

The Max-Min principle admits a very nice corollary, convenient in particular in numerical spectral analysis where operators are truncated on finite dimensional subspaces.

**Corollary 49.** [Rayleigh-Ritz method] Let $A$ be selfadjoint and bounded below. Consider $\mathcal{V} = \mathcal{V}_n \subset D(A)$ a subspace of dimension $n$, $\Pi_\mathcal{V}$ the orthogonal projector on $\mathcal{V}$, and call $A_\mathcal{V} \overset{\text{def}}{=} \Pi_\mathcal{V} A \Pi_\mathcal{V}$ the projection of $A$ on the subspace $\mathcal{V}$. The spectrum of the finite rank selfadjoint operator $A_\mathcal{V}$ is made of $n$ ordered eigenvalues $\tilde{\mu}_1 \leq \cdots \leq \tilde{\mu}_n$.

These eigenvalues can then be compared with the variational eigenvalues of $A$:

$$\forall 1 \leq j \leq n, \quad \mu_j(A) \leq \tilde{\mu}_j(A).$$
There is a dual variational principle, called the Min-Max principle, which may look more natural.

**Theorem 50. [Min-Max principle]** With the same definitions as above,

\[ \mu_n = \inf_{L_n \subset D(A)} \sup_{v \in L_n} \frac{\langle v, Av \rangle}{\|v\|^2}, \]

where \( L_n \) is any subspace of \( D(A) \) of dimension \( n \). We can also take \( L_n \) subspaces of \( D(q_A) \), replacing \( \langle v, Av \rangle \) by \( q_A(v, v) \).

The proof of this Min-Max principle is similar to the preceding one. This min-max principle allows to compare precisely the spectra of two ordered operators.

**Corollary 51.** Assume \( A, B \) are selfadjoint, bounded below, with \( D(A) \supset D(B) \) (resp. \( D(q_A) \supset D(q_B) \)) and \( A \leq B \) (resp. \( q_A \leq q_B \)). Then the variational eigenvalues of \( A \) and \( B \) satisfy the following inequalities:

\[ \forall n \geq 1, \quad \mu_n(A) \leq \mu_n(B). \]

These variational expressions are very useful in practice, for instance in applications to atomic or condensed matter physics, where one is mostly interested in the bottom of the spectrum of the Hamiltonian operator.

For any trial state \( v \in D(q_A) \), the Rayleigh quotient \( \frac{q_A(v, v)}{\|v\|^2} \) provides an upper bound for the bottom of the spectrum \( \mu_1 \). Part of condensed matter physics consists making a “good guess” for the state \( v \), such that the Rayleigh quotient is a good approximation of \( \mu_1 \).

In case we know the bottom of \( \text{Spec}_{\text{ess}}(A) \), for instance using the stability property explained in section 4.4.2, then finding a state \( v \) such that \( \frac{\langle v, Av \rangle}{\|v\|^2} < \inf \text{Spec}_{\text{ess}} \) ensures the existence of discrete eigenvalues (“bound states”) at the bottom of the spectrum.

**Example 52.** This can be the case, for instance, if the scattering potential \( V \) belongs to the Kato class (see Ex. 45) and is sufficiently negative. In dimensions \( d = 1, 2 \), being in the Kato class and assuming the condition \( \int V(x)dx < 0 \) suffices to ensure that \( \mu_1(-\Delta + V) < 0 \). On the other hand, in dimension \( d \geq 3 \), for any \( V \in L^\infty_{\text{comp}}(\mathbb{R}^d) \), there exists a coupling \( g_0 \) such that for any small enough coupling \( |g| \leq g_0 \), \( \text{Spec}(-\Delta + gV) = \text{Spec}_{\text{ess}}(-\Delta + gV) = \mathbb{R}_+ \), and there is no discrete eigenvalue, even if the potential \( V(x) \) is negative.

### 4.6 One application of variational principles: counting the eigenvalues

of the Laplacian in a bounded domain \( \Omega \)

Throughout we assume that the domain \( \Omega \subset \mathbb{R}^d \) is open, connected, bounded, and regular (meaning that its boundary is piecewise smooth and Lipschitz), so that \( H^1(\Omega) \) injects into \( L^2(\Omega) \) compactly. If we call \( P_D = -\Delta_D \), resp. \( P_N = -\Delta_N \) the Dirichlet, resp. Neumann realizations of the Laplacian on \( \Omega \), both these operators have compact resolvents, hence purely discrete spectra \( \mu_j^D \), resp. \( \mu_j^N \). (eigenvalues are counted with multiplicities, as explained in Notation 47). Remember that the domains of \( P_D, P_N \) are not included in one another, but the corresponding quadratic forms \( q_D, q_N \) have domains \( D(q_D) = H^1_0(\Omega) \), resp. \( D(q_N) = H^1(\Omega) \) (see Ex. 13). Noticing that \( D(q_D) \subset D(q_N) \), a direct application of Corollary 51 is the following comparison of the spectra of \( P_D \) and \( P_N \):
Proposition 53. [Dirichlet-Neumann ordering]

\[ \forall n \geq 1, \quad \mu_n^N(\Omega) \leq \mu_n^D(\Omega). \]

A second consequence of the Max-Min principle is the monotonicity of the Dirichlet spectrum w.r.t. \( \Omega \):

Proposition 54. Assume \( \Omega \subset \bar{\Omega}, \) with both domains regular. Then

\[ \forall n \geq 1, \quad \mu_n^D(\bar{\Omega}) \leq \mu_n^D(\Omega). \] (9)

Proof. The proof proceeds by extending trial functions \( u \in H^1_0(\Omega) \) by zero outside \( \Omega \), to form a function \( \tilde{u} \in H^1_0(\tilde{\Omega}) \).

Now, let us consider a growing sequence of \( \Omega_j \subset \Omega_{j+1} \) such that \( \Omega = \bigcup \Omega_j \). The above result shows that each eigenvalue \( \mu_n^D(\Omega_j) \) decays w.r.t. \( j \). We can actually get a more precise continuity property:

\[ \forall n \geq 1, \quad \mu_n^D(\Omega_j) \downarrow \mu_n^D(\Omega), \quad \text{as } j \to \infty. \]

Dealing with the monotonicity of Neumann eigenvalues is more difficult, because it is less obvious to extend \( u \in H^1(\Omega) \) to \( \tilde{u} \in H^1(\tilde{\Omega}) \). However, let us split the regular set \( \Omega \) by cutting it into two regular open sets \( \Omega_1, \Omega_2 \), with \( \Omega_1 \cup \Omega_2 \subset \Omega \). One easily shows that \( H^1(\Omega) \subset H^1(\Omega_1 \cup \Omega_2) \), hence the variational principle induces an inequality in the opposite direction to (9):

\[ \forall n \geq 1, \quad \mu_n^N(\Omega_1 \cup \Omega_2) \leq \mu_n^N(\Omega). \] (10)

Putting together these 3 inequalities, we obtain a Dirichlet-Neumann bracketing:

Corollary 55. [Dirichlet-Neumann bracketing]

\[ \forall n \geq 1, \quad \mu_n^N(\Omega_1 \cup \Omega_2) \leq \mu_n^N(\Omega) \leq \mu_n^D(\Omega) \leq \mu_n^D(\Omega_1 \cup \Omega_2). \] (11)

We conclude this section by mentioning the famous Weyl asymptotics for the eigenvalue count of \( P_D \) on \( \Omega \). Let us define the counting function \( N_D(\mu) = \# \{ \mu_n(P_D) \leq \mu \} = \text{rank } E(-\infty,\mu](P_D) \).

Theorem 56. [Weyl asymptotic formula] Let \( \Omega \subset \mathbb{R}^d \) be open, bounded and regular. Then the Dirichlet counting function satisfies the following asymptotics as \( \mu \to \infty \):

\[ N_D(\mu) \sim \frac{\omega_d}{(2\pi)^d} \mu^{d/2} \text{Vol}(\Omega), \] (12)

where \( \omega_d = \frac{\pi^{d/2}}{\Gamma(d/2+1)} \) is the volume of the unit ball in \( \mathbb{R}^d \).

Proof. We first explicitly compute the eigenvalues of both Neumann and Dirichlet Laplacians on a unit hypercube, and check that they satisfy the above estimate. This step uses the Gauss counting of integral points inside large balls in dimension \( d \). By scaling, we get the counting function for cubes or arbitrary sidelength \( \epsilon > 0 \).
We then pave Ω by such ε-hypercubes, either staying inside Ω, or covering all of it; namely, we may define two sets Ω_ε ⊂ Ω ⊂ ˜Ω_ε, where Ω_ε and ˜Ω_ε are unions of ε-hypercubes, and such that their volumes are Cε-close to that of Ω. Let us note ∪_j Ω_j ⊂ Ω ⊂ ∪_j ˜Ω_j the first union of hypercubes. The Dirichlet-Neumann bracketing shows that

$$\sum_j N_N(\Omega_j) = N_N(\bigcup_j \Omega_j) \geq N_N(\bigcup_j \tilde{\Omega}_j) \geq N_D(\bigcup_j \Omega_j) \geq \sum_j N_D(\Omega_j).$$

Both sides satisfy the Weyl asymptotics, hence so does $N_D(\bigcup_j \Omega_j) = N_D(\Omega_\epsilon)$. The same computation applies to $\tilde{\Omega}_\epsilon$, hence we get the corresponding asymptotics for $N_D(\tilde{\Omega}_\epsilon)$. Finally, the monotonicity property (9) induces a monotonicity of the Dirichlet counting function:

$$N_D(\Omega_\epsilon) \leq N_D(\Omega) \leq N_D(\tilde{\Omega}_\epsilon),$$

so we get two asymptotic bounds for $N_D(\Omega)$. Sending finally $\epsilon \searrow 0$ provides the announced asymptotics.

The Weyl asymptotics (12) is the first step towards more precise expansions, which have occupied PDE specialists and geometers throughout the last century (the study of Spec($-\Delta$) on Euclidean domains, or more generally on Riemannian manifolds, defines the field of spectral geometry). Microlocal methods, which use the connection between the Laplacian with the geodesic flow, is helpful in the task of obtaining more expansions expansions, the latter depending of various properties of the geometry of the domain Ω (resp. the Riemannian manifold), and of the dynamical properties of the induced geodesic flow.