Brief Summary of Lectures The first lecture is going to be introductory and general. We are going to explain some motivations of Quantum mechanics, and we are also going to explain a little bit what it means Mathematical Methods in Quantum Mechanics. We are going to motivate the use of wavefunctions, why one uses self-adjoint operators and why the notion of spectrum is important. The last two notions play a very important part in Quantum mechanics. In the first few weeks we are going to deal with background needed to study them.

1 An introduction to weak derivatives and Sobolev spaces

Let X be a vector space with a norm $\|.\|$. X is called a Banach space if every Cauchy sequence in $(X, \|.\|)$ is convergent. If in addition X is a complex vector space it is called a complex Banach space.

An important example We consider the space

$$X = \{\phi \in L^2(\mathbb{R}^n) : \phi \in C^2(\mathbb{R}^n) \text{ and } \Delta\phi \in L^2(\mathbb{R}^n)\}.$$

Then X equipped with the norm $\|\phi\|_{L^2(\mathbb{R}^n)} + \|\Delta\phi\|_{L^2(\mathbb{R}^n)}$ is not a Banach space. This motivates as to define the Sobolev spaces.

Some notation

$C_c^\infty(\mathbb{R}^n) := \{\phi : \mathbb{R}^n \to \ \mid \phi \in C^\infty(\mathbb{R}^n), \text{ and } \operatorname{supp}\phi \text{ is compact }\}$, where $\operatorname{supp}\phi := \overline{\{x \in \mathbb{R}^n : \phi(x) \neq 0\}}$.

An element of $C_c^\infty(\mathbb{R}^n)$ is called a test function.

$L^1_{\text{loc}}(\mathbb{R}^n) := \{\phi : \mathbb{R}^n \to \mathbb{C} \mid \phi \in L^1(K) \text{ for all compact sets } K\}$.

Definition 1.1 (Weak derivatives). *Suppose that $u, w \in L^1_{loc}(\mathbb{R}^n)$. We say that w is the α^{th}-weak partial derivative of u, and write $\partial^\alpha u = v$ if*

$$\int_{\mathbb{R}^n} u\partial^\alpha\phi dx = (-1)^{|\alpha|}\int_{\mathbb{R}^n} w\phi dx, \forall\phi \in C_c^\infty(\mathbb{R}^n).$$

Proposition 1.2 (Uniqueness of weak derivatives)**.** *If $u \in L^1_{loc}(\mathbb{R}^n)$ has a weak derivative then it is unique.*

Definition 1.3 (Sobolev spaces). *Let $k \in \mathbb{N}$ and $1 \leq p \leq \infty$. Then*

$$H^k(\mathbb{R}^n) := \{u \in L^2(\mathbb{R}^n) \mid \partial^\alpha u \textit{ exists and } \partial^\alpha u \in L^2(\mathbb{R}^n), \textit{ for all multiindices } \alpha, \textit{ with } |\alpha| \leq k\}.$$

We equip $H^k(\mathbb{R}^n)$ with the norm $\|.\|_{H^k(\mathbb{R}^n)}$ defined by

$$\|u\|_{H^k(\mathbb{R}^n)} := \left(\sum_{|\alpha|\leq k} \|\partial^\alpha u\|^2_{L^2}\right)^{\frac{1}{2}}.$$

Theorem 1.4. *The $H^k(\mathbb{R}^n)$ norm is equivalent to the norm*

$$\|u\| := \left(\int_{\mathbb{R}^n} (1 + |\xi|^2)^k |\hat{u}(\xi)|^2\right) d\xi, \tag{1}$$

where $\hat{u}$ is the Fourier transformation of u. In particular, the $H^2(\mathbb{R}^n)$ norm is equivalent to the norm $\|u\| := \left(\|u\|^2_{L^2(\mathbb{R}^n)} + \|\Delta u\|^2_{L^2(\mathbb{R}^n)}\right)^{\frac{1}{2}}$.

Some elementary properties of Sobolev spaces

Theorem 1.5 (Completeness)**.** *For any $k \in \mathbb{N}$ the space $(H^k(\mathbb{R}^n), \|.\|_{H^k(\mathbb{R}^n)})$ is a Banach space.*

Theorem 1.6 (Approximation by smooth functions)**.** *Let $k \in \mathbb{N}$ If $u \in H^k(\mathbb{R}^n)$, then there exists a sequence of functions $u_m \in C_c^\infty(\mathbb{R}^n)$ such that $u_m \to u$ in $H^k(\mathbb{R}^n)$.*

2 Unbounded Operators, Spectrum and Resolvent

Let $(X, \|\|)$ be a complex Banach space and $D \subset X$ a linear subspace of X. Let $A : D \to X$ be a linear operator. If $\overline{D} = X$ then we say that A is densely defined. The range of A and the Kernel of A are respectively defined by

$$\mathrm{Ran}(A) = \{Ax : x \in D\}, \quad \mathrm{Kern}(A) = \{x \in D : Ax = 0\}.$$

A is called bounded if $\|A\| := \sup\{\|Ax\| : x \in D, \|x\| = 1\} < \infty$. Otherwise A is called unbounded.

The operator A is called closed if the graph of A

$$\Gamma_A = \{(x, y) : x \in D, y = Ax\}$$

is closed in the Graph Norm $\|\phi\|_A := \|\phi\| + \|A\phi\|$.

Remark 2.1. *From the definition one can see that A is closed if and only the following property holds: If $(x_n)_{n\in\mathbb{N}}$ is a sequence in $D(A)$ with $x_n \to x$ and $Ax_n \to y$ for some $x, y \in X$ then $x \in D$ and $y = Ax$.*

The resolvent set of A is defined as

$$\rho(A) = \{z \in \mathbb{C} : (z - A) : D(A) \to X \text{ is a bijection and } (z - A)^{-1} \text{ is bounded}\}.$$

As the resolvent of A one defines the mapping $R_A : \rho(A) \to \mathcal{L}(X), R_A(z) := (z - A)^{-1}$.

The spectrum of A is defined as

$$\sigma(A) = \mathbb{C} \setminus \rho(A).$$

Lemma 2.2. *(1) If A is not a closed operator then $\sigma(A) = \mathbb{C}$.*
(2) If A is a closed operator and $D = X$ then A is bounded.

Let $\mathcal{L}(X)$ denote the set of bounded operators from X to itsself.

Lemma 2.3. *Let $K \in \mathcal{L}(X)$. If $\|K\| := \sup\{\|Kx\| : \|x\| = 1\} < 1$, then the operator $I+K$ is invertiable and*

$$(I + K)^{-1} = \sum_{k=0}^{\infty}(-K)^n.$$

Theorem 2.4. *Let X be a complex Banach space and $A : D \to X$ a linear operator. Then $\rho(A)$ is open, $\sigma(A)$ is closed and R_A is analytic in $\rho(A)$. More precisely if $z_0 \in A$ then $B(z_0, \|R_A(z_0)\|^{-1}) \subset \rho(A)$ and for all $z \in B(z_0, \|R_A(z_0)\|^{-1})$ we have*

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

In particular $\|R_A(z_0)\| \geq \frac{1}{dist(z_0, \sigma(A))}$.

Theorem 2.5. *Let $V : \mathbb{R}^n \to \mathbb{C}$ be continuous. Consider the multiplication operator $T_V : D \subset L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ defined on $D := \{f \in L^2 : Vf \in L^2\}$ where $(Vf)(x) = V(x)f(x)$ by $T_V f := Vf$. Then $\sigma(T_V) = \overline{Ran(V)}$. In particular, if V is real-valued, then $\sigma(T_V) \subset \mathbb{R}$.*

Remark 2.6. *Note that in a similar way the multiplication operator can be defined for a measurable function V and in that case $\sigma(T_V) = essran(V) = \{y \in C : \mu(V^{-1}(B(y, \epsilon))) > 0, \forall \epsilon > 0\}$.*

Remark 2.7. *From now on we will mostly denote the multiplication operator mostly by V instead of T_V.*

Theorem 2.8. *For the Laplacian operator $-\Delta : H^2(\mathbb{R}^n) \subset L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ we have that $\sigma(-\Delta) = [0, \infty)$.*

Definition 2.9. *Let X be a complex Banach space and $A : D_1 \subset X \to X, B : D_2 \subset X \to X$ linear operators. We set that B is an extension of A if and write $A \subset B$ if $D_1 \subset D_2$ and $Ax = Bx$ for all $x \in D_1$.*

Definition 2.10. *Let X be a complex Banach space and $A : D \subset X \to X$ a linear operator. We set that A is closable if it has a closed extension, namely an extension which is a closed operator.*

Theorem 2.11. *Let X be a complex Banach space and $A : D \subset X \to X$ a linear operator. Then the following statements are equivalent:*
(a) A is closable
(b) $\overline{\Gamma_A}$ (closure of the graph of A in the graph norm) is the graph of a linear operator.
(c) From $x_n \to 0$ and $Ax_n \to y$ it always follows that $y = 0$.

3 Symmetric and self-adjoint operators

Let $\mathcal{H}$ be a complex Hilbert space and $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ densely defined. Then the adjoint operator $A^* : D(A^*) \subset \mathcal{H} \to \mathcal{H}$ is defined as follows:

If for a given $\phi \in \mathcal{H}$ there exists a unique ϕ^* such that $\langle \phi, A\psi \rangle = \langle \phi^*, \psi \rangle$ for all $\psi \in D(A)$, then $\phi \in D(A^*)$ and $A^*\phi = \phi^*$. The operator A^* is linear.

Lemma 3.1. $D(A^*) = \{\phi \in \mathcal{H} : \psi \to \langle \phi, A\psi \rangle$ *is continuous in* $D(A)\}$

Remark 3.2. *If $A \subset B$ then $B^* \subset A^*$.*

Remark 3.3. *A^* is defined only because A is densely defined. Similarly A^{**} can be defined only if A^* is densely defined which is not always the case.*

Theorem 3.4. *Let $\mathcal{H}$ be a complex Hilbert space and $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ densely defined. Then*
1. A^* is a closed operator
2. If A ist closable then $(\overline{A})^* = A^*$.
3. A is closable if and only if A^* is densely defined and in this case $\overline{A} = A^{**}$.

Theorem 3.5. *Let $A : D(A) \subset \mathcal{H} \subset \mathcal{H}$ be densely defined. Then $Kern(A^*) = \mathrm{Ran}(A)^\perp$. In particular $\mathrm{Ran}(A) \subset D(A^*)$ and $Kern(A^*) = \{0\} \Leftrightarrow \overline{Ran(A)} = \mathcal{H}$.*

Definition 3.6 (Symmetry and self-adjointness)**.** *A densely defined operator $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ is called symmetric if $A \subset A^*$ and self-adjoint if $A = A^*$.*

Remark 3.7. *A densely defined operator is symmetric if and only if $\langle A\phi, \psi \rangle = \langle \phi, A\psi \rangle$ for all $\phi, \psi \in D(A)$. A is self-adjoint if and only if A is symmetric and $D(A) = D(A^*)$.*

Remark 3.8. *From the definition of self-adjointness and Theorem 3.4 it follows that a self-adjoint operator is always closed.*

We define $\mathbb{C}_+ = \{z \in \mathbb{C} : \mathrm{Im}(z) > 0\}$, $\mathbb{C}_- = \{z \in \mathbb{C} : \mathrm{Im}(z) < 0\}$.

Theorem 3.9. *Let $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ be symmetric.*
1. For all $\lambda, \mu \in \mathbb{R}$ and all $\phi \in D(A)$ we have $\|(A - \lambda - i\mu)\phi\|^2 = \|(A - \lambda)\phi\|^2 + \mu^2\|\phi\|^2$.
2. (i) If $\mathrm{Ran}(A - z_+) = \mathcal{H}$ for one $z_+ \in \mathbb{C}_+$ then $\mathbb{C}_+ \subset \rho(A)$.
(ii) If $\mathrm{Ran}(A - z_-) = \mathcal{H}$ for one $z_- \in \mathbb{C}_-$ then $\mathbb{C}_- \subset \rho(A)$.

Theorem 3.10. *Let A be a symmetric operator. Then the following statements are equivalent:*
1. $A = A^*$
2. $\sigma(A) \subset \mathbb{R}$
3. $\mathrm{Ran}(A + z_\pm) = \mathcal{H}$ for a $z_+ \in \mathbb{C}_+$ and a $z_- \in \mathbb{C}_-$.
4. A is closed and Kern$(A^* + z_\pm) = \{0\}$ for a $z_+ \in \mathbb{C}_+$ and a $z_- \in \mathbb{C}_-$.

Remark 3.11. *From $\sigma(A) \subset \mathbb{R}$ alone self-adjointness does not necessarily follow.*

Example 3.12 (Important)**.** *The operator $A : H^2(\mathbb{R}^n) \subset L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ $A\phi = -\Delta\phi$ is self-adjoint.*

Theorem 3.13 (Kato-Rellich)**.** *Let A be self-adjoint and B symmetric with $D(A) \subset D(B)$. If*

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

where $a, b \in \mathbb{R}$ and $0 < a < 1$ then is $A + B : D(A) \subset \mathcal{H} \to \mathcal{H}$ self-adjoint.

Theorem 3.14 (Hardy's inequality)**.** *Let $\psi \in H^1(\mathbb{R}^3)$. Then we have that*

$$\int \frac{|\psi(x)|^2}{|x|^2} dx = 4 \int |\nabla\psi(x)|^2 dx.$$

Example 3.15 (Important)**.** *1. The operator $A : H^2(\mathbb{R}^3) \subset L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ $(A\phi)(x) = (-\Delta - \frac{1}{|x|})\phi(x)$ is self-adjoint.*
2. We use the notation $x := (x_1, ..., x_N) \in (\mathbb{R}^3)^N = \mathbb{R}^{3N}$. The operator $B : H^2(\mathbb{R}^{3N}) \subset L^2(\mathbb{R}^{3N}) \to L^2(\mathbb{R}^{3N})$

$$(B\phi)(x) = \sum_{j=1}^{N} \left(-\Delta_{x_j} - \frac{N}{|x_j|} \right) \phi(x) + \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|} \phi(x) \tag{2}$$

is self-adjoint.

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

Theorem 3.16. *Let A be a symmetric operator. Then the following statements are equivalent:*
1. A is essentially self-adjoint.
2. $\overline{\mathrm{Ran}(A + z_\pm)} = \mathcal{H}$ for a $z_+ \in \mathbb{C}_+$ and a $z_- \in \mathbb{C}_-$.
3. Kern$(A^* + z_\pm) = \{0\}$ for a $z_+ \in \mathbb{C}_+$ and a $z_- \in \mathbb{C}_-$.

Theorem 3.17 (Kato-Rellich general form)**.** *Let A be essentially self-adjoint and B symmetric with $D(A) \subset D(B)$. If*

$$\|B\phi\| \leq a\|A\phi\| + b\|\phi\|, \quad \forall \phi \in D(A), \tag{3}$$

where $a, b \in \mathbb{R}$ and $0 < a < 1$ then is $A + B : D(A) \subset \mathcal{H} \to \mathcal{H}$ is essentially self-adjoint and $D(\overline{A + B}) = D(\overline{A})$.

4 The Schrödinger equation and Existence of dynamics

Let $H : D(H) \subset \mathcal{H} \to \mathcal{H}$ be densely defined. We consider the initial value problem

$$\begin{cases} i\frac{d}{dt}\phi_t = H\phi_t \\ \phi_0 = u \end{cases} \tag{4}$$

Let I be a nontrivial interval with $0 \in I$. A solution (4) is a differentiable function $\phi : I \to \mathcal{H}$, with the following properties
1. $\phi_t \in D(H), \quad \forall t \in I$
2. $i\frac{d}{dt}\phi_t = i\lim_{h\to 0}\frac{\phi_{t+h}-\phi_t}{h} = -iH\phi_t$.
3. $\phi_0 = u$

Theorem 4.1. *Let $H : D(H) \subset \mathcal{H} \to \mathcal{H}$ be densely defined. If (4) has for all $u \in D$ a solution with constant norm then H is symmetric. If H is symmetric then the problem has for every $u \in D(H)$ at most one solution locally in time.*

Theorem 4.2. *Let $H : D(H) \subset \mathcal{H} \to \mathcal{H}$ be symmetric. If (4) has for all $u \in D$ a unique solution which is global in time then H is essentially self-adjoint.*

Theorem 4.3 (Existence of Solution bounded case)**.** *Let $H : \mathcal{H} \to \mathcal{H}$ be bounded and self-adjoint. Then for all $u \in \mathcal{H}$ (4) has the unique solution $e^{-itH}u$, where $e^{-itH} = \sum_{n=0}^{\infty}\frac{(-itH)^n}{n!}$. The solution is global in time. The map $U : \mathbb{R} \to \mathcal{L}(\mathcal{H})$, $U(t) = e^{-iHt}$ satisfies the following properties*
1) $U(t)$ is unitary and $U(t+s) = U(t)U(s)$ for all $s,t \in \mathbb{R}$
2) $\lim_{t\to 0} U(t)\psi \to \psi$ for all $\psi \in \mathcal{H}$.

Definition 4.4. *A map $U : \mathbb{R} \to \mathcal{L}(\mathcal{H})$ satisfying the properties 1),2) of the last theorem is called a strongly continuous unitary group.*

Remark 4.5. *If U is a strongly continuous unitary group then $U(0) = I$ and $t \to U(t)\psi$ is continuous for all $\psi \in \mathcal{H}$ ($U(t)$ is strongly continuous).*

Theorem 4.6 (Existence of Solution general case)**.** *Let $H : D(H) \subset \mathcal{H} \to \mathcal{H}$ be self-adjoint. Then for all $u \in D(H)$ (4) has a unique solution. The solution ϕ_t is global in time. Moreover there exists a unique strongly continuous unitary group U such that, $\phi_t = U(t)u, \forall t \in \mathbb{R}, \forall u \in D(H)$.*

Remark 4.7. *The strongly continuous group U in the last theorem is denoted by $U(t) = e^{-iHt}$. From the last theorem one can see that the notion of the solution actually makes sense for all $u \in \mathcal{H}$ even if u is not in $D(H)$.*

Definition 4.8. *Let $U : \mathbb{R} \to \mathcal{L}(\mathcal{H})$ be a strongly continuous unitary group. The generator of U is defined to be the linear operator $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ defined through:*
1. $D(A) := \{\psi \in \mathcal{H} : \lim_{t\to 0}\frac{U(t)\psi-\psi}{t}$ exists $\}$
2. $A\psi = i\lim_{t\to}\frac{U(t)\psi-\psi}{t} = i\frac{d}{dt}U(t)\psi|_{t=0}$.

Theorem 4.9 (Stone)**.** *Let $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ be the generator of a strongly continuous unitary group $U : \mathbb{R} \to \mathcal{L}(\mathcal{H})$. Then the following statements hold:*
1. $U(t)D(A) \subset D(A)$ and for all $\phi \in D(A)$

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

2. $A = A^*$.
3. $U(t)$ is uniquely determined by A.

5 Observables, uncertainty principle, ground state energy

Physically measurable quantities, called observables correspond to self-adjoint operators acting on the Hilbert space $\mathcal{H}$ to which the wave function ψ belongs.

Definition 5.1. *(i) The expectation value associated with the self-adjoint operator A in the state ψ is given by $\langle \psi, A\psi \rangle$.*
(ii) The variance of A in $\psi \in D(A)$ is defined by

$$\Delta A_\psi := \langle \psi, (A - \langle \psi, A\psi \rangle)^2 \psi \rangle = \langle \psi, A^2 \psi \rangle - \langle \psi, A\psi \rangle^2.$$

Definition 5.2. *The commutator of two operators A, B is defined by $[A, B] = AB - BA$.*

Theorem 5.3 (Heisenberg's uncertainty principle)**.** *Let A, B be two self-adjoint operators acting on $\mathcal{H}$. Then we have for $\psi \in D(A) \cap D(B)$*

$$\Delta A_\psi \Delta B_\psi \geq \frac{1}{4} \langle \psi, [A, B]\psi \rangle.$$

We consider the Hamiltonian H of an atom with atomic number N defined similarly as in (2)

$$(H\phi)(x) = \sum_{j=1}^{N} \left(-\Delta_{x_j} - \frac{Z}{|x_j|} \right) \phi(x) + \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|} \phi(x) \tag{5}$$

We now by Kato-Rellich that H is self-adjoint with domain $H^2(\mathbb{R}^{3N})$. Each expectation value $\langle \psi, H\psi \rangle$ can be extended naturally to be defined for all $\psi \in H^1(\mathbb{R}^{3N})$. The ground state energy of H is defined by

$$E = \inf_{\psi \in H^1(\mathbb{R}^{3N}), \|\psi\|_{L^2(\mathbb{R}^{3N})} = 1} \langle \psi, H\psi \rangle.$$

If the infimum is attained then a minimizer is called a ground state.

Theorem 5.4. *We always have that $E \in \sigma(H)$. If H has a ground state ψ then $\psi \in H^2(\mathbb{R}^{3N})$ and $H\psi = E\psi$.*

Theorem 5.5. *If $N = 1, Z > 0$ then H has up to a constant a unique ground state and its ground state energy is given by $E = -\frac{Z^2}{4}$.*

6 Some tools of functional analysis

Here we will introduce some tools of the functional analysis that we will need to handle the problem of the drum in the next section. For simplicity we will explain some of the needed tools only for Hilbert spaces.

Definition 6.1. *Let $(X, \|.\|)$ be a real (respectively complex) Banach space, $x \in X$ and x_n be a sequence in x. We say that x_n converges weakly to x and we write $x_n \rightharpoonup x$, if $f(x_n) \to f(x)$ for all $f : X \to \mathbb{R}$ (respectively $f : X \to \mathbb{C}$) linear continuous.*

Remark 6.2. *If $(X, \langle ., . \rangle)$ is a Hilbert space then $x_n \rightharpoonup x$ if and only if $\langle x_n, y \rangle \to \langle x, y \rangle$ for all $y \in X$.*

Theorem 6.3. *Let $(X, \|.\|)$ be a Banach space. Then every weakly convergent sequence in X is bounded. Moreover, if $x_n \rightharpoonup x$ then $\|x\| \leq \liminf_{n \to \infty} \|x_n\|$.*

Theorem 6.4 (Banach-Alaoglu, special case)**.** *Let $(X, \langle ., . \rangle)$ be a Hilbert space. Then every bounded sequence in X has a weakly convergent subsequence.*

Theorem 6.5. *Let $(X, \langle ., . \rangle)$ be a Hilbert space. If $x_n \rightharpoonup x$ and $\|x_n\| \to \|x\|$, then $x_n \to x$.*

Definition 6.6 (Compact operators)**.** *Let X, Y be Banach spaces and $K : X \to Y$ a linear operator. K is called compact, if for every bounded sequence x_n in X Kx_n has a convergent subsequence in Y.*

Theorem 6.7. *Let X, Y be separable Hilbert spaces, and $K : X \to Y$ be a linear operator. Then K is compact if and only if for any sequence x_n in X and any $x \in X$ we have $x_n \rightharpoonup x \implies Kx_n \to Kx$.*

Theorem 6.8. *Let X, Y be Banach spaces spaces, and $K_n : X \to Y$ a sequence of compact operators. If $K : X \to Y$ is linear bounded and $K_n \to K$ in the operator norm, then K is compact.*

Theorem 6.9. *Let $f \in C_c^1(\mathbb{R}^n)$. Then the operator $T_f : H^1(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$, $T_f\psi = f\psi$ is compact.*

Theorem 6.10. *Let f be bounded with $\lim_{|x|\to\infty} f(x) = 0$. Then the operator $T_f : H^1(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$, $T_f\psi = f\psi$ is compact.*

7 Decomposition of an operator

Theorem 7.1. *Let X be a Banach space and consider a linear operator $A : D \subset X \mapsto X$. Consider a simply closed positively oriented curve γ lying in the resolvent set $\rho(A)$ of A. If inside of γ there are no points of the spectrum of A, then $\int_\gamma (z - A)^{-1} dz = 0$.*

Definition 7.2. *Let X be a Banach space and $A \in \mathcal{L}(X)$. The spectral radius of A is defined by $r_A := \limsup \|A^n\|^{\frac{1}{n}}$.*

Theorem 7.3. *Let $A \in \mathcal{L}(X)$. Then*
1) $\sigma(A) \neq \emptyset$ and $r_A = \sup_{z\in\sigma(A)} |z|$.
2) If X is a Hilbert space and A is self-adjoint then $\|A\| = \sup_{z\in\sigma(A)} |z|$.

Theorem 7.4. *Let $\mathcal{H}$ be a Hilbert space and $A : D \subset \mathcal{H} \to \mathcal{H}$ be self-adjoint. Assume that $\sigma(A) = \sigma' \cup \sigma''$ where $\sigma', \sigma'' \subset \mathbb{C}$ are disjoint and σ' is compact. Let γ be a simply closed positively oriented curve such that σ' is inside of γ but σ'' is outside of γ. We consider the operator $P = \frac{1}{2\pi i} \int_\gamma (z - A)^{-1} dz$. Then*
1) P does not depend on the choice of γ.
2) P is an orthogonal projection.
3) $PA \subset AP$. Thus A lives the range of P and the range of $1 - P$ invariant.
4) Let $A' = A|_{Ran(P)}$, $A'' = A|_{Ran(1-P)}$. Then $\sigma(A') = \sigma'$ and $\sigma(A'') = \sigma''$. Moreover A' and A'' are both self-adjoint.
5) A' is a bounded operator
6) If $\sigma' = \{\lambda\}$ for some $\lambda \in \mathbb{R}$ then $AP = \lambda P$.

Theorem 7.5. *Let $\mathcal{H}$ be a Hilbert space and $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ be self-adjoint. Let $\lambda \in \mathbb{R}$. Then $\lambda \in \sigma(A) \iff$ there exists a sequence $(\psi_n)_{n\in\mathbb{N}} \subset D(A)$ with $\|\psi_n\| = 1$ and $\|(A - \lambda)\psi_n\| \to 0$.*

8 Discrete and Essential spectrum

Definition 8.1. *Let $\mathcal{H}$, be a Hilbert space and $A : D \subset \mathcal{H} \to \mathcal{H}$ be self-adjoint. The discrete spectrum $\sigma_d(A)$ of A is defined to be the set of all isolated points of the spectrum of A that are eigenvalues of finite multiplicity. The essential spectrum $\sigma_{ess}(A)$ of A is defined by $\sigma_{ess}(A) = \sigma(A) \setminus \sigma_d(A)$*

Theorem 8.2. *For a self-adjoint operator A as above and a $\lambda \in \mathbb{R}$ we have that $\lambda \in \sigma_{ess}(A)$ if and only if there exists a sequence ψ_n in D with the following properties:*
1) $\|\psi_n\| = 1, \forall n \in \mathbb{N}$
2) $\|(H - \lambda_n)\psi_n\| \to 0$
3) $\psi_n \rightharpoonup 0$.

Theorem 8.3. *Assume that $V : \mathbb{R}^n \to \mathbb{R}$ with $\lim_{|x|\to\infty} V(x) = 0$, $H = -\Delta + V$ is self-adjoint in $H^2(R^n)$ and $\sigma_{ess}(H) = [0, \infty)$.*

Theorem 8.4. *Assume that $V : \mathbb{R}^n \to \mathbb{R}$ with $\lim_{|x|\to\infty} V(x) = \infty$, $H = -\Delta + V$ is self-adjoint with domain $D(H) = \{\psi \in L^2(\mathbb{R}^n) : -\Delta\psi + V\psi \in L^2(\mathbb{R}^n)\}$ and $\sigma_{ess}(H) = \emptyset$.*

Theorem 8.5 (IMS localization formula)**.** *Let $H : H^2(\mathbb{R}^n) \subset L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$, $H = -\Delta + V$ be self-adjoint.*

a) If $f : \mathbb{R}^n \to \mathbb{R}$ is a C^2 function with $\partial^\alpha f \in L^\infty$, for $0 \le |\alpha| \le 2$ then

$$fHf = \frac{1}{2}(f^2H + Hf^2) + |\nabla f|^2. \tag{6}$$

b) If $(J_a)_{a\in\mathcal{A}} : \mathbb{R}^n \to \mathbb{R}$ is a finite family of C^2 functions with $\partial^\alpha J_a \in L^\infty$, for $0 \le |\alpha| \le 2$, $\forall a \in \mathcal{A}$ and with $\sum_{a\in\mathcal{A}} J_a^2 = 1$ then

$$H = \sum_{a\in\mathcal{A}} J_a H J_a - \sum_{a\in\mathcal{A}} |\nabla J_a|^2.$$

Theorem 8.6 (HVZ Theorem (Hunziker- van Winter- Zhislin))**.** *We consider the operator $H_{N,Z} : H^2(\mathbb{R}^{3N}) \subset L^2(\mathbb{R}^{3N}) \to L^2(\mathbb{R}^{3N})$*

$$(H_{N,Z}\phi)(x) = \sum_{j=1}^{N} \left(-\Delta_{x_j} - \frac{Z}{|x_j|}\right)\phi(x) + \sum_{1\le i<j\le N} \frac{1}{|x_i - x_j|}\phi(x).$$

Then $\sigma_{ess}(H_{N,Z}) = [\inf \sigma(H_{N-1,Z}), \infty)$.

Theorem 8.7. *We consider two self-adjoint operators A, B with $D(A) = D(B)$. If there exists a $z \in \mathbb{C} \setminus \mathbb{R}$ such that $(z - A)^{-1} - (z - B)^{-1}$ is compact then $\sigma_{ess}(A) = \sigma_{ess}(B)$.*

Corollary 8.8. *We consider two self-adjoint operators A, B with $D(A) = D(B)$. If there exists a $z \in \mathbb{C} \setminus \mathbb{R}$ such that $(B - A)(z - A)^{-1}$ is compact then $\sigma_{ess}(A) = \sigma_{ess}(B)$.*

Definition 8.9. *Let $H = H^*$ be an operator on $L^2(\mathbb{R}^n)$ that is bounded from below and satisfies the IMS localization formula in the sense that If $f : \mathbb{R}^n \to \mathbb{R}$ is a C^2 function with $\partial^\alpha f \in L^\infty$, for $0 \le |\alpha| \le 2$ then $fD(H) \subset D(H)$ and (6) holds. For $R > 0$ let $\Sigma_R := \inf_{\psi\in D(H),\operatorname{supp}\psi\subset B_R(0)^C}$. The ionization threshold of H is defined by $\Sigma = \lim_{R\to\infty} \Sigma_R$.*

Remark 8.10. *In the next weeks we will prove that for the operator $H_{N,Z}$ we have $\Sigma = \inf \sigma_{ess}(H_{N,Z})$.*

Theorem 8.11 (Exponential decay of eigenfunctions to eigenvalues below Σ)**.** *Let H be as in Definition 8.9. If $\psi \in D(H)$ satisfies $H\psi = E\psi$ for an $E < \Sigma$ then for all $\beta > 0$ with $\beta^2 < \Sigma - E$ we have that $e^{\beta|x|}\psi \in L^2(\mathbb{R}^n)$.*

9 Spectral Theorem for self-adjoint Operators and some applications

Theorem 9.1 (Spectral Theorem multiplication operator form)**.** *Let A be a self-adjoint operator on a separable Hilbert space $\mathcal{H}$ with domain $D(A)$. Then there is a measure space $\langle M, \mu\rangle$ with μ a finite measure, a unitary operator $U : \mathcal{H} \to L^2(M, d\mu)$, and a real-valued function f on M which is finite a.e. so that*

(a) $\psi \in D(A) \iff f(U\psi) \in L^2(M, \mu)$.

(b) If $\phi \in U[D(A)]$, then $(UAU^{-1}\phi)(m) = f(m)\phi(m)$.

Theorem 9.2 (Spectral Theorem functional calculus form)**.** *Let A be a self-adjoint operator on a Hilbert space $\mathcal{H}$. Then there exists a unique map ϕ from the bounded Borel functions on $\mathbb{R}$ into $\mathcal{L}(\mathcal{H})$ with the following properties:*

*(a) $\phi(fg) = \phi(f)\phi(g), \phi(\lambda f) = \lambda\phi(f)$, $\phi(1) = I$, $\phi(\overline{f}) = \phi(f)^*$, that is ϕ is an algebraic * homomorphism.*

(b) $\|\phi(h)\|_{\mathcal{L}(\mathcal{H})} \leq \|h\|_{L^\infty}$.

(c) Let $h_n(x)$ be a sequence of bounded Borel functions with $h_n(x) \to x$ pointwise and $|h_n(x)| \leq |x|$ for all x and n. Then for all $\psi \in D(A)$ $\phi(h_n)\psi \to A\psi$.

(d) If $h_n(x) \to h(x)$ and $\|h_n\|$ is bounded, then $\phi(h_n)\psi \to \phi(h)\psi$ for all $\psi \in \mathcal{H}$.

In addition: (e) If $A\psi = \lambda\psi$ then $\phi(h)\psi = h(\lambda)\psi$.

(f) If $h \geq 0$ then $\phi(h) \geq 0$.

Theorem 9.3. *Let $P_\Omega = \phi(\chi_\Omega)$, where $\Omega \subset \mathbb{R}$ Borel and χ_Ω is the characteristic function of Ω.*

(i) The family P_Ω is a projection valued measure, namely it satisfies the following properties

(a) Each P_Ω is an orthogonal projection.

(b) $P_\emptyset = 0$, $P_\mathbb{R} = I$.

(c) If $\Omega = \cup_{n=1}^N \Omega_n$, where $N = 1, ..., \infty$ with $\Omega_n \cap \Omega_m = \emptyset$ if $n \neq m$, then $P_\Omega\psi = \sum_{n=1}^N P_{\Omega_n}\psi$.

(d) $P_{\Omega_1}P_{\Omega_2} = P_{\Omega_1\cap\Omega_2}$.

(ii) For all $\Omega \subset \mathbb{R}$ Borel we have that $P_\Omega A \subset AP_\Omega$. If Ω is open then

$$\sigma(A) \cap \Omega \subset \sigma(A|_{\mathrm{Ran}\, P_\Omega}) \subset \overline{\sigma(A) \cap \Omega}.$$

Theorem 9.4. *Let $H : D(H) \subset \mathcal{H} \to \mathcal{H}$ be self-adjoint and bounded from below. Let*

$$\mu_n(H) := \inf_{M\subset D(H), \dim(M)=n} \Big(\sup_{\phi\in M, \|\phi\|=1} \langle\phi, H\Phi\rangle\Big)$$

Then for any $n \in \mathbb{N}$ we have <u>either</u>

(a) There are at least n eigenvalues (counting multiplicity) below $\inf \sigma_{ess}(H)$ and $\mu_n(H)$ is the n-th eigenvalue from below (counting multiplicity)

<u>or</u>

(b) $\mu_n(H) = \inf \sigma_{ess}(H) = \mu_{n+1}(H) = \mu_{n+2}(H) = ...$ and there are at most $(n - 1)$ eigenvalues (counting multiplicity) below $\mu_n(H)$.

Corollary 9.5. *$\mu_1(H) = \inf_{\phi\in D(H), \|\phi\|=1}\langle\phi, H\phi\rangle$ (ground state energy of H) is in the spectrum of H.*

Corollary 9.6. *(i) If there exists a function $\phi \in D(H)$ with $\|\phi\| = 1$ and $\langle\phi, H\phi\rangle < \inf \sigma_{ess}(H)$, then H has a ground state.*

(ii) If there exists a subspace $M \subset D(H)$ of dimension $N \in \mathbb{N}\cup\{\infty\}$, with $\langle\phi, H\phi\rangle < \inf \sigma_{ess}(H)$, then H has (at least) N eigenvalues below the bottom if its essential spectrum.

Example The operator $H : H^2(\mathbb{R}^3) \subset L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$, $H = -\Delta - \frac{1}{|x|}$ has infinitely many eigenvalues below the bottom of its essential spectrum.

Definition 9.7. *Let $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ be self-adjoint with functional calculus ϕ. The map $P : \mathcal{B} \to \mathcal{L}(\mathcal{H})$ with $P(\Omega) = P_\Omega = \phi(\chi_\Omega)) = \chi_\Omega(A)$. P is called the spectral measure of A. Its support is defined by* $\mathrm{supp}(P) = \{x \in \mathbb{R} : P(U) \neq 0$ *for all neighborhoods U of x*$\}$.

Theorem 9.8. *Let $A = A^*$ with spectral measure P. Then*
1. $S := \mathrm{supp}(P)$ is closed.
2. $P_S = 1$ and $P_{\mathbb{R}\setminus S} = 0$.
3. For all f bounded continuous we have $f(A) := \phi(f) = \sup_{x\in S} |f(x)|$.
4. $S = \sigma(A)$, $\|(z - A)^{-1}\| = dist(z, \sigma(A))^{-1}, \forall z \in \rho(A)$.

Theorem 9.9. *(Spectral Theorem projection valued form) There is a 1-1 correspondence between self-adjoint operators and projection valued measures on $\mathcal{H}$ the correspondence given by*

$$A = \int_{-\infty}^{\infty} \lambda dP_\lambda = \int_{\sigma(A)} \lambda dP_\lambda.$$

If g is a real valued Borel function on $\mathbb{R}$ then

$$g(A) := \int_{-\infty}^{\infty} g(\lambda) dP_\lambda$$

defined on

$$D_g := \{\phi : \int_{-\infty}^{\infty} |g(\lambda)|^2 d(\phi, P_\lambda \phi) < \infty\},$$

is self-adjoint.

10 Newton's Theorem and Zhislin's Theorem

Theorem 10.1 (Newton's Theorem)**.** *We consider a spherically symmetric function $\rho : \mathbb{R}^3 \to \mathbb{R}$. Assume that for all $x \in R^3$ the function $g(y) = \frac{\rho(y)}{|x-y|}$ is in $L^1(\mathbb{R}^3)$. Then*

$$\int_{\mathbb{R}^3} \frac{\rho(y)}{|x-y|} dy = \int_{\mathbb{R}^3} \frac{\rho(y)}{\max\{|x|, |y|\}} dy = \frac{1}{|x|} \int_{|y|\le|x|} \rho(y) dy = \int_{|y|\ge|x|} \frac{\rho(y)}{|y|} dy$$

Theorem 10.2 (Zhislin's Theorem)**.** *We consider the operator $H_{N,Z} : H^2(\mathbb{R}^{3N}) \subset L^2(\mathbb{R}^{3N}) \to L^2(\mathbb{R}^{3N})$*

$$(H_{N,Z}\phi)(x) = \sum_{j=1}^{N} \left(-\Delta_{x_j} - \frac{Z}{|x_j|} \right) \phi(x) + \sum_{1\le i<j\le N} \frac{1}{|x_i - x_j|} \phi(x).$$

If $Z > N - 1$ then $H_{N,Z}$ has infinitely many eigenvalues below the bottom of the essential spectrum.

11 Continuous spectrum, pure point spectrum and RAGE Theorem

Definition 11.1. *Let $H : D(H) \subset \mathcal{H} \to \mathcal{H}$ be self-adjoint. We define*

$$\mathcal{H}_{pp} := \overline{span\{\psi : \psi \text{ is eigenvalue of } H\}}, \qquad \mathcal{H}_c := \mathcal{H}_{pp}^{\perp}.$$

We define as the <u>pure point</u> *spectrum $\sigma_{pp}(H)$ of H as its set of eigenvalues. We also define the* <u>continuous spectrum</u> *of H by $\sigma_c(H) := \sigma(H|_{\mathcal{H}_c})$.*

Remark 11.2. *We have $\sigma(H) = \overline{\sigma_{pp}(H)} \cup \sigma_c(H)$, where the union is not necessarily disjoint and $\overline{\sigma_{pp}(H)} = \sigma(H|_{\mathcal{H}_{pp}})$. If P is the spectral measure of H then $\phi \in \mathcal{H}_{pp}$, if and only if the measure $\Omega \to \phi, P_\Omega \phi$ has discrete support and $\phi \in \mathcal{H}_c$ if and only if the measure is continuous (namely every set with one element has measure zero).*

Theorem 11.3 (RAGE Theorem)**.** *Let Let $H : D(H) \subset \mathcal{H} \to \mathcal{H}$ be self-adjoint. Assume that the operator $\chi_R(H+i)^{-1}$ is compact for all $R > 0$, where $\chi_R = \chi_{B_R(0)}$. Then*

$$\phi \in \mathcal{H}_{pp} \iff \lim_{R\to\infty} \sup_{t\geq 0} \|(1-\chi_R)e^{-itH}\phi\| = 0$$

$$\phi \in \mathcal{H}_c \iff \lim_{T\to\infty} \frac{1}{T}\int_0^T \|\chi_R e^{-itH}\phi\|^2 dt = 0, \text{ for all } R > 0.$$

Lemma 11.4. *Let μ be a complex valued finite measure on $\mathbb{R}$. Define $\hat{\mu}(t) := \int_{\mathbb{R}} e^{-it\lambda} d\mu(\lambda)$. Then*

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T |\hat{\mu}(t)|^2 dt = \sum_{y\in\mathbb{R}} |\mu(\{y\})|^2. \tag{7}$$

Lemma 11.5. *Let Let $H : D(H) \subset \mathcal{H} \to \mathcal{H}$ be self-adjoint. If $\phi \in \mathcal{H}$ and $\psi \in \mathcal{H}_c$ then*

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T |\langle \phi, e^{-iHt}\psi\rangle|^2 dt = 0. \tag{8}$$