Mathematical Methods in Quantum Mechanics

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Winter term 2019/2020

Introduction and Disclaimer

This PDF contains the lecture notes for the lecture "Mathematical Methods in Quantum Mechanics I" (http://www.math.kit.edu/iana1/lehre/quantummech2019w/en), given by *Dr. Anapolitanos* at the Karlsruhe Institute of Technology (KIT) during the winter term 2019/20.

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The document includes an index of used terminology and symbols at the end. Symbols are, however, not in the same alphabetical order as humans would probably arrange them. If you find yourself looking for a certain symbol in the index make sure you search the complete list of symbols for it.[1]

[1] Errors, typos, and suggested improvements can be reported to `martin_at_fachschaft.physik.kit.edu` and `laurin.benz_at_student.kit.edu`.

Contents

0 Introduction

When light (from some source like a laser) shines through a small slit on a detector placed behind the slit, one observes an intensity pattern like the one shown in Figure 0.1.

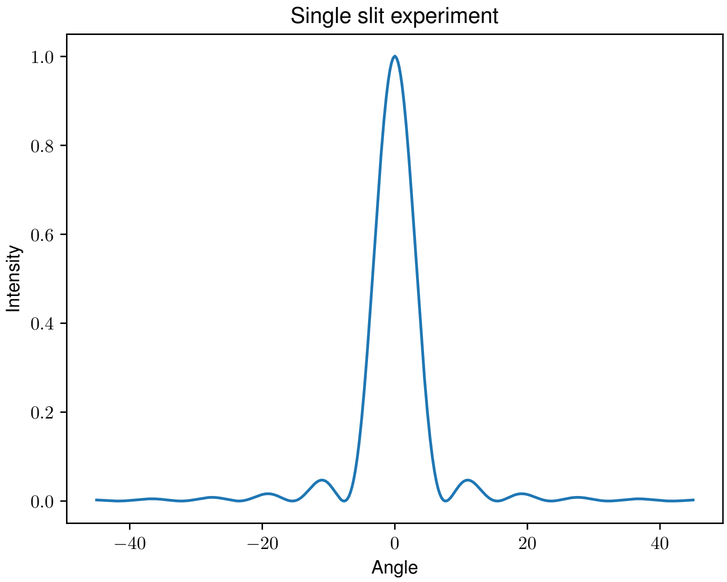

Figure 0.1: Intensity pattern of light shining through a single slit.

If instead the wall with the slit has a second slit (double slit experiment), the light waves cross both slits simultaneously and an interference pattern appears on the screen.
Now let us replace the source of light by a source of slow (nonrelativistic) electrons. Since electrons are particles, one would expect that the electron has the choice to pass through either of the slits, but not through both slits simultaneously, unlike the light waves. Thus, we would expect a pattern like Figure 0.2 in a double-slit experiment with electrons instead of light.
It came quite surprising in 1927 that electrons show the same behaviour as light in a double-slit experiment: an interference pattern, as shown in Figure 0.3.
Therefore, a beam of light seems to have some wave-like properties; in particular, there is

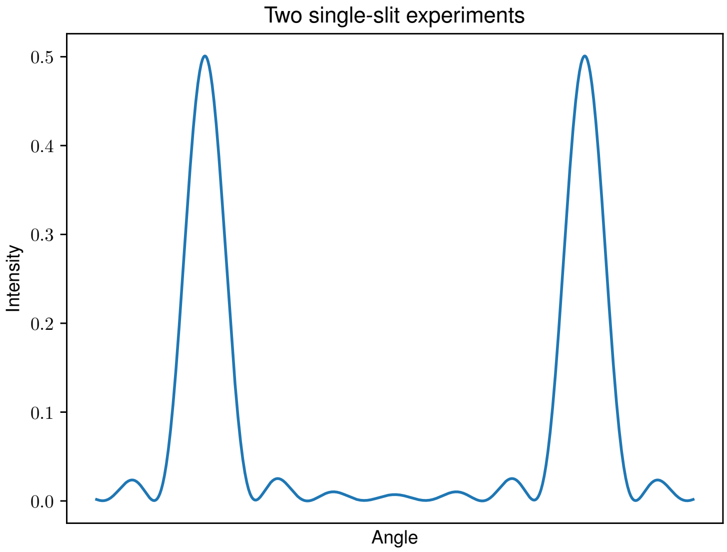

Figure 0.2: Naive expectation: the intensity pattern of the electron double-slit experiment is the sum of the intensity patterns of two electron single-slit experiments. The angle scale is much smaller than in the previous figure, the distance between the peaks is the distance between the two slits.

interference from both slits.[1] Moreover, even after reducing the flux of electrons drastically so that there was never more than electron between the source and the screen, the interference pattern appeared on the screen after enough electrons have been sent through the experiment successively. Hence, even single electrons seem to "pass both slits simultaneously", as did the light waves.

This observation had profound consequences:

1. Physicists had to abandon the idea of knowing the location where a single electron will hit the screen (and knowing through which slit the electron has passed). Instead, it is only possible to predict the (probability) distribution of locations on the screen.

2. Interference also applies to particles (and it is sizeable for small enough particles like electrons.

This phenomenon was explained with Quantum Mechanics. We describe a particle by a complex-valued *wave function* (*state vector*) $\psi(x, t)$, where $x \in \mathbb{R}^3$ is the position and $t \in \mathbb{R}$ is the time

[1] It was soon realized that both slits are necessary since the interference pattern disappeared as soon as one of the two slits was closed.

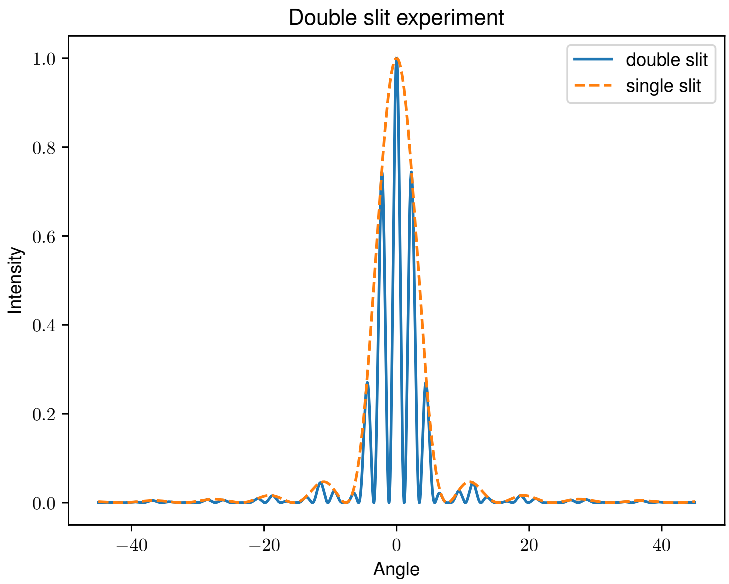

Figure 0.3: Electrons show the same interference behaviour as light.

and consider $|\psi(x,t)|^2$ as the probability distribution for fixed time t. Since particles show interference like waves, we want ψ to satisfy some wave equation.
Since we interpret $|\psi(x,t)|^2$ as the probability distribution, we need that $\int |\psi(x,t)|^2 \, \mathrm{d}x < \infty \, \forall t$; thus we embed $\psi(\cdot,t)$ into the Hilbert space, $\psi(\cdot,t) \in L^2\left(\mathbb{R}^3\right)$, where
$L^2\left(\mathbb{R}^3\right) = \left\{ \psi : R^3 \to \mathbb{C}, \int |\psi|^2 < \infty \right\}$ with the inner product $\langle \psi, \varphi \rangle = \int_{\mathbb{R}^3} \overline{\psi(x)} \varphi(x) \, \mathrm{d}x$.
The equation that ψ satisfies is a partial differential equation called the *Schrödinger equation*. We list some physically sensible properties that ψ and the Schrödinger equation should have.

1. $\psi(\cdot, t_0)$ should determine $\psi(\cdot, t)$ for all $t > t_0$.

2. If ψ and φ are evolution of states, then $a\psi + b\varphi$ (with $a, b \in \mathbb{R}$) should also be an evolution of a state (superposition principle).

3. $\int |\psi(x,t)|^2 \, \mathrm{d}x$ should be conserved.

4. Quantum mechanics should be close to classical mechanics in some limit.

From properties 1. and 2., it follows that the Schrödinger equation can be at most a first-order differential equation in t and that it has to be linear:

$$\mathrm{i}\frac{\partial}{\partial t}\psi = A\psi \tag{0.1}$$

where A is a linear operator.
From 3. we obtain $\frac{\partial}{\partial t}\langle\psi,\psi\rangle = 0 \Rightarrow \left\langle\frac{\partial\psi}{\partial t},\psi\right\rangle + \left\langle\psi,\frac{\partial\psi}{\partial t}\right\rangle = 0 \Rightarrow \langle -\mathrm{i}A\psi,\psi\rangle + \langle\psi,-\mathrm{i}A\psi\rangle = 0 \Rightarrow$ $\mathrm{i}\langle A\psi,\psi\rangle - \mathrm{i}\langle\psi,A\psi\rangle = 0 \Rightarrow \langle A\psi,\psi\rangle = \langle\psi,A\psi\rangle\ \forall\psi\in L^2\left(\mathbb{R}^3\right) \overset{\text{Exercise 2}}{\Rightarrow} \langle A\psi,\varphi\rangle = \langle\psi,A\varphi\rangle\ \forall\varphi,\psi\in L^2\left(\mathbb{R}^3\right)$. So A has to be a symmetric operator.
To assure that the initial-value problem

$$\left\{\begin{array}{l}\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\varphi_t = H\varphi_t \\ \varphi_t\big|_{t=0} = u\end{array}\right\}. \tag{0.2}$$

has exactly one solution for all $\psi_0 \in L^2\left(\mathbb{R}^3\right)$, we actually need a self-adjoint operator A (more than symmetric).

Definition 0.1 (Banach and Hilbert spaces)
Let X be a vector space with a norm $\|\cdot\|$ (respectively inner product $\langle\cdot,\cdot\rangle$). X is called a *Banach space* (respectively *Hilbert space*) if it is complete (every Cauchy sequence converges) with respect to the norm (respectively inner product). If in addition X is a complex vector space, then X is called a *complex Banach space* (respectively *complex Hilbert space*).

Example 0.1
$L^2\left(\mathbb{R}^3\right) := \left\{\psi : \mathbb{R}^3 \to \mathbb{C}, \int |\psi|^2\,\mathrm{d}x < \infty\right\}$ equipped with the inner product $\langle\psi,\varphi\rangle := \int_{\mathbb{R}^3} \overline{\psi(x)}\varphi(x)\,\mathrm{d}x$ is a complex Hilbert space and therefore a complex Banach space (see e.g. [1]).

Example 0.2
Let $X := \left\{\varphi \in L^2(\mathbb{R}) : \varphi \in C^1(\mathbb{R}) \text{ and } \varphi' \in L^2(\mathbb{R})\right\}$ with norm $\|\varphi\|_X := \|\varphi\|_{L^2} + \left\|\varphi'\right\|_{L^2}$. Then X is not a Banach space. See Exercise 8.

Hint: Let $u_n(x) := \exp\left(-\left(\frac{1}{n}+|x|^2\right)^{\frac{1}{2}}\right)$. Then u_n is a Cauchy sequence in X and not convergent in X. Indeed, if $u_n \to u$ in X for some $u \in X$, then $u_n \to u$ in L^2. But $u_n \to \exp(-|x|)$ in L^2, so $u(x) = \exp(-|x|)$. But $u \notin X$ because $u \notin C^1(\mathbb{R})$, therefore X is not complete.

1 Weak derivatives and Sobolev spaces

We will use the notation $C_c^\infty(\mathbb{R}^n) := \{\phi : \mathbb{R}^n \to \mathbb{C} : \phi \in C^\infty(\mathbb{R}^n) \text{ and } \operatorname{supp}(\phi) \text{ is compact}\}$, where $\operatorname{supp}(\phi) = \overline{\{x \in \mathbb{R}^n : \phi(x) \neq 0\}}$. A $\phi \in C_c^\infty(\mathbb{R}^n)$ is called a *test function*.

Example 1.1

Let $f : \mathbb{R} \to \mathbb{R}$, $f(x) = \begin{cases} \mathrm{e}^{-\frac{1}{x^2}} & , x > 0 \\ 0 & , x \leq 0 \end{cases}$. Then $f \in C^\infty(\mathbb{R})$ (proof by induction) and $g \in C_c^\infty(\mathbb{R})$, where $g(x) := f(x)f(1-x)$.

We write $L^p(X) := \left\{\phi : X \to \mathbb{C} : \int_X |\phi|^p < \infty\right\}$
and $L^1_{\text{loc}}(\mathbb{R}^n) := \left\{\phi : \mathbb{R}^n \to \mathbb{C} : \phi \in L^1(K) \text{ for all closed and bounded subsets } K \subseteq \mathbb{R}^n\right\}$.

Example 1.2

(i) Let $\phi(x) := \mathrm{e}^{x^2}$. Then $\phi \in L^1_{\text{loc}}(\mathbb{R})$ because ϕ is bounded on bounded closed sets (as a continuous function) and thus $\int_K |\phi| < \infty$ for all closed and bounded $K \subseteq \mathbb{R}$.

(ii) Let $f(x) := \dfrac{1}{|x|}$. Then $f \notin L^1_{\text{loc}}(\mathbb{R})$, since $f \notin L^1([-1, 1])$.

If $\alpha = (\alpha_1, \ldots, \alpha_n)$, we write $\partial^\alpha := \partial_{x_1}^{\alpha_1} \ldots \partial_{x_n}^{\alpha_n}$ and $|\alpha| := \alpha_1 + \ldots + \alpha_n$.
Let $u \in C_c^\infty(\mathbb{R}^n)$. Then we have $\forall \phi \in C_c^\infty(\mathbb{R}^n) : \int u \partial^\alpha \phi \, \mathrm{d}x = (-1)^{|\alpha|} \int (\partial^\alpha u) \phi \, \mathrm{d}x$ by integration by parts (IBP). In fact, if $u, v \in C_c^\infty(\mathbb{R}^n)$, then $\omega = \partial^\alpha u$ if and only if

$$\forall \phi \in C_c^\infty(\mathbb{R}^n) : \int_{\mathbb{R}^n} u \partial^\alpha \phi \, \mathrm{d}x = (-1)^{|\alpha|} \int_{\mathbb{R}^n} \omega \phi \, \mathrm{d}x \,. \tag{1.1}$$

Definition 1.1

Let $u, v \in L^1_{\text{loc}}(\mathbb{R}^n)$. We say that $\omega = \partial^\alpha u$ is the *α-th weak partial derivative of u* if equation (1.1) holds.

Example 1.3

Let $u : \mathbb{R} \to \mathbb{R}$, $u = \exp(-|x|) = \mathrm{e}^{-|x|}$. Then in the sense of weak derivatives $u'(x) = \frac{x}{|x|}\mathrm{e}^{-|x|}$. Indeed, let $\phi \in C_c^\infty(\mathbb{R})$, then $\operatorname{supp}(\phi) \subseteq [-M, M]$ for some $M > 0$. We have

$$\begin{aligned}\int_{\mathbb{R}} u\phi' \,\mathrm{d}x &= \int_{-M}^{M} u\phi' \,\mathrm{d}x = \int_{-M}^{0} u\phi' \,\mathrm{d}x + \int_{0}^{M} u\phi' \,\mathrm{d}x \\ &= \int_{-M}^{0} \mathrm{e}^{x}\phi' \,\mathrm{d}x + \int_{0}^{M} \mathrm{e}^{-x}\phi' \,\mathrm{d}x \overset{\text{IBP}}{=} \int_{-M}^{0} (-\mathrm{e}^{x})\phi \,\mathrm{d}x + \int_{0}^{M} \mathrm{e}^{-x}\phi \,\mathrm{d}x \\ &= \int_{-M}^{M} \frac{x}{|x|}\mathrm{e}^{-|x|}\phi \,\mathrm{d}x = \int_{\mathbb{R}} \frac{x}{|x|}\mathrm{e}^{-|x|}\phi \,\mathrm{d}x\,,\end{aligned}$$

verifying equation (1.1).

Proposition 1.2

If $u \in L^1_{\mathrm{loc}}(\mathbb{R}^n)$ has a weak derivative then it is unique.

Definition 1.3 (Sobolev space)

Let $k \in \mathbb{N}$. $H^k(\mathbb{R}^n) := \left\{u \in L^2(\mathbb{R}^n) : \partial^\alpha u \in L^2(\mathbb{R}^n)\ \forall \alpha \text{ with } |\alpha| \le k\right\}$ equipped with the norm $\|u\|_{H^k(\mathbb{R}^n)} := \left(\sum_{|\alpha|\le k} \|\partial^\alpha u\|_{L^2}^2\right)^{\frac{1}{2}}$ is called *Sobolev space of order k*.

Example 1.4

Let u be as in Example 1.3. Then $u(x) = \mathrm{e}^{-|x|}$, so $u \in L^2(\mathbb{R})$, $u' = \frac{x}{|x|}\mathrm{e}^{-|x|}$, and $u' \in L^2(\mathbb{R})$. Therefore, $u \in H^1(\mathbb{R})$. (Exercise 8: $u_n = \exp\left(-\left(\frac{1}{n} + |x|^2\right)^{\frac{1}{2}}\right) \to u$ in $H^1(\mathbb{R})$.)

Theorem 1.4

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

Theorem 1.5 (Completeness)

$H^k(\mathbb{R}^n)$ equipped with the norm $\|\cdot\|_{H^k(\mathbb{R}^n)}$ is a Banach space (without proof).

Theorem 1.6

If $u \in H^k(\mathbb{R}^n)$ there exists a sequence of functions $(u_n)_{n\in\mathbb{N}}$ in $C_c^\infty(\mathbb{R}^n)$ with $u_n \to u$ in $H^k(\mathbb{R}^n)$

(without proof). So $H^k(\mathbb{R}^n)$ is the smallest possible complete space containing $C_c^\infty(\mathbb{R}^n)$.

2 Unbounded operators, spectrum, and resolvent

Let $(X, \|\cdot\|)$ be a complex Banach space, $D \subseteq X$ a subspace of X. Let $A : D \to X$ be a linear operator. If $\overline{D} = X$, then A is called *densely defined*.
The *range* (or *image of* A is defined as $\operatorname{Ran}(A) := \{Ax : x \in D\}$.
The *kernel of* A is the inverse image of $\{0\}$: $\operatorname{Ker}(A) := \{x \in D : Ax = 0\}$.
A is called *bounded* if $\|A\| := \{\sup\|Ax\| : x \in D, \|x\| = 1\} < \infty$, otherwise A is called *unbounded*.

Remark
A is bounded $\Rightarrow$ $\|A\| = \sup\left\{\frac{\|Ax\|}{\|x\|} : x \in D, x \neq 0\right\} < \infty$ $\Rightarrow$ $\forall x \in X : \|Ax\| \leq \|A\|\|x\|$ $\Rightarrow$ $\|A(x-y)\| \leq \|A\|\|x-y\|$ $\Rightarrow$ A is Lipschitz continuous $\Rightarrow$ A is continuous.
The converse directions are also true for linear operators A.

Example 2.1
Let $A : H^2(\mathbb{R}^3) \subseteq L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$, $\quad A = -\Delta + \mathrm{i}$.
A is linear and densely defined because $\overline{H^2(\mathbb{R}^3)} = L^2(\mathbb{R}^3)$.
A is not bounded:
Let $\psi \in C_c^\infty(\mathbb{R}^3)$ with $\|\psi\|_{L^2} = 1$. Consider $(\psi_n)_{n\in\mathbb{N}}$, $\psi_n(x) = n^{\frac{3}{2}}\psi(nx)$. Then

$$\|\psi_n\|_{L^2}^2 = \int_{\mathbb{R}^3} n^3|\psi(nx)|^2 \,\mathrm{d}x \overset{y=nx}{=} \int_{\mathbb{R}^3} |\psi(y)|^2 \,\mathrm{d}y = 1.$$

For Ax we have

$$\|Ax\| = \|(-\Delta + \mathrm{i})\psi_n\| \geq \|-\Delta\psi_n\| - \|\psi_n\| = \|\Delta\psi_n\| - 1. \tag{2.1}$$

Furthermore $(\Delta\psi_n)(x) \overset{\text{chain rule}}{=} n^{\frac{3}{2}} n^2 (\Delta\psi)(nx)$.
Therefore $\|\Delta\psi_n\|_{L^2}^2 = n^4 \int_{\mathbb{R}^3} n^3 |(\Delta\psi)(nx)|^2 \,\mathrm{d}x = n^4\|\Delta\psi\|^2$ by repetition of the previous transformation argument. Thus, $\|\Delta\psi_n\|_{L^2} \to \infty$ and therefore by equation (2.1) and $\|\psi_n\| = 1$ we have that $\|A\psi_n\| \to \infty$. So A is unbounded.

We find that $\operatorname{Ker}(A) = \{0\}$ because if $A\psi = 0$, then $(-\Delta + \mathrm{i})\psi = 0 \overset{\text{F.T.}}{\Rightarrow} (|\xi|^2 + \mathrm{i})\hat{\psi}(\xi) = 0 \Rightarrow \hat{\psi} = 0 \Rightarrow \psi = 0$.
The image/range of A is $\operatorname{Ran}(A) = L^2(\mathbb{R}^3)$: Let $f \in L^2(\mathbb{R}^3)$. We will find a $g \in H^2$ with $Ag = (-\Delta + \mathrm{i})g = f$. We have $(-\Delta + \mathrm{i})g = f \Leftrightarrow (|\xi|^2 + \mathrm{i})\hat{g}(\xi) = \hat{f}(\xi) \Leftrightarrow \hat{g}(\xi) = \dfrac{\hat{f}(\xi)}{|\xi|^2 + \mathrm{i}}$.
$g \in H^2$ because

$$\|g\|_{H^2}^2 = \int_{\mathbb{R}^3} \left(1 + |\xi|^2\right)^2 |\hat{g}(\xi)|^2 \,\mathrm{d}x\, i = \int_{\mathbb{R}^3} \left(1 + |\xi|^2\right)^2 \frac{\left|\hat{f}(\xi)\right|^2}{|\xi|^4 + 1} \,\mathrm{d}x\, i \le C \int_{\mathbb{R}^3} \left|\hat{f}(\xi)\right|^2 \mathrm{d}x\, i < \infty$$

for some $C < \infty$. Thus, $\operatorname{Ran}(A) = L^2(\mathbb{R}^3)$. In particular, $A = -\Delta + \mathrm{i} : H^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ is a bijection. This will help us prove that Δ is self-adjoint later.

Definition

Let $A : D \subseteq X \to X$ be a linear 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 $\|\phi\|_A = \|\phi\| + \|A\phi\|$.
This is equivalent to the following statement: For all sequences $(x_n)_{n\in\mathbb{N}}$ in D and $x \in X$, if $\|x_n - x\| \to 0$ and $\|y - Ax - n\| \to 0$ for some $y \in X$, we have that $x \in D$ and $y = Ax$.

For bounded (continuous) linear operators, $x_n \to x$ implies $Ax_n \to Ax$.
For closed linear operators, we have: if $x_n \to x$ and Ax_n converges to some y, then $y = Ax$.

Example 2.2

Let $A : H^2(\mathbb{R}^3) \subseteq L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$, $\quad A = -\Delta$.
Then A is closed because if $(f_n)_{n\in\mathbb{N}} \subseteq H^2(\mathbb{R}^3)$ and $f_n \to f$ in L^2 and $-\Delta f_n \to g$ in L^2 for some $g \in L^2$, then f is Cauchy in the graph norm given by $\|u\|_A = \|u\|_{L^2} + \|\Delta u\|_{L^2} \approx \|u\|_{H^2}$, where $\approx$ denotes the equivalence of the two norms.
But H^2 is complete, so f_n converges to h for some $h \in H^2$. Thus, $f = h \in H^2$ and $f_n \to f$ in H^2. Therefore, $-\Delta f_n \to -\Delta f$, so $-\Delta f = g$.

Proposition (Exercise 5)

(a) Let $(X, \|\cdot\|)$ be a Banach space, $A : D \subseteq X \to X$ closed, and $g : [0, T] \to (D, \|\cdot\|_A)$ for some $T > 0$. Then $A \displaystyle\int_0^T g(t)\,\mathrm{d}t = \int_0^T Ag(t)\,\mathrm{d}t$.

(b) If $A = -\Delta$ and $g : [0, T] \to H^2(\mathbb{R}^3)$ is continuous, then $-\Delta \displaystyle\int_0^T g(t)\,\mathrm{d}t = \int_0^T -\Delta g(t)\,\mathrm{d}t$.

Definition (Resolvent and spectrum)

The *resolvent set of* A is defined as:

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

Let $\mathcal{L}(X) := \{T : X \to X : T \text{ is linear and bounded}\}$.

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

Example 2.3

Let $A : H^2(\mathbb{R}^3) \subseteq L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$, $A = \Delta$. Then $\mathrm{i} \in \rho(A)$ because $(\Delta - \mathrm{i})$ is a projection (in Example 2.1 we proved that $\operatorname{Ker}(\Delta - \mathrm{i}) = \{0\}$ and $\operatorname{Ran}(\Delta - \mathrm{i}) = L^2(\mathbb{R}^3)$).
Since $\left\|(\mathrm{i}\Delta)^{-1} f\right\|_{L^2} \leq \left\|(\mathrm{i}-\Delta)^{-1} f\right\|_{H^2} \leq C\|f\|_{L^2}$, it follows that $(\mathrm{i}-\Delta)^{-1}$ is bounded.

Lemma 2.1

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.

(without proof)

Lemma 2.2

Let $K \in \mathcal{L}(X)$. If $\|K\| := \sup\{\|Kx\| : \|x\| = 1\} < 1$, then the operator $I + K$ is invertible and $(I+K)^{-1} = \sum_{k=0}^{\infty} (-K)^n$ (Exercise 7).

Theorem 2.3

Let X be a Banach space, $D \subseteq X$ a subspace, and $A : D \to X$. Then:

1. $\rho(A)$ is open.

2. $\sigma(A)$ is closed.

3. The resolvent R_A is analytic in $\rho(A)$. More precisely, if $z_0 \in \rho(A)$, then $B\left(z_0, \frac{1}{\|R_A(z_0)\|}\right) \subseteq \rho(A)$[1] and

[1] $B(z_0, R) = \{x \in X : \|x - z_0\| < R\}$

$$\forall z \in B\left(z_0, \frac{1}{\|R_A(z_0)\|}\right) : R_A(z) = \sum_{n=0}^{\infty}(-1)^n R_A(z_0)^{n+1}(z-z_0)^n.$$

In particular, $\|R_A(z_0)\| \geq \dfrac{1}{\operatorname{dist}(z_0, \sigma(A))}$, with $\operatorname{dist}(z_0, \sigma(A)) := \inf\{|z-y| : y \in \sigma(A)\}$.

Proof. Let $z \in \mathbb{C}$. Then

$$z - A = z_0 - A + (z - z_0) = (1 + (z-z_0)R_A(z_0))(z_0 - A). \tag{2.2}$$

By Lemma 2.2 the operator $1 + (z-z_0)R_A(z_0)$ is invertible if $\|(z-z_0)R_A(z_0)\| < 1$ $\Leftrightarrow |z - z_0| < \dfrac{1}{\|R_A(z_0)\|}$. So $B\left(z_0, \dfrac{1}{\|R_A(z_0)\|}\right) \subseteq \rho(A)$, and hence $\rho(A)$ is open and $\sigma(A)$ is closed.

If equation (2.2) holds we thus have: $(z-A)^{-1} = (z_0 - A)^{-1}(1 + (z-z_0)R_A(z_0))^{-1}$
$= R_A(z_0)\sum_{n=0}^{\infty}(-(z-z_0)R_A(z_0))^n = \sum_{n=0}^{\infty}(-1)^n R_A(z_0)^{n+1}(z-z_0)^n.$

Now consider $z \in \sigma(A)$. Then $z - A$ is not invertible, and by equation (2.2) $1+(z-z_0)R_A(z_0)$ is not invertible. So $\|(z-z_0)R_A(z_0)\| \geq 1 \Rightarrow |z - z_0| \geq \dfrac{1}{\|R_A(z_0)\|} \Rightarrow \inf_{z\in\sigma(A)} |z-z_0| \geq \dfrac{1}{\|R_A(z_0)\|}$. ■

Theorem 2.4

Let $V : \mathbb{R}^d \to \mathbb{C}$ be a continuous function and $D := \left\{f \in L^2\left(\mathbb{R}^d\right) : V \cdot f \in L^2\left(\mathbb{R}^d\right)\right\}$,
$T_V : D \to L^2\left(\mathbb{R}^d\right)$, $(T_V f)(x) := V(x) \cdot f(x)$.
Then $\sigma(T_V) = \overline{\operatorname{Ran}(V)}$. In particular, if V is real-valued, then $\sigma(T_V) \subseteq \mathbb{R}$.

Proof. To prove this, it is sufficient to show

1. If $z \notin \overline{\operatorname{Ran}(V)}$, then $z \in \rho(T_V)$.
2. If $z \in \overline{\operatorname{Ran}(V)}$, then $z \in \sigma(T_V)$.

From 1. it follows that $\overline{\operatorname{Ran}(V)}^C \subseteq \rho(T_V)$, i.e. $\overline{\operatorname{Ran}(V)} \supseteq \sigma(T_V)$. We will only show 1. (2. was shown in Exercise 9): Let $z \notin \overline{\operatorname{Ran}(V)}$.

(i) $z - T_V$ is injective. Indeed $(z - T_V)(f) = 0 \Leftrightarrow (z - V(x))f(x) = 0$, so either $z - V(x) = 0$ or $f(x) = 0\, \forall x$. But since $z \notin \overline{\operatorname{Ran}(V)}$, we must have $f \equiv 0$ and thus $\operatorname{Ker}(z - T_V) = \{0\}$.

(ii) $\operatorname{Ran}(z - T_V) = L^2\left(\mathbb{R}^d\right)$. Consider a function $g \in L^2\left(\mathbb{R}^d\right)$. We want to find a function $f \in D$ such that $(z - T_V)f = g \Leftrightarrow (z - V(x))f(x) = g(x)$. Since $z - V(x) \neq 0$, we find

$$f(x) = \frac{g(x)}{z - V(x)}. \tag{2.3}$$

Since $z \notin \overline{\operatorname{Ran}(V)}$, there exists an $\varepsilon > 0$ such that $\forall x \in \mathbb{R}^d : |z - V(x)| \geq \varepsilon$. From equation (2.3) it follows that $|f(x)| = \frac{|g(x)|}{|z - V(x)|} \leq \frac{|g(x)|}{\varepsilon}$, so $\|f\|_2 \leq \frac{|g(x)|}{\varepsilon} < \infty$, and hence $f \in L^2\left(\mathbb{R}^d\right)$. Thus, we find $V(x)f(x) = zf(x) - g(x)$, so $V \cdot f \in L^2\left(\mathbb{R}^d\right)$ and $f \in D$. Finally, since $(z - T_V)^{-1}g = f$, we have $\left\|(z - T_V)^{-1}g\right\|_2 = \|f\|_2 \, \forall g \in L^2\left(\mathbb{R}^d\right)$. So $\left\|(z - T_V)^{-1}g\right\|_2 \leq \frac{\|g\|_2}{\varepsilon}$, hence $(z - T_V)^{-1} : L^2\left(\mathbb{R}^d\right) \to L^2\left(\mathbb{R}^d\right)$ is bounded.

■

Remark

For $V : \mathbb{R}^d \to \mathbb{C}$ measurable (not necessarily continuous) the multiplication operator T_V is defined as well and $\sigma(T_V) = \operatorname{ess\,sup}(V) := \left\{y \in \mathbb{C} : \forall \varepsilon > 0 : \mu(V^{-1}(B(y, \varepsilon))) > 0\right\}$, where μ is the Lebesgue measure.

Example 2.4

Let $V : \mathbb{R}^d \to \mathbb{R}$, $V(x) := |x|^2$. Then by Theorem 2.3 $\sigma(T_V) = \operatorname{Ran}(V) = [0, \infty)$.

Theorem 2.5

Let $A : H^2\left(\mathbb{R}^d\right) \to L^2\left(\mathbb{R}^d\right)$ be defined as $Af = -\Delta f$. Then $\sigma(-\Delta) = [0, \infty)$.

Proof. Denote by $\mathcal{F}$ and $\mathcal{F}^{-1}$ the Fourier transform on $\mathbb{R}^d$ and its inverse. Then $\mathcal{F}(-\Delta f)(\xi) = |\xi|^2 \hat{f}(\xi) \Rightarrow -\Delta = \mathcal{F}^{-1}|\xi|^2\mathcal{F}$. Hence, $z - (-\Delta) = \mathcal{F}^{-1}(z - |\xi|)\mathcal{F} \Rightarrow z - (-\Delta)$ is invertible $\Leftrightarrow z - |\xi|^2$ is invertible for all $\xi \Leftrightarrow z \notin [0, \infty)$. ■

Definition 2.6

Let X be a Banach space, $D_1, D_2 \subseteq X$ subspaces, and $A : D_1 \to X$, $B : D_2 \to X$ linear operators. We say that B is an *extension* of A if $D_1 \subseteq D_2$ and $\forall x \in D_1 : Ax = Bx$. We write $A \subset B$ in this case.

Definition 2.7

Let X be a Banach space, $D \subseteq X$ a subspace, and $A : D \to X$ a linear operator. A is called *closable* if there exists an extension B that is closed.

Example 2.5

Let $A : C_c^\infty(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$, $B : H^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ be defined as $Af = -\Delta f$, $Bf = -\Delta f$.

Then $A \subset B$.

Theorem 2.8

Let X be a Banach space, $D \subseteq X$ a subspace and $A : D \to X$ a linear operator. Then the following are equivalent:

1. A is closable.
2. $\overline{\Gamma_A}$ is a graph of a linear operator (which we denote by $\overline{A}$).
3. If $(x_n)_{n\in\mathbb{N}}$ is a sequence in D with $x_n \to 0$ and $Ax_n \to y$ for some $y \in X$, then $y = 0$.

Proof.

- 1. $\Rightarrow$ 3.: Let $A \subset B$ for some closed operator B. Consider a sequence $(x_n)_n$ in D with $x_n \to 0$ and $Ax_n \to y \in X$. We need to show that $y = 0$. Since B is an extension of A, we have $Bx_n \to y$, and since B is closed it follows that $y = B \cdot 0 = 0$.
- 3. $\Rightarrow$ 2.: Consider $(x, y_1), (x, y_2) \in \overline{\Gamma_A} \Rightarrow (0, y_1 - y_2) \in \overline{\Gamma_A}$. Thus, there exists a sequence $(x_n, Ax_n)_n$ in Γ_A with $x_n \to 0$ and $Ax_n \to y_1 - y_2 \overset{3.}{\Rightarrow} y_1 - y_2 = 0 \Rightarrow y_1 = y_2$.

  We define the domain of B by $D(B) := \{x \in X : \exists y \in X \text{ such that } (x, y) \in \overline{\Gamma_A}\}$ and $B : D(B) \to X$, $Bx = y$ for $(x, y) \in \overline{\Gamma_A}$. B is well-defined by the argument presented above. B is linear and $\Gamma_B = \overline{\Gamma_A}$. Furthermore, $D(B) \supseteq D = D(A)$.
- By assumption, there exists a linear operator B with $\Gamma_B = \overline{\Gamma_A}$. Thus, B is closed and $A \subset B$.

■

Example 2.6

Let $X = L^2(\mathbb{R})$, $g \in X$ with $\|g\|_2 = 1$. Define $A : C_c(\mathbb{R}) \to X$, $(Af)(x) = f(0) \cdot g(x)$.
Then A is linear, but not closable. Indeed, consider the sequence $f_n(x) = f(nx), n \in \mathbb{N}$. Then $f_n \in C_c(\mathbb{R})\, \forall n$ and $\forall n : f_n(0) = f(0), Af_n = Af$.
We have $\displaystyle\int_{\mathbb{R}} |f_n(x)|^2 \,\mathrm{d}x = \int_{\mathbb{R}} |f(nx)|^2 \,\mathrm{d}x \overset{y=nx}{=} \frac{1}{n} \int_{\mathbb{R}} |f(x)|^2 \,\mathrm{d}x$. But $\|f_n\|_2 = \dfrac{1}{n}\|f\|_2 \to 0$ as $n \to \infty$, so $f_n \to 0$ in L^2.

3 Symmetric and self-adjoint operators

In this chapter let $\mathcal{H}$ be a complex Hilbert space and $A : D(A) \subseteq \mathcal{H} \to \mathcal{H}$ a densely defined linear operator. If for some $\phi \in \mathcal{H}$ there exists one and only ϕ^* such that $\langle \phi, A\psi \rangle = \langle \phi^*, \psi \rangle \ \forall \psi \in D(A)$, then $\phi \in D(A^*)$ and $A^*\phi = \phi^*$. The operator A^* is called the *adjoint* of A.

Remark

If such a ϕ^* exists, then it is unique.

Indeed, if $\langle \phi^*, \psi \rangle = \left\langle \tilde{\phi}^*, \psi \right\rangle \ \forall \psi \in D(A)$, then $\forall \psi \in D(A) : \left\langle \phi^* - \tilde{\phi}^*, \psi \right\rangle = 0$ $\Rightarrow \forall \psi \in \overline{D(A)} = \mathcal{H} : \left\langle \phi^* - \tilde{\phi}^*, \psi \right\rangle = 0 \Rightarrow \tilde{\phi}^* = \phi^*$. So A^* is well-defined only if A is densely defined. Similarly, $A^{**} = (A^*)^*$ is well-defined only if A^* is densely defined, which is not always the case.

For $\phi \in \mathcal{H}$ let $T_\phi : D(A) \to \mathbb{C}$, $T_\phi(\psi) = \langle \phi, A\psi \rangle$.

Lemma 3.1

We have $D(A^*) = \{\phi \in \mathcal{H} : T_\phi \text{ is continuous in } D(A)\}$ (here we are considering $D(A)$ with respect to the topology induced by the inner product of $\mathcal{H}$).

Proof. If $\phi \in D(A^*)$, then there exists one (and only one) $\phi^* \in \mathcal{H}$ with $\forall \psi \in D(A) : T_\phi(\psi) = \langle \phi^*, \psi \rangle$, so $\|T_\phi(\psi)\| \leq C\|\psi\|$, where $C = \|\phi^*\| = \sqrt{\langle \phi^*, \phi^* \rangle}$. Thus, T_ϕ is continuous. If T_ϕ is continuous on $D(A)$, then since $\overline{D(A)} = \mathcal{H}$, by the Riesz representation theorem there exists one and only one $\phi^* \in \mathcal{H}$ with $T_\phi(\psi) = \langle \phi^*, \psi \rangle \ \forall \psi \in D(A)$, so $\phi \in D(A^*)$. ■

Example 3.1

Let $\mathcal{H} = L^2(\mathbb{R})$, $g \in \mathcal{H}$ with $\|g\| = 1$. Let $A : C_c(\mathbb{R}) \subseteq \mathcal{H} \to \mathcal{H}$ be defined by $Af = f(0)g$.

Then $D(A^*) = \{\varphi \in \mathcal{H} : \varphi \perp g\}$ and $A^* = 0$ in $D(A^*)$. Indeed, if $\langle \varphi, g \rangle = 0$, then $\forall f \in \mathbb{C}_c(\mathbb{R}) : \langle \varphi, Af \rangle = \langle \varphi, f(0)g \rangle = f(0) \langle \varphi, g \rangle = 0$. Thus, $\forall f \in C_c(\mathbb{R}) : \langle \varphi, Af \rangle = 0 = \langle 0, f \rangle$. Therefore, $\varphi \in D(A^*)$ and $A^*\varphi = 0$.

Exercise 10: If $A \subset B$, then $B^* \subset A^*$.

Exercise 11: If $\langle \varphi, g \rangle \neq 0$, then $\varphi \notin D(A^*)$.

Theorem 3.2

1.) A^* is closed.

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

3.) A is closable if and only if A^* is densely defined. In this case $\overline{A} = (A^*)^*$.

Proof. 1. Suppose that $(x_n)_{n\in\mathbb{N}}$ in $D(A^*)$ with $x_n \to x$ and $Ax_n \to y$ for some $x, y \in \mathcal{H}$. Then we have $\forall \varphi \in D(A) : \langle x, A\varphi \rangle = \lim_{n\to\infty} \langle x_n, A\varphi \rangle \stackrel{x\in D(A^*)}{=} \lim_{n\to\infty} \langle A^* x_n, \varphi \rangle = \langle y, \varphi \rangle$.
Thus $x \in D(A^*)$ and $A^* x = y$.

2. If A is closable then (since $A \subset \overline{A}$) we have $(\overline{A})^* \subset A^*$. It therefore suffices to prove that $D(A^*) \subseteq D\left(\overline{A}^*\right)$. Let $x \in D(A^*)$ and $\varphi \in D\left(\overline{A}\right)$. Then there exists a sequence $(\varphi_n)_{n\in\mathbb{N}} \subseteq D(A)$ with $\varphi_n \to \varphi$ and $A\varphi_n \to \overline{A}\varphi$. Then $\left\langle x, \overline{A}\varphi \right\rangle = \lim_{n\to\infty} \langle x, A\varphi_n \rangle \stackrel{x\in D(A^*)}{=} \lim_{n\to\infty} \langle A^* x, \varphi_n \rangle = \langle A^* x, \varphi \rangle$. Thus, $\forall \varphi \in D\left(\overline{A}\right) : \left\langle x, \overline{A}\varphi \right\rangle = \langle A^* x, \varphi \rangle$. It follows that $x \in D\left((\overline{A})^*\right)$, so $D(A^*) \subseteq D\left(\overline{A}^*\right)$, as desired.

3. "$\Leftarrow$": Suppose that A^* is densely defined. Assume that $(x_n)_{n\in\mathbb{N}}$ in $D(A)$ with $x_n \to 0$ and $Ax_n \to y$. Then we have

$$\forall \psi \in D(A^*) : \langle \psi, y \rangle = \lim_{n\to\infty} \langle \psi, Ax_n \rangle \stackrel{\psi\in D(A^*)}{=} \lim_{n\to\infty} \langle A^*\psi, x_n \rangle \stackrel{x_n\to 0}{=} 0.$$

Since $D(A^*)$ is dense it follows that $y = 0$.

"$\Rightarrow$": See [2] Theorem VIII.1.

■

Theorem 3.3

$\mathrm{Ker}(A^*) = \mathrm{Ran}(A)^\perp$. Thus, $\mathrm{Ran}(A) \subseteq D(A^*)$ and $\ker A^* = \{0\}$ if and only if $\overline{\mathrm{Ran}(A)} = \mathcal{H}$.

Proof. $\varphi \in \ker A^* \Leftrightarrow A^*\varphi = 0 \Leftrightarrow \forall \psi \in D(A) : \langle A^*\varphi, \psi \rangle = 0 \Leftrightarrow \forall \psi \in D(A) : \langle \varphi, A\psi \rangle = 0$
$\Leftrightarrow \varphi \in \mathrm{Ran}(A)^\perp$. ■

Definition 3.4

A linear operator A (densely defined) is called *symmetric* if $A \subset A^*$. It is called *self-adjoint* if $A = A^*$.

Remark

$A \subset A^* \Leftrightarrow D(A) \subseteq D(A^*)$ and $\forall \varphi \in D(A) : A^*\varphi = A\varphi \Leftrightarrow \forall \varphi \in D(A) : \langle \varphi, A\psi \rangle = \langle A\psi, \varphi \rangle$.
A is self-adjoint if and only if A is symmetric and $D(A) = D(A^*)$.

Remark

From Definition 3.4 and 1. of Theorem 3.2 it follows that self-adjoint operators are closed.

Example 3.2

Let $B : C_c^\infty(\mathbb{R}^n) \subseteq L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ be defined as $B\varphi = -\Delta\varphi$. B is symmetric because for all $\varphi, \psi \in C_c^\infty(\mathbb{R}^n)$ we have

$$\langle \psi, B\varphi \rangle = \int_{\mathbb{R}^n} \overline{\psi(x)}(-\Delta\varphi)(x)\,\mathrm{d}x \overset{\text{IBP}}{=} \int_{\mathbb{R}^n} \overline{(-\Delta\psi)(x)}\varphi(x)\,\mathrm{d}x = \langle B\psi, \varphi \rangle$$

by integration by parts (IBP). Similarly, $A : H^2(\mathbb{R}^n) \subseteq L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$, $A\varphi = -\Delta\varphi$ is symmetric because of the same relation and the fact that $\overline{C_c^\infty(\mathbb{R}^n)} = H^2(\mathbb{R}^n)$.

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

Theorem 3.5

Let $A : D(A) \subseteq \mathcal{H} \to \mathcal{H}$ be a symmetric operator.

1. For all $\lambda, \mu \in \mathbb{R}$ and $\phi \in D(A)$ we have

$$\|(A - \lambda - \mathrm{i}\mu)\phi\|^2 = \|(A - \lambda)\phi\|^2 + \mu^2\|\phi\|^2. \tag{3.1}$$

2. a) If $\mathrm{Ran}(A - z_+) = \mathcal{H}$ for one $z_+ \in \mathbb{C}_+$, then $\mathbb{C}_+ \subseteq \rho(A)$.

   b) If $\mathrm{Ran}(A - z_-) = \mathcal{H}$ for one $z_- \in \mathbb{C}_-$, then $\mathbb{C}_- \subseteq \rho(A)$.

Proof. 1.
$$\begin{aligned}\|(A - \lambda - \mathrm{i}\mu)\phi\|^2 &= \langle (A - \lambda - \mathrm{i}\mu)\phi, (A - \lambda - \mathrm{i}\mu)\phi \rangle \\ &= \|(A - \lambda)\phi\|^2 + \mu^2\|\phi\|^2 + \underbrace{\langle (A - \lambda)\phi, -\mathrm{i}\mu\phi \rangle}_{=0,\text{ since } A \text{ is symmetric}}.\end{aligned}$$

2. We will prove (a), (b) can be proven analogously:

   a) Equation (3.1) implies that $\|(A - z_+)\phi\| \geq |\mathrm{Im}(z_+)|\|\phi\|$. If $(A - z_+)\phi = 0$, then $\|\phi\|^2 = 0 \Rightarrow \phi = 0 \Rightarrow A - z_+$ is 1-1 (injective). By assumption, it is onto. If $\psi = (A - z_+)\phi$, then $\|\psi\| \geq |\mathrm{Im}(z_+)|\|\phi\| \Rightarrow \|\phi\| \leq \dfrac{\|\psi\|}{|\mathrm{Im}(z_+)|} \Rightarrow \left\|(A - z_+)^{-1}\psi\right\| \leq$

$\frac{\|\psi\|}{|\mathrm{Im}(z_+)|} \Rightarrow (A - z_+)^{-1}$ is bounded. Thus $z_+ \in \rho(A)$ and $\left\|(A - z_+)^{-1}\right\| \leq \frac{1}{|\mathrm{Im}(z_+)|}$. By Theorem 2.3 $B\left(z_+, \left\|(A - z_+)^{-1}\right\|^{-1}\right) \subseteq \rho(A) \Rightarrow B(z_+, |\mathrm{Im}(z_+)|) \subseteq \rho(A)$. Iterating this argument for some $z'_+ \in B(z_+, |\mathrm{Im}(z_+)|) \in \rho(A)$ we can prove that $\mathbb{C}_+ \subseteq \rho(A)$.

■

Theorem 3.6 (Basic criterion of self-adjointness)
Let A be a symmetric operator. Then the following are equivalent:

1. $A = A^*$.
2. $\sigma(A) \subseteq \mathbb{R}$.
3. $\mathrm{Ran}(A + z_\pm) = \mathcal{H}$ for one $z_+ \in \mathbb{C}_+$ and one $z_- \in \mathbb{C}_-$.
4. A is closed and $\mathrm{Ker}(A^* + z_\pm) = \{0\}$ for one $z_+ \in \mathbb{C}_+$ and one $z_- \in \mathbb{C}_-$.

Proof.

- 1. $\Rightarrow$ 4.: $A = A^* \Rightarrow A$ is closed by Theorem 3.2. Also, $\mathrm{Ker}(A^* + z_\pm) = \mathrm{Ker}(A + z_\pm) = \{0\}$ because $A + z_\pm$ is injective by 2.) of the proof of Theorem 3.5.
- 4. $\Rightarrow$ 3.: We have that $\mathrm{Ran}(A - \overline{z}_\pm)^\perp = \mathrm{Ker}(A + z_\pm) = \{0\}$. Thus $\overline{\mathrm{Ran}(A + \overline{z}_\pm)} = \mathcal{H}$. It remains to prove that $\mathrm{Ran}(A + \overline{z}_\pm)$ is closed. Let $y \in \overline{\mathrm{Ran}(A + z_\pm)}$. Then there exists a sequence $(\varphi_n)_{n\in\mathbb{N}}$ in $D(A)$ such that $(A + z_\pm)\varphi_n \to \varphi$. Thus $(A + z_\pm)\varphi_n$ is a Cauchy sequence. Since $\|(A + z_\pm)(\varphi_n - \varphi_m)\| \geq |\mathrm{Im}(z_\pm)|\|\varphi_n - \varphi_m\|$, it follows that φ_n is a Cauchy sequence. Thus, there exists a $\varphi \in \mathcal{H}$ such that $\varphi_n \to \varphi$. From this and from $(A + z_\pm)\varphi_n \to y$, it follows (since $(A + z_\pm)$ is closed) that $\varphi \in D(A)$ and $(A + z_\pm)\varphi = y$, so $y \in \mathrm{Ran}(A + z_\pm)$.
- 3. $\Rightarrow$ 2.: $\mathrm{Ran}(A + z_\pm) = \mathcal{H} \overset{\text{Thm. 3.5}}{\Rightarrow} \mathbb{C}_+ \subseteq \rho(A)$ and $C_- \subseteq \rho(A)$. Thus $\sigma(A) = \mathbb{C} \setminus \rho(A) \subseteq \mathbb{R}$.
- 2. $\Rightarrow$ 1.: We want to prove that $D(A^*) \subseteq D(A)$. Let $\varphi \in D(A^*)$. We have $-\mathrm{i} \in \rho(A)$ (by assumption), so $\mathrm{Ran}(A + \mathrm{i}) = \mathcal{H}$. Thus, there exists $\eta \in D(A)$ such that $(A + \mathrm{i})\eta = (A + \mathrm{i})\varphi \overset{A \subseteq A^*}{\Rightarrow} (A^* + \mathrm{i})\eta = (A^* + \mathrm{i})\varphi \Rightarrow (A^* + \mathrm{i})(\varphi - \eta) = 0$, so $\varphi - \eta \in \mathrm{Ker}(A^* + \mathrm{i}) = \mathrm{Ran}(A - \mathrm{i})^\perp = \mathcal{H}^\perp = \{0\}$. Thus $\varphi = \eta \in D(A)$.

■

Remark 3.7

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

Example 3.3

$A : H^2(\mathbb{R}^3) \subseteq L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$, $A\phi = -\Delta\phi$ is self-adjoint. Indeed, by Example 3.2, A is symmetric. By Example 2.1, $\operatorname{Ran}(A + \mathrm{i}) = L^2(\mathbb{R}^3)$ and similarly $\operatorname{Ran}(A - \mathrm{i}) = L^2(\mathbb{R}^3)$. Thus, by Theorem 3.6, A is self-adjoint.

Theorem 3.8 (Kato-Rellich)

Let $A : D(A) \subseteq \mathcal{H} \to \mathcal{H}$ be a self-adjoint operator and B symmetric with $D(B) \supseteq D(A)$. If $\forall\varphi \in D(A) : \|B\varphi\| \leq a\|A\varphi\| + b\|\varphi\|$, where $a, b \in \mathbb{R}$ with $a < 1$, then $A + B : D(A) \to \mathcal{H}$ is self-adjoint.

Proof. Clearly $A + B$ is symmetric on $D(A)$. By Theorem 3.6, it is enough to prove $\operatorname{Ran}(A + B + \mu\mathrm{i}) = \mathcal{H}$ for $\mu \in \mathbb{R}$ with $|\mu|$ large enough. Notice that $(A + B + \mathrm{i}\mu)$ $= (I + B(A + \mu\mathrm{i})^{-1})(A + \mu\mathrm{i})$. We will show that $\left\|B(A + \mu\mathrm{i})^{-1}\right\| < 1$ for $|\mu|$ large enough. If this holds, then Lemma 2.2 implies that $(I + B(A + \mathrm{i}\mu)^{-1})$ is invertible. Since A is self-adjoint, by Theorem 3.6 we have that $\operatorname{Ran}(A + \mathrm{i}\mu) = \mathcal{H} \Rightarrow \operatorname{Ran}(A + B + \mathrm{i}\mu) = \mathcal{H}$, as desired. It therefore remains to prove that $\left\|B(A + \mu\mathrm{i})^{-1}\right\| < 1$. Let $\varphi \in \mathcal{H}$ and define $\psi := (A + \mu\mathrm{i})^{-1}\varphi \in D(A)$. Then $\left\|B(A + \mu\mathrm{i})^{-1}\varphi\right\| = \|B\psi\| \leq a\|A\psi\| + b\|\psi\|$. But $\|A\psi\| \leq \|(A + \mu\mathrm{i})\psi\| = \|\varphi\|$ and $\|\varphi\| = \|(A + \mu\mathrm{i})\psi\| \geq |\mu|\|\psi\|$, so $\|\psi\| \leq \dfrac{\|\varphi\|}{|\mu|}$. Combining both, we find $\left\|B(A + \mu\mathrm{i})^{-1}\varphi\right\| \leq a\|\varphi\| + \dfrac{b}{|\mu|}\|\varphi\| \leq \left(a + \dfrac{b}{|\mu|}\right)\|\varphi\|$ for all $\varphi \in \mathcal{H}$. Thus $\left\|B(A + \mu\mathrm{i})^{-1}\right\| \leq a + \dfrac{b}{|\mu|}$ and since by assumption $a < 1$, choosing $|\mu|$ large enough we obtain $\left\|B(A + \mu\mathrm{i})^{-1}\right\| < 1$, as desired. ■

A detour in convergence theorems

Theorem (Dominated convergence (DCT))

Let $(f_n)_{n\in\mathbb{N}}$ be a sequence in $L^1(\mathbb{R}^n)$ (complex-valued functions). If

1. $f_n \to f$ almost everywhere
2. $\exists g \in L^1$ such that $|f_n| \leq g$ almost everywhere for all n,

then $\displaystyle\int f \,\mathrm{d}\mu = \lim_{n\to\infty} \int f_n \,\mathrm{d}\mu$.

Theorem (Monotonic convergence (MCT))

If $f_n : \mathbb{R}^n \to [0, \infty)$ is a pointwise increasing sequence of measurable functions and $\lim_{n\to\infty} f_n(x) = f(x)$, then $\int f \, \mathrm{d}\mu = \lim_{n\to\infty} \int f_n \, \mathrm{d}\mu$.

Lemma (Fatou)

If $f_n : \mathbb{R}^n \to [0, \infty)$ is a sequence of measurable functions, we have: $\int \liminf_{n\to\infty} f_n \, \mathrm{d}\mu \leq \liminf_{n\to\infty} \int f_n \, \mathrm{d}\mu \,.$

Example

$f : \mathbb{R} \to \mathbb{R},\ f(x) = \begin{cases} \frac{1}{2}\sin x, & x \in [0,\pi] \\ 0, & x \notin [0,\pi] \end{cases}$, $f_n(x) = nf(nx)$. Then $\forall x \in \mathbb{R} : f_n(x) \to 0$ as $n \to \infty$. But $\int_{\mathbb{R}} f_n(x) \, \mathrm{d}x = \int_{\mathbb{R}} n(nx) \, \mathrm{d}x = \int_{\mathbb{R}} f(y) \, \mathrm{d}y = 1$. So $\lim_{n\to\infty} \int_{\mathbb{R}} f_n(x) \, \mathrm{d}x \neq 0 = \int_{\mathbb{R}} \lim_{n\to\infty} f_n(x) \, \mathrm{d}x$ (we cannot always exchange limits with integrals).

We conclude: If convergence is dominated or monotone, we can exchange the limit and the integral.

<u>Proof</u> that monotonic convergence implies Fatou's Lemma:

Let $g(x) := \liminf_{n\to\infty} f_n(x) = \lim_{m\to\infty} \underbrace{\inf k \geq m f_k(x)}_{:=g_m(x)}$. Then $\forall k \geq m : g_m \leq f_k \Rightarrow \forall k \geq m : \int g_m \, \mathrm{d}\mu \leq \int f_k \, \mathrm{d}\mu \Rightarrow \int g_m \, \mathrm{d}\mu \leq \liminf_{n\to\infty} \int f_n \, \mathrm{d}\mu$. But (g_m) is an increasing positive sequence and $g_m(x) \to g(x)$ almost everywhere, so $\int g \, \mathrm{d}\mu = \lim_{m\to\infty} \int g_m \, \mathrm{d}\mu \leq \liminf_{n\to\infty} \int f_n \, \mathrm{d}\mu$.

Theorem 3.9 (Hardy inequality)

For all $\psi \in H^1\left(\mathbb{R}^3\right)$ we have that

$$\int \frac{|\psi(x)|}{|x|^2} \, \mathrm{d}x \leq 4 \int |\boldsymbol{\nabla} \psi(x)|^2 \, \mathrm{d}x \,. \tag{3.2}$$

Proof. We first assume that $\psi \in C_c^\infty\left(\mathbb{R}^3\right)$. Then we have:

$$\begin{aligned} \int \left(\partial_i \frac{x_i}{|x_i|^2}\right) |\psi(x)|^2 \, \mathrm{d}x &= \int \frac{|\psi(x)|^2}{|x|^2} \, \mathrm{d}x + \int \frac{x_i \left(-\partial_i |x|^2\right)}{|x|^4} |\psi\,(x)|^2 \, \mathrm{d}x \\ &= \int \frac{|\psi(x)|^2}{|x|^2} \, \mathrm{d}x - \int \frac{2x_i^2}{|x|^4} |\psi(x)|^2 \, \mathrm{d}x \,. \end{aligned}$$

Thus,

$$
\begin{aligned}
&\sum_{i=1}^{3}\int\left(\partial_i\frac{x_i}{|x|^2}\right)|\psi(x)|^2\,\mathrm{d}x = 3\int\frac{|\psi(x)|^2}{|x|^2}\,\mathrm{d}x - 2\int\frac{|\psi(x)|^2}{|x|^2}\,\mathrm{d}x\\
&\Rightarrow\int\frac{|\psi(x)|^2}{|x|^2} = \sum_{i=1}^{3}\int\left(\partial_i\frac{x_i}{|x|^2}\right)|\psi\,(x)|^2\,\mathrm{d}x \overset{\text{IBP}}{=} \int\sum_{i=1}^{3}\frac{x_i}{|x|^2}\partial_i|\psi\,(x)|^2\,\mathrm{d}x\\
&= \int\sum_{i=1}^{3}\frac{x_i}{|x|^2}2\,\mathrm{Re}\left(\overline{\psi(x)}\partial_i\psi(x)\right)\mathrm{d}x \le 2\int\left|\frac{\overline{\psi\,(x)}}{|x|}\frac{\sum_{i=1}^{3}x_i\partial_i\psi\,(x)}{|x|}\right|\mathrm{d}x\\
&\le 2\int\frac{|\psi(x)|}{|x|}\left|\frac{x\cdot\boldsymbol{\nabla}\psi(x)}{|x|}\right|\mathrm{d}x \le 2\int\frac{|\psi(x)|}{|x|}|\boldsymbol{\nabla}\psi(x)|\,\mathrm{d}x
\end{aligned}
$$

From the Cauchy-Schwarz inequality it follows that

$$
\int\frac{|\psi(x)|^2}{|x|^2}\,\mathrm{d}x \le 2\left(\int\frac{|\psi(x)|^2}{|x|^2}\,\mathrm{d}x\right)^{\frac{1}{2}}\left(\int|\boldsymbol{\nabla}\psi(x)|^2\,\mathrm{d}x\right)^{\frac{1}{2}},
$$

which implies equation (3.2) for all $\psi\in C_c^\infty\left(\mathbb{R}^3\right)$.
Assume now that $\psi\in H^1\left(\mathbb{R}^3\right)$. Then by Theorem 1.6 there exists a sequence $(\psi_n)_{n\in\mathbb{N}}$ in $C_c^\infty\left(\mathbb{R}^3\right)$ with $\psi_n\to\psi$ in H^1.
But then $\displaystyle\int\frac{|\psi_n(x)|^2}{|x|^2}\,\mathrm{d}x \le \int|\boldsymbol{\nabla}\psi_n(x)|^2\,\mathrm{d}x \overset{n\to\infty}{\to} \int|\boldsymbol{\nabla}\psi(x)|^2\,\mathrm{d}x$. Since $\psi_n\to\psi$ in L^2, there exists a subsequence ψ_{n_k} with $\psi_{n_k}\to\psi$ almost everywhere. Then by Fatou's Lemma:
$\displaystyle\int\frac{|\psi(x)|^2}{|x|^2}\,\mathrm{d}x \le \liminf_{n_k\to\infty}\int\frac{|\psi_{n_k}(x)|^2}{|x|^2}\,\mathrm{d}x \le \int|\boldsymbol{\nabla}\psi(x)|^2\,\mathrm{d}x$, as desired. ■

Example 3.4

Let $A: H^2\left(\mathbb{R}^3\right)\subseteq L^2\left(\mathbb{R}^3\right)\to L^2\left(\mathbb{R}^3\right)$ with $A=-\Delta+V$, where $V(x)=-\dfrac{1}{|x|}$ (up to physical units, this is the Hamiltonian of the hydrogen atom). Then A is self-adjoint.

Proof. From Example 3.3 we know that $-\Delta: H^2\left(\mathbb{R}^3\right)\subseteq L^2\left(\mathbb{R}^3\right)\to L^2\left(\mathbb{R}^3\right)$ is self-adjoint. With help of the Hardy inequality we will prove that $\forall\varepsilon>0$ there exists a $C_\varepsilon>0$ such that for all $\psi\in H^2\left(\mathbb{R}^3\right)$ we have $V\psi\in L^2\left(\mathbb{R}^3\right)$ and $\|V\psi\|\le\varepsilon\|-\Delta\psi\|+C_\varepsilon\|\psi\|$. Once we have this, we can apply Theorem 3.8 to conclude that A is self-adjoint. For all $\psi\in H^2\left(\mathbb{R}^3\right)$ we have that $\displaystyle\|V\psi\|^2=\int\frac{|\psi(x)|^2}{|x|^2}\,\mathrm{d}x \overset{\text{Hardy}}{\le} 4\int|\boldsymbol{\nabla}\psi(x)|^2\,\mathrm{d}x$. But $\displaystyle\int|\boldsymbol{\nabla}\psi(x)|^2\,\mathrm{d}x \overset{\text{FT}}{=} \int\left|\xi\hat{\psi}(\xi)\right|^2\mathrm{d}x = \int\xi^2\left|\hat{\psi}(\xi)\right|^2\mathrm{d}x \overset{\xi^2\le\varepsilon^2\xi^4+\frac{1}{4\varepsilon^2}}{\le} \int\varepsilon^2\xi^4\left|\hat{\psi}(\xi)\right|^2\mathrm{d}x+\frac{1}{4\varepsilon^2}\int\left|\hat{\psi}(\xi)\right|^2\mathrm{d}x = \varepsilon^2\|-\Delta\psi\|^2+\frac{1}{4\varepsilon^2}\|\psi\|^2 \le \left(\varepsilon\|-\Delta\psi\|+\frac{1}{2\varepsilon}\|\psi\|\right)^2$, so $\|V\psi\|\le\varepsilon\|-\Delta\psi\|+\dfrac{1}{2\varepsilon}\|\psi\|$. ■

Exercise 13: Let $x := (x_1, \dots, x_n) \in (\mathbb{R}^3)^N = \mathbb{R}^{3N}$. The operator

$$B : H^2\left(\mathbb{R}^{3N}\right) \subseteq L^2\left(\mathbb{R}^{3N}\right) \to L^2\left(\mathbb{R}^{3N}\right),$$
$$(B\phi)(x) := \sum_{j=1}^{N}\left(-\Delta_{x_j} - \frac{N}{|x|}\right)\phi(x) + \sum_{1\le i<j\le N}\frac{1}{|x_i - x_j|}\phi(x)$$

is self-adjoint (up to physical units, this is the Hamilton operator for an atom with N electrons)

Definition 3.10

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

Example 3.5

Let $B : C_c^\infty(\mathbb{R}^n) \subseteq L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$, $B\varphi = -\Delta\varphi$. Then B is essentially self-adjoint.
Indeed, $A : H^2(\mathbb{R}^n) \subseteq L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$, $A\varphi = \Delta\varphi$ is self-adjoint by Example 3.3. So it suffices to show that $\overline{B} = A$ (B is closable since e.g. A is closed as a self-adjoint operator and $B \subset A$). Since $B \subset A$ and A is closed, we have that $\overline{B} \subset A$. Let $(\varphi, -\Delta\varphi) \in \Gamma_A$. Then $\varphi \in H^2(\mathbb{R}^n)$. But by Theorem 1.6 there exists a sequence $(\varphi_n)_{n\in\mathbb{N}}$ in $C_c^\infty(\mathbb{R}^n)$ with $\varphi_n \to \varphi$ in $H^2(\mathbb{R}^n)$, so $\varphi_n \to \varphi$ and $-\Delta\varphi_n \to -\Delta\varphi \Rightarrow (\varphi, -\Delta\varphi) \in \overline{\Gamma_B}$. Thus $A \subset \overline{B}$. Hence $A = \overline{B}$, as desired.

Theorem 3.11

Let A be a symmetric operator. Then the following statements are equivalent:

1. A is essentially self-adjoint.
2. $\overline{\operatorname{Ran}(A - z_\pm)} = \mathcal{H}$ for a $z_+ \in \mathbb{C}_+$ and a $z_- \in \mathbb{C}_-$.
3. $\operatorname{Ker}(A^* - z_\pm) = \{0\}$ for a $z_+ \in \mathbb{C}_+$ and a $z_- \in \mathbb{C}_-$.

Proof.

- 1. $\Rightarrow$ 3.: $\overline{A}$ is self-adjoint by assumption and $(\overline{A})^* \overset{\text{Thm. 3.2}}{=} A^*$.
  So $\operatorname{Ker}(A^* - z_\pm) = \operatorname{Ker}\left((\overline{A})^* - z_\pm\right) \overset{\text{Thm. 3.6}}{\Rightarrow} \operatorname{Ker}(A^* - z_\pm) = \{0\}$.
- 3. $\Rightarrow$ 2.: $\operatorname{Ran}(A - z_\pm)^\perp \overset{\text{Thm. 3.3}}{=} \operatorname{Ker}(A^* - z_\pm) = \{0\}$.
- 2. $\Rightarrow$ 1.: Since A is symmetric, A is closable (by Theorem 3.2 3.)). Let $\overline{A}$ be its closure.
  Claim: $\overline{\operatorname{Ran}\left(\overline{A} - z_\pm\right)} \subseteq \operatorname{Ran}\left(\overline{A} - z_\pm\right)$. Once this is proven it follows that $\operatorname{Ran}\left(\overline{A} - z_\pm\right) =$

$\mathcal{H}$, so by Theorem 3.6 $\overline{A}$ is self-adjoint. Since $\operatorname{Ran}(A - z_\pm) \subseteq \operatorname{Ran}\left(\overline{A} - z_\pm\right)$, it remains to prove that $\operatorname{Ran}\left(\overline{A} - z_\pm\right)$ is closed.

This can be done as in the proof of Theorem 3.6 "4. $\Rightarrow$ 3.".

■

Theorem 3.12 (Kato-Rellich, general form)
Let A be essentially self-adjoint and B symmetric with $D(A) \subseteq D(B)$. If $\|B\phi\| \leq a\|A\phi\| + b\|\phi\| \, \forall \phi \in D(A)$, where $a, b \in \mathbb{R}$ with $0 < a < 1$, then $A + B : D(A) \subseteq \mathcal{H} \to \mathcal{H}$ is essentially self-adjoint and $D\left(\overline{A+B}\right) = D\left(\overline{A}\right)$.

Proof. B is symmetric, thus closable by Theorem 3.2, so let $\overline{B}$ be its closure. We show:

(i) $D\left(\overline{A}\right) \subseteq D\left(\overline{B}\right)$ and $D\left(\overline{A}\right) \subseteq D\left(\overline{A+B}\right)$.

(ii) $\overline{A} + \overline{B}$ is self-adjoint.

(iii) $\overline{A+B} \subset \overline{A} + \overline{B}$, $D\left(\overline{A+B}\right) = D\left(\overline{A}\right)$, and $\overline{A+B} = \overline{A} + \overline{B}$.

(i) Let $\varphi \in D\left(\overline{A}\right)$. Then there exists a sequence $(\varphi_n)_{n\in\mathbb{N}}$ in $D(A)$ with $\varphi_n \to \varphi$ and $A\varphi_n \to \overline{A}\varphi$. But since $\|B(\varphi_n - \varphi_m)\| \leq a\|A(\varphi_n - \varphi_m)\| + b\|\varphi_n - \varphi_m\|$, $B\varphi_n$ is a Cauchy sequence and thus convergent. Thus $\varphi \in D\left(\overline{B}\right)$ (and $B\varphi_n \to \overline{B}\varphi$). Similarly, $\varphi \in D\left(\overline{A+B}\right)$, since $(A+B)\varphi_n$ is a Cauchy sequence.

(ii) Since $\|B\varphi_n\| \leq a\|A\varphi_n\| + b\|\varphi_n\| \, \forall n \in \mathbb{N}$, we find $\left\|\overline{B}\varphi\right\| \leq \left\|\overline{A}\varphi\right\| + b\|\varphi\|$ for $n \to \infty$. Since $\varphi \in D\left(\overline{A}\right) \subseteq D\left(\overline{B}\right)$ was arbitrary, by Theorem 3.8 it follows that $\overline{A} + \overline{B}$ is self-adjoint in $D\left(\overline{A}\right)$.

(iii) Clearly, $A + B \subset \overline{A} + \overline{B}$, and since $\overline{A} + \overline{B}$ is self-adjoint (and therefore closed), we have $\overline{A+B} \subset \overline{A} + \overline{B}$. Since $D\left(\overline{A} + \overline{B}\right) = D\left(\overline{A}\right) \subseteq D\left(\overline{A+B}\right)$, it follows that $\overline{A+B} = \overline{A} + \overline{B}$, thus $\overline{A+B}$ is self-adjoint.

■

Example 3.6
$A : C_c^\infty\left(\mathbb{R}^3\right) \subseteq L^2\left(\mathbb{R}^3\right) \to L^2\left(\mathbb{R}^3\right)$, $A\varphi = (-\Delta + V)\varphi$, where $V(x) = -\dfrac{1}{|x|}$, is essentially self-adjoint in $C_c^\infty\left(\mathbb{R}^3\right)$, since by Example 3.5 the operator $-\Delta$ is essentially self-adjoint and by Example 3.4 $\|V\psi\| \leq \varepsilon\|-\Delta\psi\| + \dfrac{1}{2\varepsilon}\|\psi\|$. Thus, the general form of Kato-Rellich is applicable.

4 The Schrödinger equation and existence of dynamics

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

$$\left\{ \begin{array}{l} \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\varphi_t = H\varphi_t \\ \varphi_t\big|_{t=0} = u \end{array} \right\}. \tag{4.1}$$

The partial differential equation $\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\varphi_t = H\varphi_t$ is known as the *Schrödinger equation*. Let I be a nontrivial interval with $0 \in I$. A solution of equation (4.1) is a differentiable function $\varphi_t : I \to \mathcal{H}$ with

1. $\forall t \in I : \varphi_t \in D(H)$.
2. $\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\varphi_t := \lim_{h\to 0} \mathrm{i}\frac{\varphi_{t+h} - \varphi_t}{h} = H\varphi_t$.
3. $\varphi_0 = u$.

Theorem 4.1

(i) If equation (4.1) has for all $u \in D(H)$ a solution with constant norm, then H is symmetric.

(ii) If H is symmetric then equation (4.1) has for all $u \in D(H)$ at most one solution locally in time.

Proof.

(i) $\frac{\mathrm{d}}{\mathrm{d}t}\langle\varphi_t, \varphi_t\rangle = 0 \Rightarrow \left\langle \frac{\mathrm{d}}{\mathrm{d}t}\varphi_t, \varphi_t \right\rangle + \left\langle \varphi_t, \frac{\mathrm{d}}{\mathrm{d}t}\varphi_t \right\rangle = 0 \Rightarrow \langle -\mathrm{i}H\varphi_t, \varphi_t\rangle + \langle \varphi_t, -\mathrm{i}H\varphi_t\rangle = 0 \Rightarrow \mathrm{i}\langle H\varphi_t, \varphi_t\rangle - \mathrm{i}\langle\varphi_t, H\varphi_t\rangle = 0 \Rightarrow \langle\varphi_t, H\varphi_t\rangle = \langle H\varphi_t, \varphi_t\rangle$. In particular, $\forall u \in D(H) : \langle u, Hu\rangle = \langle Hu, u\rangle$. From Exercise 2 it follows that $\langle u, Hv\rangle = \langle Hu, v\rangle\ \forall u, v \in D(H)$, so H is symmetric.

(ii) If for some $u \in D(H)$ equation (4.1) has the two solutions φ_t and $\tilde{\varphi}_t$, then

$$\left\{ \begin{array}{l} \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}(\varphi_t - \tilde{\varphi}_t) = H(\varphi_t - \tilde{\varphi}_t) \\ (\varphi_t - \tilde{\varphi}_t)|_{t=0} = 0 \end{array} \right\}.$$

Arguing similarly as in (i) we obtain $\frac{\mathrm{d}}{\mathrm{d}t}\langle \varphi_t - \tilde{\varphi}_t, \varphi_t - \tilde{\varphi}_t \rangle = 0$.
Thus $\|\varphi - \tilde{\varphi}_t\| = \|(\varphi_t - \tilde{\varphi}_t)|_{t=0}\| = 0 \Rightarrow \varphi = \tilde{\varphi}_t$.

■

Theorem 4.2

If H is symmetric and equation (4.1) has a solution in $I = \mathbb{R}\,\forall u \in D(H)$, then H is essentially self-adjoint.

Proof. We will prove that $\operatorname{Ker}(H^* + \mathrm{i}) = \{0\}$ (and similarly $\operatorname{Ker}(H^* - \mathrm{i}) = \{0\}$). Let $w \in \operatorname{Ker}(H^* + \mathrm{i})$. Then $H^* w = -\mathrm{i}w$. Thus, for any $u \in D(H)$, if φ_t is a solution of equation (4.1), then $\frac{\mathrm{d}}{\mathrm{d}t}\langle w, \varphi_t \rangle = \langle w, -\mathrm{i}H\varphi_t \rangle = \langle \mathrm{i}H^* w, \varphi_t \rangle = \langle w, \varphi_t \rangle$. Solving the differential equation, we find $\langle w, \varphi_t \rangle = \mathrm{e}^t \langle w, \varphi_0 \rangle = \mathrm{e}^t \langle w, u \rangle$. But $|\langle w, \varphi_t \rangle| \overset{\text{Cauchy-Schwarz}}{\leq} \|w\|\|\varphi_t\| \overset{\text{Thm. 4.1}}{\leq} \|w\|\|u\|$. Thus $\forall t \in \mathbb{R} : \left|\mathrm{e}^t \langle w, u \rangle\right| \leq \|w\|\|u\| \Rightarrow \forall u \in D(H) : \langle w, u \rangle = 0 \overset{D(H)\text{ dense}}{\Rightarrow} w = 0$. ■

Example 4.1

Let $P : H_0^1(\mathbb{R}_+) \to L^2(\mathbb{R}_+)$, $Pf = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}f$. Then P is symmetric, but not essentially self-adjoint (shown in Exercise 14). Thus, if $H = P$, then equation (4.1) does not have a solution for all $u \in H_0^1(\mathbb{R}_+)$ and for all $t \in \mathbb{R}$ in $L^2(\mathbb{R}_+)$ by Theorem 4.2. This is not surprising because $\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\varphi_t = P\varphi_t \Rightarrow \frac{\mathrm{d}}{\mathrm{d}t}\varphi = -\frac{\mathrm{d}}{\mathrm{d}x}\varphi_t$. So if u is smooth and φ_t is a solution of equation (4.1), then $\varphi_t(x) = u(x+t)$, but $\operatorname{supp}(\varphi_t)$ is not a subset of $\mathbb{R}_+$.

Let us denote by $\mathcal{L}(\mathcal{H})$ the set of all bounded linear operators from $\mathcal{H}$ to $\mathcal{H}$.

Theorem 4.3 (Existence and properties of a solution, bounded case)

Let $H : \mathcal{H} \to \mathcal{H}$ be bounded and self-adjoint. Then equation (4.1) has $\forall u \in D(H) = \mathcal{H}$ the unique solution $\mathrm{e}^{-\mathrm{i}Ht}u$, where $\mathrm{e}^{-\mathrm{i}Ht} = \sum_{n=0}^{\infty} \frac{(-\mathrm{i}Ht)^n}{n!}$. This solution is global in time. The map $U : \mathbb{R} \to \mathcal{L}(\mathcal{H})$, $U(t) = \mathrm{e}^{-\mathrm{i}Ht}$, fulfills

(1) $\forall s, t \in \mathbb{R}\ U(t)$ is unitary and $U(t+s) = U(t)U(s)$,

(2) $\lim_{t\to 0} U(t)\psi = \psi \, \forall \psi \in \mathcal{H}$.

Proof. (1) That $U(t+s) = U(t)\,U(s)$ can be proven using the Cauchy product of power series as in the case of real numbers. $U(t)$ is unitary since $U^*(t) = \left(\sum_{n=0}^{\infty} \frac{(-\mathrm{i}Ht)^n}{n!}\right)^* = \sum_{n=0}^{\infty} \frac{(\mathrm{i}Ht)^n}{n!} = U(-t)$. Thus $U^*(t)U(t) = U(-t)U(t) = U(-t+t) = U(0) = I$ by definition.

(2) $U(t)\psi - \psi = \sum_{n=1}^{\infty} \frac{(-\mathrm{i}Ht)^n}{n!}\psi = -iHt \sum_{n=1}^{\infty} \frac{(-\mathrm{i}Ht)^{n-1}}{n!}\psi$

$$\Rightarrow \|U(t)\psi - \psi\| \leq t\|H\| \left\| \sum_{n=1}^{\infty} \frac{(\mathrm{i}Ht)^{n-1}}{n!}\psi \right\| \overset{t\to 0}{\to} 0,$$

so $\lim_{t\to 0} U(t)\psi - \psi = 0$.

We now prove that $\varphi_t = U(t)u = \mathrm{e}^{-\mathrm{i}Ht}u$ is a solution of equation (4.1) for all $t \in \mathbb{R}$ and uniqueness follows from Theorem 4.1. Trivially $\varphi_0 = \mathrm{e}^{-\mathrm{i}H\cdot 0}u = u$. We have

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\varphi_t = \lim_{h\to 0} \mathrm{i}\frac{\varphi_{t+h} - \varphi_t}{h} = \mathrm{i}\lim_{h\to 0} \frac{U(t+h)u - U(t)u}{h} = \mathrm{i}\lim_{h\to 0} \frac{U(h)U(t)u - U(t)u}{h}$$
$$= \mathrm{i}\lim_{h\to 0} \left(\frac{U(h) - I}{h}\right) U(t)u.$$

But $\mathrm{i}\frac{U(h) - I}{h} = \frac{\mathrm{i}}{h}\sum_{n=1}^{\infty} \frac{(-\mathrm{i}Hh)^n}{n!} = \frac{\mathrm{i}(-\mathrm{i}Hh)}{h}\sum_{n=1}^{\infty} \frac{(-\mathrm{i}Hh)^{n-1}}{n!} \overset{h\to 0}{\to} H,$

so indeed $\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\varphi_t = H\varphi_t$ and $\varphi_t|_{t=0} = u$. ■

A map $U : \mathbb{R} \to \mathcal{L}(\mathcal{H})$ satisfying

(1) $\forall s, t \in \mathbb{R} : U(t)$ is unitary and $U(t+s) = U(t)U(s) = U(s)U(t)$, (4.2)

(2) $\lim_{t\to 0} U(t)\psi = \psi \, \forall \psi \in \mathcal{H}$. (4.3)

is called a *strongly continuous unitary group* .

Example 4.2

The map $U : \mathbb{R} \to \mathcal{L}(L^2(\mathbb{R}))$ defined by $[U(t)\varphi](x) = \varphi(x+t)$ is a strongly continuous unitary group.

Proof. $[U(t+s)\varphi](x) = \varphi(x+t+s) = [U(s)\varphi](x+t) = [U(t)U(s)\varphi](x) \Rightarrow U(t+s) = U(t)U(s)$. $\langle U(t)\varphi, U(t)\varphi\rangle = \int \overline{\varphi(t+x)}\varphi(x+t)\,\mathrm{d}x \overset{y:x+t}{=} \int \overline{\varphi(y)}\varphi(y)\,\mathrm{d}y = \langle y, y\rangle$, so $U(t)$ is unitary for all $t \in \mathbb{R}$.

If $\psi \in C_c^\infty(\mathbb{R})$, then $|U(t)\psi(x)| \leq f \,\forall t \in [-1,1]$, where $f = \max|\psi|\chi_{\bigcup_{t\in[-1,1]}\operatorname{supp}(U(t)\psi)} \in L^1$. Thus, since $U(t)\psi \to \psi$ pointwise, we can apply the dominated convergence theorem to conclude that $\|U(t)\psi - \psi\|_{L^1} \to 0$. But $\|U(t)\psi - \psi\|_{L^2} \leq \|U(t)\psi - \psi\|_{L^\infty}\|U(t)\psi - \psi\|_{L^1} \to 0$. Let $\varphi \in L^2$, $\varepsilon > 0$. Then there exists a $\varphi_0 \in C_c^\infty(\mathbb{R})$ with $\|\varphi - \varphi_0\| < \frac{\varepsilon}{3}$. But then $U(t)\varphi - \varphi = U(t)(\varphi - \varphi_0) + U(t)\varphi - \varphi_0 + \varphi_0 - \varphi \to \|U(t)\varphi - \varphi\| \leq 2\|\varphi - \varphi_0\| + \|U(t)\varphi_0 - \varphi_0\|$. Choosing $t_0 > 0$ such that $\forall t \in (-t_0, t_0) : \|U(t)\varphi_0 - \varphi_0\| < \frac{\varepsilon}{3}$, we find $\|U(t)\varphi - \varphi\| < \varepsilon \,\forall t \in (-t_0, t_0)$. ■

Remark 4.4

(i) If U is a strongly continuous unitary group then $t \mapsto U(t)\psi$ is continuous $\forall t \in \mathbb{R}$.

(ii) To verify $\forall \psi \in \mathcal{H} : \lim_{t\to 0} U(t)\psi = \psi$ it is enough to check it for all ψ in a dense subset of $\mathcal{H}$.

Proof.

(i) $\lim_{h\to 0} U(t+h)\psi - U(t)\psi = \lim_{h\to 0} U(h)U(t)\psi - U(t)\psi = \lim_{h\to 0}(U(h) - I)U(t)\psi = 0$, by equation (4.3).

(ii) This can be proven by approximation as in Example 4.2.

■

Theorem 4.5 (Existence of a solution, general case)

(a) Let $H : D(H) \subseteq \mathcal{H} \to \mathcal{H}$ be a self-adjoint operator (not necessarily bounded). Then $\forall u \in D(H)$ equation (4.1) has a unique solution. This solution is global in time.

(b) There exists a strongly continuous unitary group $U(t)$ such that $\forall u \in D(H)\ \forall t \in \mathbb{R} : \varphi_t = U(t)u$.

Proof. Let $H_n := B_n H B_{-n}$, $B_n := \mathrm{i}n(H + \mathrm{i}n)^{-1}$ (intuition: if H were a real number, then $\lim_{n\to\infty} B_n = 1$. Thus we hope that $\lim_{n\to\infty} B_n = I$ in a certain sense and that "$\lim_{n\to\infty} H_n = H$"). The uniqueness of the solution (if it exists) has already been proven. We will prove Theorem 4.5 in five steps:

(1) H_n is bounded and self-adjoint for all $n \in \mathbb{N}$.

(2) $H_n\psi \to H\psi \,\forall \psi \in D(H)$.

(3) $\lim_{n\to\infty} \mathrm{e}^{-\mathrm{i}H_n t}\psi$ exists for all $\psi \in D(H)$. For fixed $\psi \in D(H)$ the limit is uniform on compact sets $[-M, M]\,\forall M > 0$.

(4) $\lim_{n\to\infty} \mathrm{e}^{-\mathrm{i}H_n t}\psi$ exists for all $\psi \in \mathcal{H}$ and $U : \mathbb{R} \to \mathcal{L}(\mathcal{H})$ with $U(t)\psi = \lim_{n\to\infty} \mathrm{e}^{-\mathrm{i}H_n t}\psi$ is a strongly continuous unitary group.

(5) $\varphi_t := U(t)u$ is a solution of

$$\left\{ \begin{aligned} \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\varphi_t &= H\varphi_t \\ \varphi_t\big|_{t=0} &= u \end{aligned} \right\} . \tag{4.4}$$

(1) $B_{\pm n}$ is bounded because $\pm n \in \rho(H)$. $\|B_n H B_m\| \le \|B_n\| \left\| H\mathrm{i}n\,(H - \mathrm{i}n)^{-1} \right\|$

$$\le n\|B_n\| \left\| H\,(H-\mathrm{i}n)^{-1} \right\| \le n\|B_n\|$$

because $\|H\psi\| \overset{\text{Thm. 3.9}}{\le} \|(H - \mathrm{i}n)\psi\|\ \forall \psi \in D(H)$. If $\psi \in D(H)$ then $\psi = (H-\mathrm{i}n)^{-1}\varphi$ for some $\varphi \in \mathcal{H}$, thus $\|H\psi\| = \left\|H(H-\mathrm{i}n)^{-1}\varphi\right\| \le \|\varphi\|$. So H_n is bounded. Let $\varphi, \psi \in \mathcal{H}$. Then $\langle \varphi, H_n\psi\rangle = \langle \varphi, B_n H B_{-n}\psi\rangle \overset{H=H^*\Rightarrow B_n^*=B_{-n}}{=} \Big\langle \underbrace{B_{-n}\varphi}_{\in D(H)}, H\, \underbrace{B_{-n}\psi}_{\in D(H)} \Big\rangle$ $\overset{H \text{ self-adjoint}}{=} \langle HB_{-n}\varphi, B_{-n}\psi\rangle = \langle B_n H B_{-n}\varphi, \psi\rangle = \langle H_n\varphi, \psi\rangle$. Thus H_n is self-adjoint.

(2) For all $\psi \in D(H)$ we have $\lim_{n\to\infty} B_{\pm n}\psi = \psi$.
$B_n\psi - \psi = \mathrm{i}n(H+\mathrm{i}n)^{-1}\psi - (H+\mathrm{i}n)(H+\mathrm{i}n)^{-1}\psi = -H(H+\mathrm{i}n)^{-1}\psi$. Thus, by Exercise 4,(3) and since $\psi \in D(H)$ we have that $B_n\psi - \psi = -(H+\mathrm{i}n)^{-1}H\psi$. Thus $\|B_n\psi - \psi\| \le \left\|(H+\mathrm{i}n)^{-1}\right\| \|H\psi\| \le \frac{1}{|n|}\|H\psi\| \overset{n\to\infty}{\to} 0$. Similarly for B_{-n}. Hence $B_{\pm n}\psi \overset{n\to\infty}{\to} \psi\ \forall\psi \in D(H)$. So if $\psi \in \mathcal{H}$, let $\psi_0 \in D(H), \varepsilon > 0$ with $\|\psi - \psi_0\| < \frac{\varepsilon}{3}$. Then $B_n\psi - \psi = B_n\psi - B_n\psi_0 + B_n\psi_0 - \psi_0 + \psi_0 - \psi$ and $\|B_n\psi - \psi\| \le (\|B_n\| + 1)\|\psi_0 - \psi\| + \|B_n\psi_0 - \psi\| \le \frac{2\varepsilon}{3} + \|B_n\psi_0 - \psi\|$, since $\|B_n\| = \left\|\mathrm{i}n(H+\mathrm{i}n)^{-1}\right\| \le 1$. Now choose n large enough. We have $H_n\psi = B_n H B_{-n}\psi \overset{\psi\in D(H)}{=} B_n B_{-n} H\psi$. Thus $H_n\psi - H\psi = B_nB_{-n}H\psi - H\psi = B_nB_{-n}H\psi - B_nH\psi + B_nH\psi - H\psi = B_n(B_{-n}H\psi - H\psi) + B_nH\psi - H\psi$. But $B_n(B_{-n}H\psi - H\psi) \to 0$ and $B_nH\psi - H\psi \to 0$ since $B_{\pm n}\psi \to \psi$ and $\|B_n\| = 1 < \infty$.

(3) By Theorem 4.3 $\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{-\mathrm{i}H_n t}\psi = \mathrm{e}^{-\mathrm{i}H_n t}(-\mathrm{i}H_n)\psi = (-\mathrm{i}H_n)\mathrm{e}^{-\mathrm{i}H_n t}\psi$. Let $\psi \in D(H)$. Then

$$\left\|\mathrm{e}^{-\mathrm{i}H_n t}\psi - \mathrm{e}^{-\mathrm{i}H_m t}\psi\right\| \overset{\mathrm{e}^{-\mathrm{i}H_m t}\text{ unitary}}{=} \left\|\mathrm{e}^{\mathrm{i}H_m t}\mathrm{e}^{-\mathrm{i}H_n t}\psi - \psi\right\|.$$

$$\mathrm{e}^{\mathrm{i}H_m t}\mathrm{e}^{-\mathrm{i}H_n t}\psi - \mathrm{e}^{\mathrm{i}H_m \cdot 0}\mathrm{e}^{-\mathrm{i}H_n \cdot 0}\psi = \int_0^t \frac{\mathrm{d}}{\mathrm{d}s}\left(\mathrm{e}^{\mathrm{i}H_m s}\mathrm{e}^{-\mathrm{i}H_n s}\psi\right)\mathrm{d}s$$

$$= \int_0^t \mathrm{e}^{\mathrm{i}H_m s}(\mathrm{i}H_m - \mathrm{i}H_n)\mathrm{e}^{-\mathrm{i}H_n s}\psi\,\mathrm{d}s \overset{\text{Exercise}}{=} \int_0^t \mathrm{e}^{\mathrm{i}H_m s}\mathrm{e}^{-\mathrm{i}H_m s}\mathrm{i}(H_m - H_n)\psi\,\mathrm{d}s\,,$$

$$\text{therefore } \left\| e^{iH_m t} e^{-iH_n t}\psi - \psi \right\| \le |t| \|(H_n - H_m)\psi\| \\ \le M\|(H_n - H_m)\psi\| \, \forall t \in [-M, M] \, \forall M > 0.$$

Thus $e^{-iH_n t}\psi$ is uniformly Cauchy in $t \in [-M, M]$ and thus uniformly convergent.

(4) The existence follows by approximation similarly as in Example 4.2.
Now we prove $\forall \psi \in \mathcal{H} : U(t+s)\psi = U(t)U(s)\psi$. By approximation it suffices to prove it $\forall \psi \in D(H)$. Let $U_n(t) := e^{-iH_n t}$. Then $U_n(s+t)\psi \overset{\text{Thm. 4.3}}{=} U_n(t)U_n(s)$.

But $U_n(t+s)\psi \overset{n\to\infty}{\to} U(t+s)\psi$ by (3) and $U_n(t)U_n(s)\psi \overset{n\to\infty}{\to} U(t)U(s)\psi$ since

$U_n(t)U_n(s)\psi - U(t)U(s)\psi = U_n(t)(U_n(s) - U_n(s))\psi + (U_n(t) - U(t))U(s)\psi \to 0$ by (3) and the fact that $\|U_n(t)\| \le 1$.

We now show that $U(t)$ is unitary: $\langle \varphi, U(t)\psi \rangle = \lim_{n\to\infty} \langle \varphi, U_n(t)\psi \rangle \overset{U_n \text{ unitary}}{=} \lim_{n\to\infty} \langle U_n^*(t)\varphi, \psi \rangle$ $= \lim_{n\to\infty} \langle U_{-n}(t)\varphi, \psi \rangle = \langle U(-t)\varphi, \psi \rangle$. Thus $(U(t))^* = U(-t)$ and it follows that $(U(t))^* U(t)$ $= U(-t)U(t) = U(-t+t) = U(0) = I$. Similarly, $U(t)(U(t))^*$, hence $U(t)$ is unitary for all $t \in \mathbb{R}$. To prove that $U(t)$ is a strongly continuous unitary group it suffices to prove that $\lim_{t\to 0} U(t)\psi = \psi \, \forall \psi \in D(H)$ (because $\overline{D(H)} = \mathcal{H}$). Let $f_n(t) = U_n(t)\psi$, where $U_n(t) = e^{-iH_n t}$. Then $f_n(t)$ is continuous by Theorem 4.3 (solution if the operator is bounded and self-adjoint). By (3), $f_n(t) \to U(t)\psi$ uniformly in $t \in [-M, M] \, \forall M > 0$. Since f_n is continous for all n it follows that $U(t)\psi$ is continuous.

(5) Let $\varphi_t := U(t)v$. We have to show: φ_t is a solution of equation (4.1) $\forall t \in \mathbb{R}, \forall v \in D(H)$. We have $i\frac{d}{dt}\varphi_t = i\lim_{h\to 0} \frac{\varphi_{t+h} - \varphi_t}{h} = i\lim_{h\to 0} \frac{U(t+h)v - U(t)v}{h} = iU(t)\lim_{h\to 0} \frac{U(h) - I}{h} v$. For fixed $h \ne 0$, $\frac{U(h) - I}{h} v = \lim_{m\to\infty} \frac{U_m(h) - U_m(0)}{h} v = \lim_{m\to\infty} \frac{1}{h} \int_0^h \left(\frac{d}{ds} U_m(s)v \right) ds$ $\overset{\text{Thm. 4.3}}{=} \lim_{m\to\infty} \frac{1}{h} \int_0^h U_m(s)(-iH_m)v \, ds \overset{\text{to show}}{=} \frac{1}{h} \int_0^h U(s)(-iH_m)v \, ds$. Once we have this, we find $\lim_{h\to 0} \frac{U(h) - I}{h} v = \lim_{h\to 0} \frac{1}{h} \int_0^h U(s)(-iH)v \, ds = U(0)(-iH)v = -iHv$. Thus, it follows that $i\frac{d}{dt}\varphi_t = U(t)Uv = HU(t)v = H\varphi_t$. To prove the last identity indicated above, we

write

$$\begin{aligned}
&\int_0^h (U_m(s)(-\mathrm{i}H_m)v - U(s)(-\mathrm{i}Hv))\,\mathrm{d}s \\
&= \int_0^h U_m(s)(-\mathrm{i}H_m + \mathrm{i}H)v\,\mathrm{d}s + \int_0^h (U_m(s) - U(s))Hv\,\mathrm{d}s \\
&\Rightarrow \left\| \int_0^h (U_m(s)(-\mathrm{i}H_m)v - U(s)(-\mathrm{i}H)v)\,\mathrm{d}s \right\| \\
&\overset{U_{(m)} \text{ unitary}}{\leq} \underbrace{|h|\|(-\mathrm{i}H_m + \mathrm{i}H)v\|}_{\overset{m\to\infty}{\to} 0 \text{ by } (2)} + \int_0^h \underbrace{\|(U(s) - U(s))Hv\|}_{\overset{m\to\infty}{\to} 0\, \forall s \in [0,h] \text{ pointwise}} \mathrm{d}s\,.
\end{aligned}$$

We have $\|(U_m(s) - U(s))Hv\| \leq \|U_m(s)Hv\| + \|U(s)Hv\| \leq 2\|Hv\|$, so we can apply the dominated convergence theorem to the last term on the right-hand side in the above inequality.

■

Remark 4.6

The strongly continuous unitary group $U(t)$ of Theorem 4.5 is denoted by $\mathrm{e}^{-\mathrm{i}Ht}$. With its help one can make sense of a solution of equation (4.1) $\forall v \in \mathcal{H}$ (even if $v \notin D(H)$).

Definition 4.7

Let $U : \mathbb{R} \to \mathcal{L}(\mathcal{H})$ be a strongly continuous unitary group. The *generator* of U is the linear operator $A : D(A) \subseteq \mathcal{H} \to \mathcal{H}$, defined by

1.) $D(A) = \left\{ \psi \in \mathcal{H} : \lim\limits_{h\to 0} \dfrac{U(h) - I}{h}\psi \text{ exists} \right\}$

2.) $A\psi = \mathrm{i}\dfrac{\mathrm{d}}{\mathrm{d}t}U(t)\,\psi\big|_{t=0} = \mathrm{i}\lim\limits_{h\to 0} \dfrac{U(h) - I}{h}\psi.$

Example 4.3

In Example 4.2 we showed that $U : \mathbb{R} \to L^2(\mathbb{R})$, $[U(t)\psi](x) = \psi(x - t)$ is a strongly continuous unitary group. The generator of it is $A : H^1(\mathbb{R}) \to L^2(\mathbb{R})$, $A\varphi = -\mathrm{i}\dfrac{\mathrm{d}}{\mathrm{d}x}\varphi$.

Proof. Let $v \in C_c^\infty(\mathbb{R})$ and $\psi \in L^2(\mathbb{R})$.
Then $\left\langle \dfrac{U(h) - I}{h}\psi, v \right\rangle \overset{U^*(h)=U(-h)}{=} \left\langle \psi, \dfrac{U(-h) - I}{h}v \right\rangle \overset{h\to 0 \text{ (Exercise)}}{\to} \int \psi(x)v'(x)\,\mathrm{d}x$. Therefore

$\lim_{h\to 0}\frac{U(h)-I}{h}\psi = f$ in L^2 for some $f \Leftrightarrow \langle f,v\rangle = \langle \psi, v'\rangle\ \forall v\in C_c^\infty(\mathbb{R}) \Leftrightarrow \psi' = f$ (in the sense of weak derivatives) $\Leftrightarrow \psi\in H^1$ and $\psi' = f$. In this case $A\psi = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}\psi$. ■

Theorem 4.8 (Stone)

Let $A : D(H) \subseteq \mathcal{H}\to\mathcal{H}$ be the generator of a strongly continuous unitary group. Then:

(1) $U(t)D(A)\subseteq D(A)$ and $\forall\varphi\in D(A)$ we have $\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}U(t)\varphi = AU(t)\varphi = U(t)A\varphi$

(2) $A = A^*$

(3) $U(t)$ is uniquely determined by A

Proof.

(1) $A\varphi = \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}U(t)\left.\varphi\right|_{t=0}$. If $\varphi\in D(A)$ then:

$\mathrm{i}\lim_{h\to 0}\frac{U(t+h)-U(t)}{h}\varphi = U(t)\mathrm{i}\lim_{h\to 0}\frac{U(h)-I}{h}\varphi = U(t)A\varphi.$

Thus $U(t)\varphi\in D(A)$ and $AU(t)\varphi = \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}U(t)\varphi = AU(t)\varphi$.

(2) (i) A is densely defined.

(ii) A is symmetric.

(iii) A is essentially self-adjoint.

(iv) A is closed.

(i) Let $\varphi\in\mathcal{H}$. Then $\varphi = \lim_{t\to 0}\frac{1}{t}\int_0^t U(s)\varphi\,\mathrm{d}s$. Thus it suffices to show that $\forall t\neq 0$: $\frac{1}{t}\int_0^t U(s)\varphi\,\mathrm{d}s\in D(A)$.

For fixed t we have:

$$\begin{aligned}
&\frac{U(h)-I}{h}\frac{1}{t}\int_0^t U(s)\varphi\,\mathrm{d}s = \frac{1}{t}\int_0^t\frac{U(s+h)-U(s)}{h}\varphi\,\mathrm{d}s\\
&= \frac{1}{t}\left(\int_h^{t+h}\frac{U(s)}{h}\varphi\,\mathrm{d}s - \int_0^t\frac{U(s)}{h}\varphi\,\mathrm{d}s\right)\\
&= \frac{1}{t}\int_t^{t+h}\frac{U(s)}{h}\varphi\,\mathrm{d}s - \int_0^h\frac{U(s)}{h}\varphi\,\mathrm{d}s \overset{h\to 0}{\to} \frac{1}{t}(U(t)\varphi - U(0)\varphi).
\end{aligned}$$

(ii) Since A is densely defined it remains to prove that $\langle A\varphi, \psi\rangle = \langle \varphi, A\psi\rangle \, \forall \varphi, \psi \in D(A)$. We have $\langle A\varphi, \psi\rangle = \lim_{h\to 0} \left\langle \mathrm{i}\frac{U(h)-I}{h}\varphi, \psi \right\rangle = \lim_{h\to 0} \left\langle \varphi, -\mathrm{i}\frac{U(-h)-I}{h}\psi \right\rangle$
$= \left\langle \varphi, \mathrm{i}\lim_{h\to 0} \frac{U(-h)-I}{-h}\psi \right\rangle = \langle \varphi, A\psi\rangle$.

(iii) A is symmetric and by (1) equation (4.1) has a solution for all times. Thus, by Theorem 4.2 A is essentially self-adjoint.

(iv) Let $(\varphi_n)_{n\in\mathbb{N}}$ be a sequence in $D(A)$ with $\varphi_n \to \varphi$ and $A\varphi_n \to A\psi$ for some $\psi \in \mathcal{H}$. We have to show: $\varphi \in D(A)$ and $A\varphi = \psi$. For fixed $h \neq 0$ we have:

$$\mathrm{i}\frac{U(h)-I}{h}\varphi = \mathrm{i}\lim_{n\to\infty} \frac{U(h)\varphi_n - U(0)\varphi_n}{h} = \lim_{n\to\infty} \frac{1}{h}\int_0^h \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}s}U(s)\varphi_n \,\mathrm{d}s$$
$$= \lim_{n\to\infty} \frac{1}{h}\int_0^h U(s)A\varphi_n \,\mathrm{d}s \overset{A\varphi_n\to\psi \text{ uniformly}}{=} \frac{1}{h}\int_0^h U(s)\psi \,\mathrm{d}s \overset{h\to 0}{\to} \psi.$$

Thus $\varphi \in D(A)$ and $A\varphi = \psi$.

(3) For all $\varphi \in D(A)$ $U(t)\varphi$ is a solution of $\left\{ \begin{array}{l} \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\varphi_t = H\varphi_t \\ \varphi_t|_{t=0} = \varphi \end{array} \right\}$ (4.5) by (1). If $W(t)$ is another strongly continuous unitary group generated by A, then $\forall \varphi \in D(A) : U(t)\varphi = W(t)\varphi$ because equation (4.5) has at most one solution by the symmetry of A. Since $D(A)$ is dense, we find $U(t) = W(t)$.

■

Example 4.4

From Example 4.2 and Example 4.3 it follows that $A : H^1(\mathbb{R}) \to L^2(\mathbb{R})$, $A\varphi = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}\varphi$ is self-adjoint.

5 Observables, Uncertainty Principle, Ground state energy

Observables are physically measurable quantities that correspond to self-adjoint operators acting on the Hilbert space of the states (also called wave functions).
Let A be a self-adjoint operator acting on a Hilbert space $\mathcal{H}$.

Definition 5.1

1. The *expectation* of A in the state ψ is given by $\langle \psi, A\psi \rangle$.

2. The *variance* of A in $\psi \in D(A)$ is defined by $\Delta A_\psi = \left\langle \psi, (A - \langle \psi, A\psi \rangle)^2 \psi \right\rangle = \left\langle \psi, A^2 \psi \right\rangle - \langle \psi, A\psi \rangle^2$.

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

Example 5.1
We compute the expectation (value) of

(i) the position operator (j-th component): $\langle \psi, x_j \psi \rangle = \int x_j |\psi(x)|^2 \, \mathrm{d}x$

(ii) the momentum operator (j-th component): $\langle \psi, -\mathrm{i}\partial_{x_j} \psi \rangle = \left\langle \hat{\psi}, \xi_j \hat{\psi} \right\rangle = \int \xi_j \left| \hat{\psi}(\xi) \right|^2 \mathrm{d}x$ after Fourier transformation and using Plancherel's identity $\langle f, g \rangle = \left\langle \hat{f}, \hat{g} \right\rangle$

(iii) the energy operator: $\langle \psi, H\psi \rangle$, where $H = \dfrac{-\Delta}{2m} + V$. Here $\dfrac{-\Delta}{2m}$ is the kinetic energy (classically, it is given by $\dfrac{p^2}{2m}$, $p = mv$) and V is the potential energy.

Notation: When we write $\langle\psi, x\psi_t\rangle$, where $x = (x_1, x_2, x_3)$, we mean $\langle\psi, x\psi_t\rangle := \begin{pmatrix}\langle\psi_t, x_1\psi_t\rangle\\ \langle\psi_t, x_2\psi_t\rangle\\ \langle\psi_t, x_3\psi_t\rangle\end{pmatrix}$.
Analogous short-hand notations hold for the momentum operator and other finite-dimensional vector-like operators.

Example 5.2

We compute the commutator of the Hamilton operator H with x_j: $[H, x_j] = \left[-\frac{\Delta}{2m} + V, x_j\right] = \left[-\frac{\Delta}{2m}, x_j\right]$, since V is a real number and therefore commutes with x_j. For ψ smooth, $\left[-\frac{\Delta}{2m}, x_j\right]\psi = -\frac{-\Delta}{2m}x_j\psi + x_j\frac{\Delta}{2m}\psi = \frac{1}{2m}\sum_{k=1}^{n}(-\partial^2_{x_k}(x_j\psi) + x_j\partial^2_{x_k}\psi)$
$\overset{\text{product rule}}{=} \sum_{k=1}^{n} -\frac{1}{m}\delta_{jk}(\partial_{x_k}x_j)\partial_{x_k}\psi = -\frac{1}{m}\partial_{x_j}\psi$, where we have used the Kronecker symbol $\delta_{ij} := \begin{cases}1, i = j\\ 0, i \neq j\end{cases}$.

Example 5.3 (Informal computations for the evolution of observables)

If $i\frac{\mathrm{d}}{\mathrm{d}t}\psi_t = H\psi_t$, how does $\langle\psi_t, A\psi_t\rangle$ (A self-adjoint and t-independent!) evolve in time? We have $\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi_t, A\psi_t\rangle = \langle -\mathrm{i}H\psi_t, A\psi_t\rangle + \langle\psi_t, A(-\mathrm{i}H)\psi_t\rangle \overset{H=H^*}{=} \langle\psi_t, (\mathrm{i}HA - \mathrm{i}AH)\psi_t\rangle$
$= \langle\psi_t, \mathrm{i}[H, A]\psi_t\rangle$. Thus

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi_t, A\psi_t\rangle = \langle\psi_t, \mathrm{i}[H, A]\psi_t\rangle}. \tag{5.1}$$

Thus, e.g. $\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi_t, x_j\psi_t\rangle = \langle\psi_t, \mathrm{i}[H, x_j]\psi_t\rangle \overset{\text{Ex. 5.2}}{=} \frac{1}{m}\langle\psi_t, -\mathrm{i}\partial_{x_j}\psi_t\rangle$, and hence $\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi_t, x\psi_t\rangle = \frac{1}{m}\langle\psi_t, -\mathrm{i}\boldsymbol{\nabla}\psi_t\rangle$. If we take one more derivative, we obtain $\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle\psi_t, x\psi_t\rangle = \frac{1}{m}\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi_t, -\mathrm{i}\boldsymbol{\nabla}\psi_t\rangle = \frac{1}{m}\langle\psi_t, \mathrm{i}[H, -\mathrm{i}\boldsymbol{\nabla}]\psi_t\rangle = \frac{1}{m}\langle\psi_t, [H, \boldsymbol{\nabla}]\psi_t\rangle \overset{[\Delta, -\mathrm{i}\boldsymbol{\nabla}]=0}{=} \frac{1}{m}\langle\psi_t, [V, \boldsymbol{\nabla}]\psi_t\rangle$. Thus $\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle\psi_t, x\psi_t\rangle = \frac{1}{m}\langle\psi, (-\boldsymbol{\nabla}V)\psi_t\rangle$. [1]

Remark

We can write $\psi_t = \mathrm{e}^{-\mathrm{i}Ht}\psi_0$, where $\psi_t|_{t=0} = \psi_0$ and ψ_t solves the Schrödinger equation

[1] This means that while position and momentum operators do not necessarily obey the equations of motion of classical mechanics (Newton's laws), $\frac{\mathrm{d}}{\mathrm{d}t} = \frac{1}{m}p$, $a = \frac{\mathrm{d}^2}{\mathrm{d}t^2}x = \frac{1}{m}(-\boldsymbol{\nabla}V) = \frac{1}{m}F$, at least their expectation values do. This result is known as the Ehrenfest theorem[3].

$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\psi_t = H\psi_t$. For an observable A we define $A(t) := \mathrm{e}^{\mathrm{i}Ht}A\mathrm{e}^{-\mathrm{i}Ht}$. Then

$$\langle\psi_t, A\psi_t\rangle = \left\langle \mathrm{e}^{-\mathrm{i}Ht}\psi_0, A\mathrm{e}^{-\mathrm{i}Ht}\psi_0\right\rangle = \langle\psi_0, A(t)\psi_0\rangle\ . \tag{5.2}$$

The left-hand side is called the Schrödinger picture of the expectation of A, while the right-hand side is called the Heisenberg picture. In the Schrödinger picture, only ψ evolves in time, while A is constant for all t. In the Heisenberg picture, only the operator $A(t)$ evolves in time, while ψ_0 is constant for all t. Note that we have continued to assume that A (Schrödinger picture) is t-independent.

At least non-rigorously we have $A'(t) = \mathrm{i}H\mathrm{e}^{\mathrm{i}Ht}A\mathrm{e}^{-\mathrm{i}Ht} - \mathrm{e}^{\mathrm{i}Ht}A\mathrm{e}^{-\mathrm{i}Ht}\mathrm{i}H$, so $A'(t) = \mathrm{i}[H, A(t)]$.

Theorem 5.3

Let A, B be self-adjoint operators acting on $\mathcal{H}$. Then for $\psi \in D(A) \cap D(B)$ we have [2]

$$\Delta A_\psi \Delta B_\psi \geq \frac{1}{4}|\langle\psi, [A,B]\psi\rangle|^2. \tag{5.3}$$

Proof. $\langle\psi, [A,B]\psi\rangle = \langle A\psi, B\psi\rangle - \langle B\psi, A\psi\rangle = \langle A\psi, B\psi\rangle - \overline{\langle A\psi, B\psi\rangle} = 2\mathrm{i}\,\mathrm{Im}\,\langle A\psi, B\psi\rangle$. So $\left|\frac{1}{2}\langle\psi, [A,B]\psi\rangle\right| = |\mathrm{Im}\,\langle A\psi, B\psi\rangle| \leq |\langle A\psi, B\psi\rangle| \leq \|A\psi\|\|B\psi\|$ by use of the Cauchy-Schwarz inequality. Squaring, we obtain $\frac{1}{4}|\langle\psi, [A,B]\psi\rangle|^2 \leq \left\langle\psi, A^2\psi\right\rangle\left\langle\psi, B^2\psi\right\rangle$. If $\langle\psi, A\psi\rangle = \langle\psi, B\psi\rangle = 0$, then the right-hand side equals $\Delta A_\psi\Delta B_\psi$. If A or B does not have the expectation value 0, we use translation invariance of the commutator ($\forall c, d \in \mathbb{R} : [A-c, B-d] = [A,B]$) to define $\tilde{A} = A - \langle\psi, A\psi\rangle$, $\tilde{B} = B - \langle\psi, B\psi\rangle$, where $\langle\psi, A\psi\rangle, \langle\psi, B\psi\rangle \in \mathbb{R}$ since $\langle\psi, A\psi\rangle = \langle A\psi, \psi\rangle = \overline{\langle\psi, A\psi\rangle}$ (and analogously for $\langle\psi, B\psi\rangle$). Then we apply the Cauchy-Schwarz inequality to $\tilde{A}, \tilde{B}$. ■

In particular, for $A = x_j$, $B = \partial_{x_k}$ we find $\Delta A_\psi\Delta B_\psi \geq \frac{1}{4}|\langle\psi, [x_j, \mathrm{i}\partial_{x_k}]\psi\rangle|^2$. The commutator vanishes if $j \neq k$ because $\partial_{x_k}x_j = 0$ for $j \neq k$. If $j = k$, $[x_j, \mathrm{i}\partial_{x_k}]\psi = x_k\mathrm{i}\partial_{x_k}\psi - \mathrm{i}\partial_{x_k}(x_k\psi) = -\mathrm{i}\psi$ by application of the product rule of differentiation. Thus, $[x_j, \mathrm{i}\partial_{x_k}] = \delta_{jk}(-\mathrm{i})I$. Hence $\Delta A_\psi\Delta B_\psi \geq \frac{1}{4}\delta_{jk}|\langle\psi,\psi\rangle|^2$. In particular, if $j = k$ and if the wavefunction ψ is normalized to $\|\psi\| = 1$, then

$$\Delta A_\psi \Delta B\psi \geq \frac{1}{4}\,. \tag{5.4}$$ [3]

[2] By $\langle\psi, A^2\psi\rangle$ we mean $\langle A\psi, A\psi\rangle$, and by $\langle\psi, AB\psi\rangle$ we mean $\langle A\psi, B\psi\rangle$.

[3] This inequality has profound consequences in physics: suppose that the position of a particle can be measured to arbitrary precision. In classical physics, there is nothing that prevents the momentum from being measured to arbitrary precision as well. However, in Quantum Mechanics, the above inequality implies that the variance

Remark

Here we repeat the argument used in the proof above. If A is a self-adjoint operator $\langle \psi, A\psi \rangle = \langle A\psi, \psi \rangle = \overline{\langle \psi, A\psi \rangle}$, so $\langle \psi, A\psi \rangle \in \mathbb{R}$. Hence, the expectation values of self-adjoint operators are real-valued (or vector-valued with real components).

We consider $H : H^2\left(\mathbb{R}^{3N}\right) \subseteq L^2\left(\mathbb{R}^{3N}\right) \to L^2\left(\mathbb{R}^{3N}\right)$,

$$H = \sum_{j=1}^{N} \left(-\Delta_{x_j} - \frac{Z}{|x_j|} \right) + \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|}\,, \tag{5.5}$$

where $x_1, \ldots, x_N \in \mathbb{R}^3$. equation (5.5) is the Hamiltonian (the Hamilton operator) of an ion with N electrons and a nucleus of charge Z. If $N = Z$, the system is electrically neutral and is called an atom.

For notational simplicity, we will write $H = -\Delta + V$, where $-\Delta = -\sum_{j=1}^{N} \Delta_{x_j}$ is the total kinetic energy, i.e. the sum of the kinetic energies of all electrons. Then for all $\psi \in H^2\left(\mathbb{R}^{3N}\right)$ we have $\langle \psi, H\psi \rangle = \langle \psi, -\Delta\psi \rangle + \langle \psi, V\psi \rangle = \langle \nabla\psi, \nabla\psi \rangle + \langle \psi, V\psi \rangle$, so actually $\langle \psi, H\psi \rangle$ makes sense for all $\psi \in H^1\left(\mathbb{R}^{3N}\right)$. It was proven in Exercise 13 that H is bounded from below, namely $\exists C \in \mathbb{R}$ such that $\langle \psi, H\psi \rangle \geq C\|\psi\|^2$. [4]

Definition

The *ground state energy* of H is defined by $E_0 := \inf_{\substack{\psi \in H^1\left(\mathbb{R}^{3N}\right) \\ \|\psi\|_{L^2} = 1}} \langle \psi, H\psi \rangle$. The infimum exists because by the above argument there exists a lower bound on $\langle \psi, H\psi \rangle$. If the infimum is attained for some $\psi_0 \in H^1\left(\mathbb{R}^{3N}\right)$, then ψ_0 is called a *ground state*.

Theorem 5.4

If H has a ground state ψ_0, then $\psi_0 \in H^2\left(\mathbb{R}^{3N}\right)$ and $H\psi_0 = E_0\psi_0$.

---

of the momentum becomes arbitrarily large, i.e. it is not possible to constrain the momentum of the particle in the limit that the uncertainty of the position goes to zero.

[4] In classical physics, the total energy is given by $\frac{p^2}{2m} - \frac{1}{|x-y|}$ and it is possible to fix p while decreasing $|x-y|$. Thus it is possible for the energy to become arbitrarily negative by fixing p and taking $x \to y$. In Quantum Mechanics, however, this is forbidden by the Heisenberg Uncertainty Principle: if we take $|x-y|$ smaller and smaller, the variance of p $\left(\langle \psi, p^2\psi \rangle - \langle \psi, p\psi \rangle^2\right)$ increases due to Equation 5.4. Since $\langle \psi, p\psi \rangle = 0$ if $\langle \psi, \psi \rangle$ is symmetric in $p \to -p$, we obtain that $\left\langle \psi, p^2\psi \right\rangle$ increases as $|x-y|$ becomes small. Thus, the energy $\frac{p^2}{2m} - \frac{1}{|x-y|}$ cannot become arbitrarily negative in Quantum Mechanics and H is bounded from below.

Proof. Let $v \in C_c^\infty\left(\mathbb{R}^{3N}\right)$, $f(s) := \langle(\psi_0 + sv), H(\psi_0 + sv)\rangle - E_0\langle\psi_0 + sv, \psi_0 + sv\rangle$. Then by assumption $f(0) = 0$, and by definition of E_0 we have $f(s) \geq 0\,\forall s \in \mathbb{R}$. Therefore

$$f'(0) = 0. \tag{5.6}$$

But $f(s) = \langle\psi_0, H\psi_0\rangle + 2s\operatorname{Re}\langle v, H\psi_0\rangle + s^2\langle v, Hv\rangle - E_0\langle\psi_0,\psi_0\rangle - 2sE_0\operatorname{Re}\langle v,\psi_0\rangle - E_0 s^2\langle v, v\rangle$, so

$$f'(0) = 2\operatorname{Re}\langle v, H\psi_0\rangle - 2E_0\langle v,\psi_0\rangle = 2\operatorname{Re}(\langle v, H\psi_0\rangle - \langle v, E_0\psi_0\rangle). \tag{5.7}$$

Equation (5.6) and equation (5.7) imply that $\operatorname{Re}(\langle v, H\psi_0\rangle - \langle v, E_0\psi_0\rangle) = 0\,\forall v \in C_c^\infty\left(\mathbb{R}^{3N}\right)$. So $\langle v, H\psi_0\rangle - \langle v, E_0\psi_0\rangle = 0\,\forall v \in C_c^\infty\left(\mathbb{R}^{3N}\right)$. We have $\langle\nabla v, \nabla\psi_0\rangle + \langle v, V\psi_0\rangle = v\langle E_0,\psi_0\rangle$ $\overset{v\in C_c^\infty(\mathbb{R}^{3N})}{\Rightarrow}$ $\langle-\Delta v,\psi_0\rangle = \langle v, -V\psi_0 + E_0\psi_0\rangle\ \forall v \in C_c^\infty\left(\mathbb{R}^{3N}\right)$. Since $-V\psi_0 + E_0\psi_0 \in L^2\left(\mathbb{R}^{3N}\right)$ by Hardy's inequality, by the definition of weak derivatives we have $-\Delta\psi_0 \in L^2\left(\mathbb{R}^{3N}\right)$ and $-\Delta\psi_0 = -V\psi_0 + E_0\psi_0$, so $H\psi_0 = E_0\psi_0$. ■

Theorem 5.5 (Existence and uniqueness of the ground state of the hydrogen atom)
The Hamiltonian $H = -\Delta - \dfrac{1}{|x|}$, $H : H^2\left(\mathbb{R}^3\right) \subseteq L^2\left(\mathbb{R}^3\right) \to L^2\left(\mathbb{R}^3\right)$ has (up to a constant) a unique ground state.

Proof. We write $E(\psi) = \langle\psi, H\psi\rangle$ and $E_0 = \inf\limits_{\substack{\psi\in H^1(\mathbb{R}^3)\\ \|\psi\|_{L^2}=1}} E(\psi)$. We have $E(\psi) = \|\nabla\psi\|_{L^2}^2 - \int_{\mathbb{R}^3}\dfrac{|\psi(x)|^2}{|x|}\,\mathrm{d}x$. By the Coulomb uncertainty principle (Exercise 17) we have $\int_{\mathbb{R}^3}\dfrac{|\psi(x)|}{|x|}\,\mathrm{d}x \leq \|\nabla\psi\|_{L^2}\|\psi\|_{L^2}$ with equality if and only if $\psi(x) = D\mathrm{e}^{-c|x|}$. Thus

$$E(\psi) \geq \|\nabla\psi\|_{L^2}^2 - \|\nabla_\psi\|_{L^2}\|\psi\|_{L^2} = \left(\|\nabla\psi\|_{L^2} - \frac{1}{2}\|\psi\|_{L^2}\right)^2 - \frac{1}{4}\|\psi\|_{L^2}^2 \tag{5.8}$$

with equality if and only if $\|\nabla\psi\|_{L^2} = \dfrac{1}{2}\|\psi\|_{L^2}$. But in $E(\psi) \geq \|\nabla\psi\|_{L^2}^2 - \|\nabla\psi\|_{L^2}\|\psi\|_{L^2}$ equality holds if and only if

$$\psi(x) = D\mathrm{e}^{-c|x|} \tag{5.9}$$

for some $D \in \mathbb{C}$ and $c > 0$. Since $\nabla\mathrm{e}^{-c|x|} = -c\dfrac{x}{|x|}\mathrm{e}^{-c|x|}$, we obtain

$$\left\|\nabla\mathrm{e}^{-c|x|}\right\|_{L^2} = |c|\left\|\mathrm{e}^{-c|x|}\right\|_{L^2}. \tag{5.10}$$

Thus, equation (5.9) and equation (5.10) hold simultaneously if and only if $\psi(x) = D\mathrm{e}^{-\frac{1}{2}|x|}$. Thus, equation (5.8) holds with equality if and only if $\psi(x) = D\mathrm{e}^{-\frac{|x|}{2}}$ for some $D \in \mathbb{C}$. ■

If we require $\|\psi\|_{L^2} = 1$, we obtain $|D| = \dfrac{1}{\sqrt{8\pi}}$, so $E_0 \sim \dfrac{1}{\sqrt{8\pi}}\mathrm{e}^{-\frac{|x|}{2}}$.

6 Some tools of functional analysis

In finite dimensions, the property that every bounded sequence has a convergent subsequence is very useful (e.g. for showing that a function has a minimum or maximum).
However, in infinite dimensions we encounter the problem that this property is not true anymore, e.g. in a Hilbert space an orthonormal basis (ONB) $(e_n)_{n\in\mathbb{N}}$ is bounded, but does not have a convergent subsequence.
We try to "weaken" the definition of convergence in infinite dimensions hoping that we will again have a property similar to the existence of convergent subsequences, as is the case for finite dimensions.

Definition 6.1

Let $(X, \|\cdot\|)$ be a real (resp. complex) Banach space and $y \in X$. Let $(y_n)_{n\in\mathbb{N}}$ be a sequence in X. We say that y_n *converges weakly* to y, $y_n \rightharpoonup y$ if $f(y_n) \to f(y)$ for all linear and continuous functions $f : X \to \mathbb{R}$ (resp. $f : X \to \mathbb{C}$).

Remark 6.2

Let $(X, \langle\cdot,\cdot\rangle)$ is a Hilbert space. Then $f : X \to \mathbb{R}$ ($f : X \to \mathbb{C}$) is linear and continuous if and only if there exists a $y \in X$ with $\forall v \in X : f(v) = \langle y, v\rangle$ (Riesz representation theorem). Therefore, $y_n \rightharpoonup y \Leftrightarrow \langle v, y_n\rangle \overset{n\to\infty}{\to} \langle v, y\rangle \; \forall v \in X$.

Example 6.1

Let $(X, \langle\cdot,\cdot\rangle)$ be a Hilbert space and $(x_n)_{n\in\mathbb{N}}$ be an orthonormal sequence, i.e. $\langle x_n, x_m\rangle = \delta_{mn} = \begin{cases} 1, & n = m \\ 0, & n \neq m \end{cases}$. Then $x_n \rightharpoonup 0$.

Proof. Let $v \in X$. Then by Parseval's identity $\sum_{n\in\mathbb{N}} |\langle x_n, v\rangle|^2 \leq \|v\|^2$. Thus $\sum_{n\in\mathbb{N}} |\langle x, v\rangle|^2$ is convergent $\Rightarrow \langle x_n, v\rangle \to 0$ as $n \to \infty$. However, $x_n \not\to 0$ because $\|x_n\| = 1 \, \forall n \in \mathbb{N}$. ■

Theorem 6.3

Let X be a Banach space. If $x_n \rightharpoonup x$ for some $x \in X$, then x_n is bounded and

$$\|x\| \leq \liminf_{n\to\infty} \|x_n\| . \tag{6.1}$$

Proof. While this holds for Banach spaces, we will only prove it for Hilbert spaces: In this case $\|x\|^2 = \langle x, x\rangle = \lim_{n\to\infty} \langle x_n, x\rangle \leq \liminf_{n\to\infty} \|x_n\|\|x\|$. ■

Theorem 6.4 (Banach-Alaoglu, special case)

Let $(X, \langle\cdot,\cdot\rangle)$ be a Hilbert space. Then every bounded sequence in X has a weakly convergent subsequence.

Theorem 6.5

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

Proof. $\|x_n - x\|^2 = \langle x_n - x, x_n - x\rangle = \langle x_n, x_n\rangle - \langle x_n, x\rangle - \langle x, x_n\rangle + \langle x, x\rangle$. But $\langle x_n, x\rangle \to \langle x, x\rangle$ as $n \to \infty$, so $\|x_n - x\|^2 \to \langle x_n, x_n\rangle - \langle x, x\rangle \to 0$ as $n \to \infty$, since $\|x_n\| \to \|x\|$. ■

Definition 6.6 (Compact operators)

Let X, Y be Banach spaces and $K : X \to Y$ be a linear operator. K is called *compact* if for every bounded sequence $(x_n)_{n\in\mathbb{N}}$ in X Kx_n has a convergent subsequence in Y.

Theorem 6.7

Let X, Y be Hilbert spaces and $K : X \to Y$ linear. Then K is compact if and only if $x_n \rightharpoonup x$ implies that $Kx_n \to Kx$ for all sequences $(x_n)_{n\in\mathbb{N}}$ in X and for all $x \in X$.

Proof.

- "$\Rightarrow$": Let $f : Y \to \mathbb{R}$ (resp $\mathbb{C}$) be linear and continuous. Then $(f \circ K) : X \to \mathbb{R}$ (resp. $\mathbb{C}$) is continuous as a composition of continuous functions. Since $x_n \rightharpoonup x$, we find $f(Kx_n) \to f(Kx)$. Since f was arbitrary, it follows that

  $$Kx_n \rightharpoonup Kx . \tag{6.2}$$

  To show that $Kx_n \to Kx$ we prove that every subsequence Kx_{n_l} has a (sub-)subsequence $Kx_{n_{l_m}}$ with $Kx_{n_{l_m}} \to Kx$. x_{n_l} is bounded, and since K is compact Kx_{n_l} has a convergent subsequence

  $$Kx_{n_{l_m}} \to y \tag{6.3}$$

for some y in Y, so $x_{n_{l_m}} \rightharpoonup y$. (6.4)

From equation (6.2) and equation (6.4) it follows that $y = Kx$. (6.5)

equation (6.3) and equation (6.5) complete the proof.

- "$\Leftarrow$": Let $(x_n)_{n\in\mathbb{N}}$ be bounded. By Theorem 6.4 there exists $x \in X$ and a subsequence x_{n_k} with $x_{n_k} \rightharpoonup x$. But $Kx_{n_k} \to Kx$, so Kx_n has a convergent subsequence.

■

Theorem 6.8

Let X, Y be Hilbert spaces (actually, Banach spaces are sufficient) and $K_n : X \to Y$ a sequence of compact operators. If $K : X \to Y$ is linear and $\|K_n - K\| \overset{n\to\infty}{\to} 0$, then K is also compact.

Sketch of proof. Let $(x_m)_{m\in\mathbb{N}}$ be a bounded sequence in X. If K_1 is compact, then there exists a subsequence $(x_m)_{m\in A_1}$, $A_1 \subseteq \mathbb{N}$, such that $(K_1 x_m)_{m\in A_1}$ converges. If K_2 is compact and $(x_m)_{m\in A_1}$ bounded, then there exists a subsequence $(x_m)_{m\in A_2}$, $A_2 \subseteq \mathbb{N}$, such that $(K_2 x_m)_{m\in A_2}$ converges. Repeating the argument we find a family of subsequences $A_1 \supseteq A_2 \supseteq A_3 \supseteq \ldots \supseteq \ldots A_n \supseteq \ldots$ such that $(K_n x_m)_{m\in A_n}$ is convergent. Choose $m_1 \in A_1$, $m_2 \in A_2, \ldots, m_n \in A_n, \ldots$ such that $m_1 < m_2 < \ldots < m_n < \ldots$. Then $(K_n x_{m_l})_{l\in\mathbb{N}}$ is convergent for all $n \in \mathbb{N}$. Let $y_n := \lim_{n\to\infty} K_n x_{m_l}$. Then $y_n \to y$ for some $y \in Y$ and $Kx_{m_l} \to y$. ■

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.

Idea. Let $T_f := J \circ G_f$, $G_f : H^1(\mathbb{R}^n) \to B := \{g \in H^1(\mathbb{R}^n) : \operatorname{supp}(g) \subseteq \operatorname{supp}(f)\}$,
$G_f := f\psi$, $J : B \to L^2(\mathbb{R}^n)$, $Jg := g$. G_f is continuous by the Leibniz rule, B is compact by the Rellich-Kondrachov theorem, so T_f is compact as a composition of a continuous and a compact operator. ■

Theorem 6.10

Let $f \in C(\mathbb{R}^n)$ with $\lim_{|x|\to\infty} f(x) = 0$. Then $T_f : H^1(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$, $T_f\psi = f\psi$ is compact.

Proof. Exercise 31. Hint: Combine Theorems 6.8 and 6.9. ■

7 Decomposition of an operator

Theorem 7.1

Let X be a complex-valued Banach space and $A : D \subseteq X \to X$ a linear operator. Let γ be a simply closed [1] positively oriented (counter-clockwise) curve lying in the resolvent set of A. If inside of γ there is no point of $\sigma(A)$, then

(i) $\oint_\gamma (z - A)^{-1} \,\mathrm{d}z = 0$ (Cauchy)

(ii) If $w \in \mathbb{C}$ is inside of γ, then

$$(w - A)^{-1} = \frac{1}{2\pi\mathrm{i}} \oint_\gamma \frac{(z - A)^{-1}}{z - w} \,\mathrm{d}z \qquad \text{(Cauchy integral formula).} \tag{7.1}$$

Proof. (i) Let $f(z) := (z - A)^{-1}$. Then $\lim_{z\to z_0} \frac{f(z) - f(z_0)}{z - z_0} = \lim_{z\to z_0} \frac{(z - A)^{-1} - (z_0 - A)^{-1}}{z - z_0}$ $= \lim_{z\to z_0} \frac{(z - A)^{-1}[(z_0 - A) - (z - A)](z_0 - A)^{-1}}{z - z_0} = -(z_0 - A)^{-2}$. Thus f is complex differentiable in γ and inside of γ and therefore $\oint f(z)\,\mathrm{d}z = 0$ by repeating the arguments of the proof of the traditional theorem of Cauchy.

(ii) Since $\frac{1}{2\pi\mathrm{i}} \oint_\gamma \frac{1}{z - w} \,\mathrm{d}z = 1$, equation (7.1) is equivalent to $\frac{1}{2\pi\mathrm{i}} \oint_\gamma \frac{(w - A)^{-1}}{z - w} \,\mathrm{d}z$ $= \frac{1}{2\pi\mathrm{i}} \oint_\gamma \frac{(z - A)^{-1}}{z - w} \,\mathrm{d}z \Leftrightarrow \oint_\gamma \frac{(w - A)^{-1} - (z - A)^{-1}}{z - w} \,\mathrm{d}z = 0$ $\Leftrightarrow \oint_\gamma (w - A)^{-1}(z - A)^{-1} \,\mathrm{d}z = 0$, which holds by part (i). ■

Definition 7.2

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

[1] By "simply closed" we mean that γ is closed and that the set enclosed by γ is connected.

Note: $\|A^n\|^{\frac{1}{n}} \leq \|A\| \, \forall n \in \mathbb{N}$.

Theorem 7.3

Let $A \in \mathcal{L}(X)$. Then

(1) $\sigma(A) \neq \emptyset$ and $r_A = \sup\limits_{c \in \sigma(A)} |c|$

(2) If X is a Hilbert space and A self-adjoint and bounded, then $\|A\| = r_A = \sup\limits_{c \in \sigma(A)} |c|$.

Proof. (1) It was shown in Exercise 23 that $\sigma(A) \neq \emptyset$. If $|z| > r_A$, then $\limsup\limits_{n\to\infty} \left\| \frac{A^n}{z^n} \right\|^{\frac{1}{n}} = \frac{r_a}{|z|} < 1$. Therefore $\sum\limits_{n=0}^{\infty} \frac{A^n}{z^n}$ converges absolutely and therefore also in the operator norm. In particular, $\frac{A^n}{z^n} \overset{n\to\infty}{\to} 0$. Thus we can repeat the argument of Exercise 7 to conclude that $\left(I - \frac{A}{z}\right)$ is invertibel and $\left(I - \frac{A}{z}\right)^{-1} = \sum\limits_{n=0}^{\infty} \frac{A^n}{z^n}$. Thus $z - A = z\left(1 - \frac{A}{z}\right)$ is invertible for $|z| > r_A \Rightarrow r_A \geq \sup\limits_{c\in\sigma(A)} |c|$. It remains to prove that $r_A \leq \sup\limits_{c\in\sigma(A)} |c|$. Let $f(s) := (1 - sA)^{-1}$. $f(s)$ is well-defined and bounded for $s < \frac{1}{\sup_{c\in\sigma(A)} |c|}$ (because then $\frac{1}{s} \notin \sigma(A)$). It follows from Exercise 24 that $\sum\limits_{n=0}^{\infty} s^n A^n$ is absolutely convergent. In particular, $\forall s < \frac{1}{\sup_{c\in\sigma(A)} |c|}$: $\limsup\limits_{n\to\infty} \|s^n A^n\|^{\frac{1}{n}} \leq 1$. Therefore $\forall s < \frac{1}{\sup_{c\in\sigma(A)} |c|} : r_A \leq \frac{1}{s}$. Hence $r_A \leq \sup\limits_{c\in\sigma(A)} |c|$.

(2) We showed in (1) that $r_A = \sup\limits_{c\in\sigma(A)} |c|$. By definition, $r_A = \limsup\limits_{n\to\infty} \|A^n\|^{\frac{1}{n}} \leq \|A\|$ (this also holds if A is not self-adjoint). If A is self-adjoint and bounded and $\eta \in D(A)$ ($= \mathcal{H}$, since A is bounded) with $\|\eta\| = 1$, then $\|A\eta\|^2 = \langle A\eta, A\eta\rangle \overset{A \text{ bounded and self-adjoint}}{=} \langle \eta, A^2\eta\rangle \leq \|\eta\|\|A^2\eta\| \leq \|A^2\|$. Thus $\|A^2\| = \sup\limits_{\|\eta\|=1} \|A\eta\|^2 \leq \|A^2\|\|A\|^2$. Hence $\|A\|^2 = \|A^2\|$. By induction, we find $\|A\|^{2^n} = \|A^{2^n}\|$. Therefore, $\forall n \in \mathbb{N} : \|A^{2^n}\|^{\frac{1}{2^n}} = \|A\|$. Hence $\limsup\limits_{n\to\infty} \|A^n\|\frac{1}{n} \geq \|A\| \Rightarrow r_A \geq \|A\|$.

■

Theorem 7.4

Let $\mathcal{H}$ be a complex Hilbert space and $A : D(A) \subseteq \mathcal{H} \to \mathcal{H}$ self-adjoint. Assume that $\sigma(A) = \sigma' \cup \sigma''$, where $\sigma', \sigma'' \subseteq \mathbb{R}$ with $\sigma' \cap \sigma'' = \emptyset$ and σ' is compact. Let γ be a simply closed, positively oriented curve such that σ' is inside of γ and σ'' is outside of γ. Let $P := \frac{1}{2\pi \mathrm{i}} \oint_\gamma (z-A)^{-1}\,\mathrm{d}z$. Then

(1) P is independent of the choice of γ (as long as γ satisfies the conditions stated above)

(2) P is an orthogonal projection

(3) $PA \subset AP$ (AP is an extension of PA). In particular, A leaves $\mathrm{Ran}\,(P)$ and $\mathrm{Ran}\,(1-P) = \mathrm{Ran}\,(P)^\perp$ invariant

(4) Let $A' = A|_{\mathrm{Ran}(P)} : D\,(A) \cap \mathrm{Ran}\,(P) \to \mathrm{Ran}\,(P)$ and $A'' = A|_{\mathrm{Ran}(P)^\perp} : D\,(A) \cap (\mathrm{Ran}\,(P))^\perp \to (\mathrm{Ran}\,(P))^\perp$. Then $\sigma\left(A'\right) = \sigma', \sigma\left(A''\right) = \sigma''$ and A', A'' are self-adjoint

(5) A' is bounded

(6) If $\sigma' = \{\lambda\}$ for some $\lambda \in \mathbb{R}$, then $A' = \lambda P$

Proof. (1) We may assume without loss of generality that one curve is inside of the other (see below; if not, we can find a third curve inside of both curves) and deform it into the contour shown on the right-hand side of the figure below. Applying Cauchy's theorem for δ_1, δ_2 we find $\oint_{\delta_1} (z-A)^{-1}\,\mathrm{d}z + \oint_{\delta_2} (z-A)^{-1}\,\mathrm{d}z = 0$. Therefore $\oint_\gamma (z-A)^{-1}\,\mathrm{d}z = \oint_{\tilde\gamma} (z-A)^{-1}\,\mathrm{d}z$. Thus P is independent of the choice of γ.

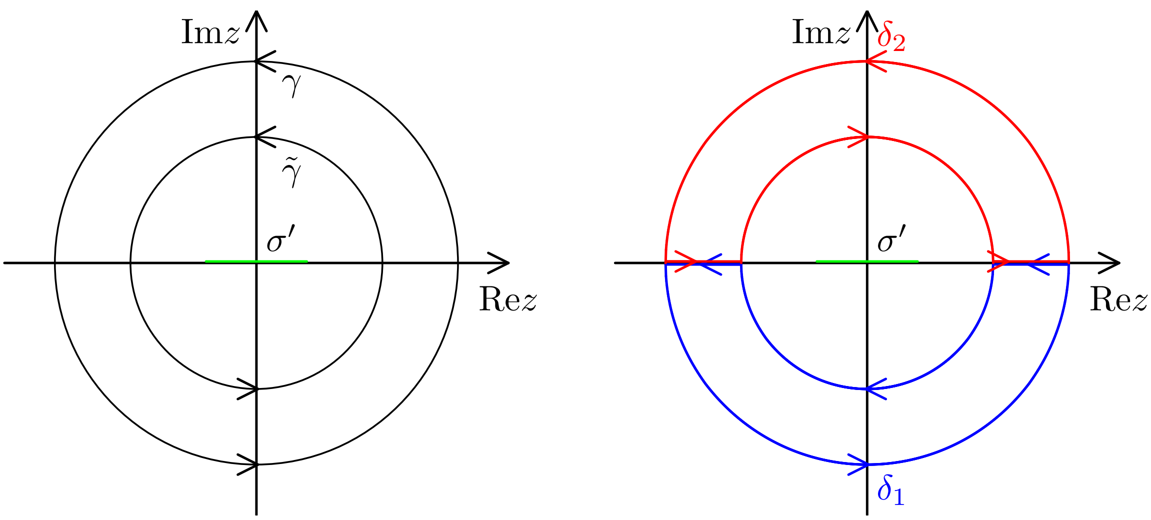

Figure 7.1: Deformation of the integration contour; created with MGA-TeX 2.4 by K. Fritzsche [4].

(2) We have to show: $P^2 = P$, $P^* = P$ (this implies that $\langle (1-P)\varphi, P\psi\rangle = \langle P(1-P)\varphi, \psi\rangle = \big\langle (P-P^2)\varphi, \psi\big\rangle = 0$). Clearly P is bounded because $(z-A)^{-1}$ is continuous and therefore bounded in γ. Let γ_1 and γ_2 be two simply closed, positively oriented curves with σ' in the inside of both curves and γ_2 inside of γ_1. Then

$$\begin{aligned} P^2 &= \frac{1}{(2\pi\mathrm{i})^2}\oint_{\gamma_1}(z-A)^{-1}\,\mathrm{d}z\oint_{\gamma_2}(s-A)^{-1}\,\mathrm{d}s = \frac{1}{(2\pi\mathrm{i})}\oint_{\gamma_1}\oint_{\gamma_2}(z-A)^{-1}(s-A)^{-1}\,\mathrm{d}s\,\mathrm{d}z \\ &\overset{\text{Exercise 4}}{=} \frac{1}{(2\pi\mathrm{i})^2}\oint_{\gamma_1}\left[\oint_{\gamma_2}\left(\frac{(z-A)^{-1}}{s-z} - \frac{(s-A)^{-1}}{s-z}\right)\mathrm{d}s\right]\mathrm{d}z\,. \end{aligned}$$

The first contribution vanishes by Cauchy's theorem, so we obtain $P^2 = \frac{1}{(2\pi\mathrm{i})^2}\oint_{\gamma_1}\oint_{\gamma_2}\frac{(s-A)^{-1}}{z-s}\,\mathrm{d}s\,\mathrm{d}z \overset{\text{Fubini}}{=} \frac{1}{(2\pi\mathrm{i})^2}\oint_{\gamma_2}\oint_{\gamma_1}\frac{(s-A)^{-1}}{z-s}\,\mathrm{d}z\,\mathrm{d}s = \frac{1}{2\pi\mathrm{i}}\oint_{\gamma_2}(s-A)^{-1} = P$, where we have used the Cauchy integral formula in the second-to-last step. Thus P is a projection. Choosing γ to be a circle, $\gamma(\theta) = c + r\mathrm{e}^{\mathrm{i}\theta}$ with $\theta \in [0, 2\pi], c \in \mathbb{R}, d > 0$, we find $P = \frac{1}{2\pi\mathrm{i}}\int_0^{2\pi}\left(c + r\mathrm{e}^{\mathrm{i}\theta} - A\right)^{-1} r\mathrm{i}\mathrm{e}^{\mathrm{i}\theta}\,\mathrm{d}\theta$.

Thus $P^* = -\frac{1}{2\pi\mathrm{i}}\int_0^{2\pi}\left(c + r\mathrm{e}^{-\mathrm{i}\theta} - A\right)^{-1}(-\mathrm{i}r)\,\mathrm{e}^{-\mathrm{i}\theta}\,\mathrm{d}\theta$

$\overset{\tilde\theta = 2\pi-\theta}{=} \frac{1}{2\pi\mathrm{i}}\int_0^{2\pi}\left(c + r\mathrm{e}^{\mathrm{i}\tilde\theta} - A\right)^{-1}\mathrm{i}r\mathrm{e}^{\mathrm{i}\tilde\theta}\,\mathrm{d}\theta = P.$

(3) We prove: if $\psi \in D(A)$, then $AP\psi = PA\psi$. We have $P\psi = \left(\frac{1}{2\pi\mathrm{i}}\oint_\gamma (z-A)^{-1}\,\mathrm{d}z\right)\psi = \frac{1}{2\pi\mathrm{i}}\oint_\gamma (z-A)^{-1}\psi\,\mathrm{d}z$ (Left as an exercise).

$$A(z-A)^{-1} \overset{\text{Exercise 4}}{=} -I + z(z-A)^{-1} \tag{7.2}$$

is bounded it follows that $(z-A)^{-1}\psi : \mathbb{C} \to \mathcal{H}$ is continuous in the graph norm of A. Thus

$$\begin{aligned} AP\psi &\overset{A=A^*\Rightarrow A=A^*\text{ closed, Exercise 5}}{=} \frac{1}{2\pi\mathrm{i}}\oint_\gamma A(z-A)^{-1}\psi\,\mathrm{d}z \\ &\overset{\psi\in D(A),\text{ Exercise 4}}{=} \frac{1}{2\pi\mathrm{i}}\oint_\gamma (z-A)^{-1}A\psi\,\mathrm{d}z\,. \end{aligned} \tag{7.3}$$

Hence $AP\psi = \frac{1}{2\pi\mathrm{i}}\oint_\gamma (z-A)^{-1}\,\mathrm{d}z\,A\psi = PA\psi$. Thus $PA \subset AP$. Let $\varphi \in D(A) \cap \operatorname{Ran}(P)$. Then $A\varphi \overset{P\varphi=\varphi}{=} AP\varphi \in \operatorname{Ran}(P)$. So

$$A(D(A) \cap \operatorname{Ran}(P)) \subseteq \operatorname{Ran}(P)\,. \tag{7.4}$$

Similarly one shows that

$$A\left(D(A) \cap (\operatorname{Ran}(P))^\perp\right) \subseteq (\operatorname{Ran}(P))^\perp\,. \tag{7.5}$$

(4) In view of equations (7.4) and (7.5) $A' = A|_{\text{Ran}(P)}$ and $A'' = A|_{(\text{Ran}(P))^\perp}$ are well-defined. A' is bounded because $A' = AP|_{\text{Ran}(P)}$, but $AP \overset{\text{equation (7.3)}}{=} \frac{1}{2\pi \mathrm{i}} \oint_\gamma A(z-A)^{-1}\,\mathrm{d}z$ $\overset{\text{equation (7.2)}}{=} \frac{1}{2\pi \mathrm{i}} \oint_\gamma \left(-I + z(z-A)^{-1}\right)\mathrm{d}z$, and $-I + z(z-A)^{-1}$ is uniformly bounded on γ. Thus AP is bounded. Let $z \in \mathbb{C}$. Then $z \in \rho(A) \Leftrightarrow (z-A) : D(A) \subseteq \mathcal{H} \to \mathcal{H}$ is a bijection with bounded inverse since A leaves $\text{Ran}(P)$ and $(\text{Ran}(P))^\perp$ invariant $\Leftrightarrow \begin{cases} z - A' : D(A) \cap \text{Ran}(P) \to \text{Ran}(P) \\ z - A'' : D(A) \cap (\text{Ran}(P))^\perp \to (\text{Ran}(P))^\perp \end{cases}$ are bijections with bounded inverses $\Leftrightarrow$ $z \in \rho(A') \cap \rho(A'')$. Thus

$$\rho(A) = \rho(A') \cap \rho(A'') \Rightarrow \sigma(A') \cup \sigma(A'') = \sigma(A). \tag{7.6}$$

We will prove $\sigma(A') \subseteq \sigma', \sigma(A'') \subseteq \sigma''$. Let $z \in \rho(A) \setminus \text{tr}\{\gamma\}$.

$$\begin{aligned}(w-A)^{-1}P &= \frac{1}{2\pi \mathrm{i}} \oint_\gamma (w-A)^{-1}(z-A)^{-1}\,\mathrm{d}z \\ &\overset{\text{Exercise 4}}{=} \frac{1}{2\pi \mathrm{i}} \oint_\gamma \left(\frac{(w-A)^{-1}}{z-w} - \frac{(z-A)^{-1}}{z-w}\right)\mathrm{d}z\,. \end{aligned} \tag{7.7}$$

Assume that w is outside of γ, then $\oint_\gamma \frac{(w-A)^{-1}}{z-w}\,\mathrm{d}z = 0$, thus $(w-A)^{-1}P$ $= \frac{1}{2\pi \mathrm{i}} \oint_\gamma \frac{(z-A)^{-1}}{w-z}\,\mathrm{d}z$. This formula gives an expression for $(w-A)^{-1}$ for all $w \in \rho(A) \setminus \text{tr}\{\gamma\}$, but it can be naturally extended for all $w \in \text{tr}\{\gamma\}^C$. Thus

$$w \in \rho(A) \Rightarrow \sigma(A') \subseteq \sigma'. \tag{7.8}$$

If w is inside of γ, then $\frac{1}{2\pi \mathrm{i}} \oint_\gamma \frac{1}{z-w}\,\mathrm{d}z = 1$ and thus $(w-A)^{-1}P$ $= (w-A)^{-1} - \frac{1}{2\pi \mathrm{i}} \oint_\gamma \frac{(z-A)^{-1}}{z-w}\,\mathrm{d}z \Rightarrow (w-A)^{-1}(1-P) = \frac{1}{2\pi \mathrm{i}} \oint_\gamma \frac{(z-A)^{-1}}{z-w}\,\mathrm{d}z$. We have $(w-A'')^{-1} = \left(\frac{1}{2\pi \mathrm{i}} \oint_\gamma \frac{(z-A)^{-1}}{z-w}\,\mathrm{d}z\right)\Big|_{(\text{Ran}(P))^\perp}$ for all $w \in \rho(A)$ inside of γ. Since this formula can be naturally extended for all w inside γ, we find that

$$\sigma(A'') \subseteq \sigma''. \tag{7.9}$$

Equations (7.6), (7.8) and (7.9) imply that $\sigma(A') \cup \sigma(A'') = \sigma(A) = \sigma' \cup \sigma'' \Rightarrow \sigma' = \sigma(A')$ and $\sigma'' = \sigma(A'')$.

(5) That A' is bounded was already proven in (4).

(6) If $\sigma' = \{\lambda\}$ for some $\lambda \in \mathbb{R}$, then $\sigma\left(A'\right) = \{\lambda\} \Rightarrow \sigma\left(A' - \lambda P\right) = \{0\}$. Since $A' - \lambda P$ is bounded and self-adjoint, it follows from Theorem 7.3 that $\left\|A' - \lambda P\right\| = 0 \Rightarrow A' - \lambda P = 0$, hence $AP = \lambda P$.

■

Theorem 7.5 (Identification of the spectrum with sequences)
Let $A : D(A) \subseteq \mathcal{H} \to \mathcal{H}$ be self-adjoint (then $\sigma(A) \subseteq \mathbb{R}$) and $\lambda \in \mathbb{R}$. Then $\lambda \in \sigma(A) \Leftrightarrow$ there exists a sequence $(\psi_n)_{n\in\mathbb{N}}$ in $D(A)$ with $\|\psi_n\| = 1$ and $\|(A-\lambda)\psi_n\| \stackrel{n\to\infty}{\to} 0$ (there exists a sequence of "approximate eigenfunctions").

Proof. • "$\Leftarrow$": If λ were in $\rho(A)$, then $(A-\lambda) : D(A) \subseteq \mathcal{H} \to \mathcal{H}$ would be a bijection with a bounded inverse. So $\exists c > 0$ with

$$\left\|(A-\lambda)^{-1}\varphi\right\| \leq c\|\varphi\| \forall \varphi \in \mathcal{H}. \tag{7.10}$$

If $\psi \in D(A)$ then $\exists \varphi \in \mathcal{H}$ with $\psi = (A-\lambda)^{-1}\varphi$. Thus $\|\psi\| = \left\|(A-\lambda)^{-1}\varphi\right\| \stackrel{\text{eqn. (7.10)}}{\leq} c\|\varphi\| = c\|(A-\lambda)\psi\| \Rightarrow \|(A-\lambda)\psi\| \geq c\|\psi\| \forall \psi \in D(A)$, contradicting that $\|\psi_n\| = 1$ and $\|(A-\lambda)\psi\| \stackrel{n\to\infty}{\to} 0$. Thus $\lambda \in \sigma(A)$.

• "$\Rightarrow$": Assume $\lambda \in \sigma(A)$. If there is no sequence $(\psi_n)_{n\in\mathbb{N}}$ in $D(A)$ with $\|\psi_n\| = 1$ and $\|(A-\lambda)\psi_n\| \to 0$, then $c := \inf\limits_{\substack{\psi \in D(A) \\ \|\psi\|=1}} \|(A-\lambda)\psi\| > 0$. Therefore

$$\forall \psi \in D(A) : \|(A-\lambda)\psi\| < c\|\psi\|. \tag{7.11}$$

We will prove

(i) $A - \lambda$ is injective.

(ii) $\operatorname{Ran}(A-\lambda)$ is closed.

(iii) $\operatorname{Ran}(A-\lambda)$ is dense, thus $A-\lambda$ is a bijection.

(iv) $(A-\lambda)^{-1}$ is bounded, contradicting $\lambda \in \sigma(A)$.

Proof:

(i) $(A-\lambda)\psi = 0 \Rightarrow \|\psi\| = 0 \Rightarrow \psi = 0$.

(ii) Exercise.

(iii) Exercise.

(iv) Since $(A - \lambda)^{-1}$ is well-defined and $\forall \psi \in D(A) : \|(A - \lambda)\psi\| > c\|\psi\|$, we find $\forall \varphi \in \mathcal{H} : \left\|(A - \lambda)^{-1}\varphi\right\| \leq \frac{1}{c}\|\varphi\|$.

■

8 Discrete and essential spectrum

Definition 8.1

Let $\mathcal{H}$ be a complex Hilbert space, $A : D(A) \subseteq \mathcal{H} \to \mathcal{H}$ self-adjoint.

The *discrete spectrum* $\sigma_d(A)$ of A is defined by

$\sigma_d(A) := \{\lambda \in \sigma(A) : \lambda$ eigenvalue of finite multiplicity and isolated in the spectrum$\}$.

The *essential spectrum* $\sigma_{\text{ess}}(A)$ of A is defined by $\sigma_{\text{ess}}(A) := \sigma(A) \setminus \sigma_d(A)$.

If H is the Hamiltonian of an atom or an ion, we define $\Sigma_R := \inf\limits_{\substack{\psi \in H^1 \\ \|\psi\|_{L^2}=1 \\ \text{supp}(\psi) \subseteq (B_R(0))^c}} \langle \psi, H\psi \rangle$,
$\Sigma := \lim\limits_{R\to\infty} \Sigma_R$. Then $\Sigma = \inf \sigma_{\text{ess}}(H)$. Σ is called *ionisation threshold (energy)*.
Let $E = \inf\limits_{\substack{\psi \in H^1 \\ \|\psi\|_{L^2}}} \langle \psi, H\psi \rangle$.
Case 1: $E = \Sigma$. In this case, it does not cost energy to remove an electron to infinite spatial distance (measured from the location of the nucleus).
Case 2: $E < \Sigma$: In this case, it costs energy to remove the electron to infinite spatial distance. Moreover $E \in \sigma_d(H)$ and a ground state exists.

Theorem 8.2 (Weyl's criterion)

Let $A : D \subseteq \mathcal{H} \to \mathcal{H}$ be self-adjoint, $\mathcal{H}$ a complex Hilbert space. Let $\lambda \in \mathbb{R}$.

Then $\lambda \in \sigma_{\text{ess}}(A) \Leftrightarrow$ there exists a sequence $(\psi_n)_{n\in\mathbb{N}}$ in D with

(1) $\|\psi_n\| = 1$

(2) $\|(A - \lambda)\psi_n\| \to 0$

(3) $\psi_n \rightharpoonup 0$.

Intuition: If $\|\psi_n\| = 1$ and $\psi_n \rightharpoonup 0$, then the sequence $(\psi_n)_{n\in\mathbb{N}}$ "lives" in an infinite-dimensional space (if not it would have a strongly convergent subsequence $\psi_{n_k} \to \psi$ for some $\psi \in \mathcal{H}$ with $\|\psi\| = 1$, contradicting $\psi_n \rightharpoonup 0$.

Remark

A sequence $(\psi_n)_{n\in\mathbb{N}}$ with the properties (1)-(3) from Theorem 8.2 is called a *Weyl sequence* for A, λ.

Proof. • "$\Leftarrow$": If there is a Weyl sequence for A and λ, then by Theorem 7.5 $\lambda \in \sigma(A)$. Assume that $\lambda \in \sigma_d(A)$. By Theorem 7.4 we can decompose A to A', A'' choosing $\sigma' = \{\lambda\}$. Since λ is an eigenvalue of finite multiplicity it follows that $\dim \operatorname{Ran}(P) < \infty$ (because $AP = \lambda P$). But $\underbrace{(A-\lambda)\psi_n}_{\to 0} = (A-\lambda)P\psi_n + (A-\lambda)P^{\perp}\psi_n = (A'-\lambda)P\psi_n + (A''-\lambda)P^{\perp}\psi_n$. Now $P\psi_n \to 0$ by Theorem 6.7 because $\psi_n \rightharpoonup 0$ and P is compact, so $(A'-\lambda)P\psi_n \to 0$, because A' is bounded by Theorem 7.4. Hence it follows that $(A''-\lambda)P^{\perp}\psi_0 \to 0$ (but $\left\|P^{\perp}\psi_n\right\| \to 1$). Thus $(A''-\lambda)\dfrac{P^{\perp}\psi_n}{\|P^{\perp}\psi_n\|} \to 0$, contradicting (by Theorem 7.5) the fact that $\lambda \notin \sigma\left(A''\right)$.

• "$\Rightarrow$": Assume $\lambda \in \sigma_{\text{ess}}(A)$.

(i) If λ is an eigenvalue of infinite multiplicity then there exists a sequence $(\psi_n)_{n\in\mathbb{N}}$ orthonormal with $(A-\lambda)\psi_n = 0$. But $\psi_n \rightharpoonup 0$ by Example 6.1.

(ii) If λ is not an eigenvalue of infinite multiplicity, then it is not an isolated point of the spectrum. Thus there exists a sequence $(a_n)_{n\in\mathbb{N}}$ in $\mathbb{R}$ with $a_n \to 0$, $a_n \neq 0\,\forall n \in \mathbb{N}$ and $\forall n \in \mathbb{N} : \lambda + a_n \in \sigma(A)$. Without loss of generality we can assume that $a_n > 0$ and

$$a_{n+1} < \frac{a_n}{2}. \tag{8.1}$$

By Theorem 7.5, for all $n \in \mathbb{N}$ there exists a $\psi_n \in D$ with

$$\|(A-\lambda-a_n)\psi_n\| \leq \mathrm{e}^{-\frac{1}{a_n}}. \tag{8.2}$$

From this it follows that $\|(A-\lambda)\psi_n\| \leq a_n + \mathrm{e}^{-\frac{1}{a_n}} \overset{n\to\infty}{\to} 0$. By the self-adjointness of A we have $\langle\psi_n, (a_n - a_m)\psi_m\rangle = \langle\psi_n, (A-\lambda-a_m)\psi_m\rangle - \langle(A-\lambda-a_n)\psi_n, \psi_m\rangle$. Thus, for $m \neq n$ we have $|\langle\psi_n, \psi_m\rangle| \leq \dfrac{\mathrm{e}^{-\frac{1}{a_n}} + \mathrm{e}^{-\frac{1}{a_m}}}{|a_n - a_m|}$ by use equation (8.1) and the triangle and Cauchy-Schwarz inequalities. Thus, if $m > n$, then $(a_n - a_m) \geq \dfrac{a_n}{2}$, and thus

$$|\langle\psi_n, \psi_m\rangle| \leq \frac{4\mathrm{e}^{-\frac{1}{a_n}}}{a_n}. \tag{8.3}$$

Since $\|\psi_m\| = 1$, by Theorem 6.4 we may assume that $\psi_m \rightharpoonup V$ for some $V \in \mathcal{H}$ after passing to a subsequence. Keeping n fixed in the limit $m \to \infty$, we obtain (using equation (8.3)) $|\langle\psi_n, V\rangle| \le \dfrac{4\mathrm{e}^{-\frac{1}{a_n}}}{a_n}$. But the limit $n \to \infty$ gives $|\langle V, V\rangle| = 0 \Rightarrow \|V\|^2 = 0$. Therefore $\psi_n \rightharpoonup 0$.

■

Example 8.1

Let $H : H^2(\mathbb{R}^3) \subseteq L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$, $H\psi = \left(-\Delta - \dfrac{1}{|x|}\right)\psi$. Then $\sigma_{\text{ess}}(H) = [0, \infty)$. In particular, the ground-state energy (which is $-\dfrac{1}{4}$ by Theorem 5.5) is in the discrete spectrum of H.

Proof. Let $\lambda \in \sigma_{\text{ess}}(H)$. Then by Weyl's criterion Theorem 8.2 there exists a sequence $(\psi_n)_{n\in\mathbb{N}}$ in $H^2(\mathbb{R}^3)$ with $\|\psi_n\|_{L^2} = 1$, $\|(H-\lambda)\psi_n\| \to 0$ and $\psi_n \rightharpoonup 0$. In particular, $\langle\psi_n, (H-\lambda)\psi_n\rangle \le \|\psi_n\|\|(H-\lambda)\psi_n\| \to 0$, so $\langle\psi_n, H\psi_n\rangle \to \lambda$. Therefore $\displaystyle\int_{\mathbb{R}^3} |\nabla\psi_n(x)|^2\,\mathrm{d}x - \int_{\mathbb{R}^3} \frac{|\psi_n(x)|^2}{|x|}\,\mathrm{d}x \to \lambda$ as $n \to \infty$. We have to show:

(i) ψ_n is bounded in $H^1(\mathbb{R}^3)$.

(ii) $\displaystyle\int_{\mathbb{R}^3} \frac{|\psi_n(x)|^2}{|x|}\,\mathrm{d}x \to 0$.

It then follows that $\lambda \ge 0$.

(i) $\displaystyle\int_{\mathbb{R}^3} \frac{|\psi_n(x)|^2}{|x|}\,\mathrm{d}x \overset{\text{Exercise}}{\le} \|\nabla\psi_n\|\|\psi_n\| = \|\nabla\psi_n\| \Rightarrow \int_{\mathbb{R}^3} |\nabla\psi_n|^2\,\mathrm{d}x - \int_{\mathbb{R}^3} \frac{|\psi_n(x)|^2}{|x|}\,\mathrm{d}x$ $\ge \|\nabla\psi_n\|^2 - \|\nabla\psi_n\| \ge \left(\|\nabla\psi_n\| - \dfrac{1}{2}\right)^2 - \dfrac{1}{4}$. Thus $\limsup\limits_{n\to\infty}\left(\|\nabla\psi_n\| - \dfrac{1}{2}\right)^2 - \dfrac{1}{4} \le \infty$. Thus $(\psi_n)_{n\in\mathbb{N}}$ is a bounded sequence in $H^1(\mathbb{R}^3)$. [1]

(ii) Let $\varepsilon > 0$ and choose $R > \dfrac{2}{\varepsilon}$. Then

$$\int_{\mathbb{R}^3} \frac{|\psi_n(x)|^2}{|x|}\,\mathrm{d}x = \int_{|x|\le R} \frac{|\psi_n(x)|^2}{|x|}\,\mathrm{d}x + \int_{|x|\ge R} \frac{|\psi_n(x)|^2}{|x|}\,\mathrm{d}x \overset{\|\psi_n\|=1}{=} \int_{|x|\le R} \frac{|\psi_n(x)|^2}{|x|}\,\mathrm{d}x + \frac{\varepsilon}{2}. \tag{8.4}$$

---

[1]Alternatively, one can prove this using Hardy's inequality: $\dfrac{1}{|x|} = 2\sqrt{\varepsilon}\dfrac{1}{2\sqrt{\varepsilon}|x|} \overset{\text{Binomi}}{\le} \dfrac{\varepsilon}{|x|^2} + \dfrac{1}{4\varepsilon}$. Thus $\displaystyle\int_{\mathbb{R}^3} \frac{(\psi_n(x))^2}{|x|}\,\mathrm{d}x \le \varepsilon\int_{\mathbb{R}^3} \frac{|\psi_n(x)|^2}{|x|}\,\mathrm{d}x + \frac{|\psi_n|^2}{4\varepsilon} \overset{\text{Hardy}}{\le} 4\varepsilon\int |\nabla\psi_n|^2\,\mathrm{d}x + \frac{1}{4\varepsilon}$. For $\varepsilon = \dfrac{1}{8}$ we find $\displaystyle\int_{\mathbb{R}^3} \frac{|\psi_n(x)|^2}{|x|}\,\mathrm{d}x \le \frac{1}{2}\|\nabla\psi_n\|^2 + 2$. Thus $\displaystyle\int_{\mathbb{R}^3} |\nabla\psi_n|^2\,\mathrm{d}x - \int_{\mathbb{R}^3} \frac{|\psi_n(x)|^2}{|x|}\,\mathrm{d}x \ge \|\nabla\psi_n\|^2 - \frac{\|\nabla\psi_n\|^2}{2} - 2 \Rightarrow \limsup_{n\to\infty} \frac{\|\nabla\psi_n\|^2}{2} - 2 \le \lambda < \infty$.

We have

$$\int_{|x|\le R} \frac{|\psi_n(x)|^2}{|x|}\,\mathrm{d}x = \int_{|x|\le R} |\psi_n| \frac{|\psi_n|}{|x|}\,\mathrm{d}x \overset{\substack{\text{Cauchy-}\\ \text{Schwarz}}}{\le} \left(\int_{|x|\le R} |\psi_n|^2\,\mathrm{d}x\right)^{\frac{1}{2}} \left(\int_{|x|\le R} \frac{|\psi_n|^2}{|x|^2}\,\mathrm{d}x\right)^{\frac{1}{2}}$$
$$\overset{\text{Hardy}}{\le} \left(\int_{|x|\le R} |\psi_n|^2\,\mathrm{d}x\right)^{\frac{1}{2}} 2\|\nabla\psi_n\| \overset{\text{(i)}}{\le} C\left(\int_{|x|\le R} |\psi_n|^2\,\mathrm{d}x\right)^{\frac{1}{2}}. \tag{8.5}$$

We have $\left|\chi_{B_R(0)}\psi_n\right| \le \left|\tilde{\chi}_{B_R(0)}\psi_n\right|$, where $\chi_A(x) = \begin{cases} 1, & x \in A \\ 0, & x \notin A \end{cases}$ is the indicator function and $\tilde{\chi}$ a "smoothed-out" version of the indicator function (an extension of χ_A that goes smoothly to zero outside of A). But $T_{\tilde{\chi}_{B_R(0)}} : H^1(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ is compact by Theorem 6.9, $\psi_n \rightharpoonup 0$ and ψ_n is bounded in H^1. Hence $T_{\tilde{\chi}_{B_R(0)}}\psi_n \overset{L^2}{\to} 0$. Thus $\int_{|x|\le R} |\psi_n(x)|^2\,\mathrm{d}x \to 0$. By equations (8.4) and (8.5) it follows that $\int_{\mathbb{R}^3} \frac{|\psi_n(x)|^2}{|x|}\,\mathrm{d}x < \varepsilon$ for n large enough.

So far we have shown that $\sigma_{\text{ess}}(H) \subseteq [0,\infty)$. Let $\lambda \in [0,\infty)$. Then by Theorem 2.5 $\lambda \in \sigma(-\Delta)$. Let $\varepsilon > 0$. By Theorem 7.5 there exists a $\psi_\varepsilon \in H^2(\mathbb{R}^3)$ with $\|\psi_\varepsilon\|_{L^2} = 1$ such that $\|(-\Delta-\lambda)\psi_\varepsilon\| < \frac{\varepsilon}{2}$. Let $\psi_{\varepsilon,h}(x) := \psi_\varepsilon(x-h)$. $\Rightarrow \|(H-\lambda)\psi_{\varepsilon,h}\| \le \underbrace{\|(-\Delta-\lambda)\psi_{\varepsilon,h}\|}_{=\|(-\Delta-\lambda)\psi_\varepsilon\|} + \left\|\frac{\psi_{\varepsilon,h}}{|x|}\right\|_{L^2}$.

<u>Exercise 30:</u> $\lim_{|h|\to\infty} \left\|\frac{\psi_{\varepsilon,h}}{|x|}\right\|_{L^2} = 0$. So, choosing h large enough, we find $\|(H-\lambda)\psi_{\varepsilon,h}\| < \varepsilon \Rightarrow \lambda \in \sigma(H)$. Thus $[0,\infty) \subseteq \sigma(H) \Rightarrow [0,\infty) \subseteq \sigma_{\text{ess}}(H)$. ■

Theorem 8.3

Let $H := -\Delta + V$, $V \in C(\mathbb{R}^n)$, $\lim_{|x|\to\infty} V(x) = 0$. Then H is self-adjoint in $H^2(\mathbb{R}^n)$ and $\sigma_{\text{ess}}(H) = [0,\infty)$.

Proof. That $[0,\infty) \subseteq \sigma_{\text{ess}}(H)$ can be shown as in the previous proof. The self-adjointness of H follows from Theorem 3.8 since $\|V\| < \infty$, so V is a bounded multiplication operator. Let $\lambda \in \sigma_{\text{ess}}(H)$. Then there exists a sequence $(\psi_n)_{n\in\mathbb{N}}$ in $H^2(\mathbb{R}^n)$ with $\|\psi_n\| = 1$, $\|(H-\lambda)\psi_n\| \to 0$ and $\psi_n \rightharpoonup 0$. Thus $\langle\psi_m, (H-\lambda)\psi_n\rangle \to 0 \Rightarrow \int_{\mathbb{R}^n} |\nabla\psi_n|^2\,\mathrm{d}x + \int_{\mathbb{R}^n} V|\psi_n|^2\,\mathrm{d}x \to \lambda$ as in the previous proof (in fact, more easily, ψ_n is bounded in the H^1 norm). Moreover, $\int_{\mathbb{R}^n} |\psi_n|^2\,\mathrm{d}x \le \left(\int_{\mathbb{R}^n} |V\psi_n|^2\,\mathrm{d}x\right)^{\frac{1}{2}} \left(\int_{\mathbb{R}^n} |\psi_n(x)|^2\,\mathrm{d}x\right)^{\frac{1}{2}}$. By Theorem 6.10 $T_V : H^1(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$, $T_V\psi = V\psi$

is compact. It similarly follows that $\int_{\mathbb{R}^n} |V\psi_n|^2 \,\mathrm{d}x \to 0$ and thus $\lambda \geq 0$. ■

Remark

This theorem can be quite easily generalized for V bounded with $\lim_{|x|\to\infty} V(x) = 0$.

Theorem 8.4

Assume that $V \in C(\mathbb{R}^n)$ with $\lim_{|x|\to\infty} V(x) = \infty$. Then $H = -\Delta + V$ with $D(H) = \left\{\psi \in L^2(\mathbb{R}^n) : (-\Delta + V)\psi \in L^2(\mathbb{R}^n)\right\}$ is self-adjoint on $L^2(\mathbb{R}^n)$ and $\sigma_{\text{ess}}(H) = \emptyset$.

Proof. For now, we omit the proof of self-adjointness and that $D(H) \subseteq H^2(\mathbb{R}^n)$ (maybe later). Assume $\lambda \in \sigma_{\text{ess}}(H)$. Then there exists a sequence $(\psi_n)_{n\in\mathbb{N}}$ in $D(H)$ such that $\|(H-\lambda)\psi_n\| \to 0$, $\|\psi_n\| = 1$, $\psi_n \rightharpoonup 0$ by Theorem 8.2. Since $\lim_{|x|\to\infty} V(x) = \infty$, there exists a $D > 0$ with $V(x) \geq -D \,\forall x \in \mathbb{R}^n$; by adding D we assume $V \geq 0$. Since $\|(H-\lambda)\psi_n\| \to 0$, we have $|\langle \psi_n, (H-\lambda)\psi_n\rangle| \leq \|\psi_n\|\|(H-\lambda)\psi_n\| \to 0$. Hence

$$\|\boldsymbol{\nabla}\psi_n\|_{L^2}^2 + \int V|\psi_n|^2 \to \lambda\,. \tag{8.6}$$

Thus $\limsup \|\boldsymbol{\nabla}\psi_n\|^2 \leq \lambda$ ($V \geq 0$) and ψ_n is bounded in $H^1(\mathbb{R}^n)$ because $\|\psi_n\| = 1$. By Theorem 6.9 we find that $\chi_{B_R(0)}\psi_n \to 0$ in L^2 because $\psi_n \rightharpoonup 0$ in L^2 and $T_{\tilde{\chi}_{B_R(0)}} : H^1(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ is compact. Thus, if $R > 0$, there exists $n_0 \in \mathbb{N}$ such that $\left\|\chi_{B_R(0)}\psi_n\right\|_{L^2}^2 < \frac{1}{3} \,\forall n \geq n_0$. Hence $\int V|\psi_n|^2 \,\mathrm{d}x \geq \int_{|x|\geq R} V|\psi_n|^2 \,\mathrm{d}x \geq \inf_{|x|\geq R} V(x) \int |\psi_n| \,\mathrm{d}x \geq \frac{2}{3} \inf_{|x|\geq R} V(x)$. Thus, choosing R arbitrarily large, $\int V|\psi_n| \,\mathrm{d}x$ can become arbitrarily large and $\lim_{n\to\infty} \int V|\psi_n|^2 \,\mathrm{d}x = \infty$, contradicting equation (8.6). Thus $\sigma_{\text{ess}}(H) = \emptyset$.

To show that $\chi_{B_R(0)}\psi_n \to 0$, we show: every subsequence has a further (sub)subsequence converging to zero. Denote a subsequence by $\chi_{B_R(0)}\psi_{n_k}$. Since ψ_{n_k} is bounded in H^1, it has a further subsequence $\psi_{n_{k_l}}$ with $\psi_{n_{k_l}} \rightharpoonup v$ in H^1 for some $v \in H^1(\mathbb{R}^n)$ by Theorem 6.4. We also have $\psi_{n_{k_l}} \rightharpoonup 0$ in $L^2(\mathbb{R}^n)$, so $v = 0$ since $\psi_{n_{k_l}} \rightharpoonup v$ in H^1. Thus $\psi_{n_{k_l}} \rightharpoonup 0$ in $H^1(\mathbb{R}^n)$ and $T_{\tilde{\chi}_{B_R(0)}} : H^1(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ is compact. Hence $\chi_{B_R(0)}\psi_0 \to 0$ in $L^2(\mathbb{R}^n)$. ■

Example 8.2

The Hamilton operator of the quantum harmonic oscillator is given by[2] $H = -\Delta + |x|^2$ and $\lim_{|x|\to\infty} |x|^2 = \infty$, so the spectrum of H consists only of discrete eigenvalues.

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[2]We obtain this operator from the physical one $H = -\frac{\hbar^2}{2m}\Delta + \frac{m\omega^2}{2}|x|^2$ by choosing $\hbar = 1$, $m = \frac{1}{2}$, and $\omega = 2$.

Theorem 8.5 (IMS localization formula)

Let $H : H^2(\mathbb{R}^n) \subseteq L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$, $H = -\Delta + V$ be self-adjoint.

(a) If $f : \mathbb{R}^n \to \mathbb{R}$ is a C^2-function with $\partial^\alpha f \in L^\infty(\mathbb{R}^n)$ for $0 \le |\alpha| \le 2$, then [3]

$$fHf = \frac{1}{2}\left(f^2H + Hf^2\right) + |\boldsymbol{\nabla} f|^2. \tag{8.7}$$

(b) If $(J_a)_{a\in A} : \mathbb{R}^n \to \mathbb{R}$ is a family of C^2-functions with $\partial^\beta J_a \in L^\infty(\mathbb{R}^n)$ for $0 \le |\beta| \le 2\,\forall a \in A$, and $\sum_{a\in A} J_a^2 = 1$, then [4]

$$H = \sum_{a\in A} J_a H J_a - \sum_{a\in A} |\boldsymbol{\nabla} J_a|^2. \tag{8.8}$$

Proof. (a) By the properties of f, $T_f : H^2(\mathbb{R}^n) \to H^2(\mathbb{R}^n)$, $T_f\psi = f\psi$ is bounded ($\|T_f\psi\|_{L^2} = \|f\psi\|_{L^2} \le \|f\|_{L^\infty}\|\psi\|_{L^2}$). We have $\|\boldsymbol{\nabla}(f\psi)\|_{L^2} \le \|(\boldsymbol{\nabla} f)\psi\|_{L^2} + \|f\boldsymbol{\nabla}\psi\|_{L^2}$ $\le (\|\boldsymbol{\nabla} f\|_{L^\infty} + \|f\|_{L^\infty})\|\psi\|_{H^2}$. Similarly one can control $\|\boldsymbol{\nabla}(f\psi)\| \le C\|\psi\|_{H^2}$ for some $C \ge 0$; in particular, $fH^2(\mathbb{R}^n) \subseteq H^2(\mathbb{R}^n)$. $fHf - \frac{1}{2}(f^2H + Hf^2) = \frac{1}{2}(fHf - f^2H + fHf - H^2f) = \frac{1}{2}(f(fH - Hf) + (fH - Hf)f) = \frac{1}{2}f[H,f] - \frac{1}{2}[H,f]f$, so

$$fHf - \frac{1}{2}(f^2H - Hf^2) = \frac{1}{2}[f,[H,f]]\,. \tag{8.9}$$

This holds (at least formally) independently of H. So it suffices to prove $[f,[H,f]] = 2|\boldsymbol{\nabla} f|^2$. We have $[H,f] = [(-\Delta + V), f] = [-\Delta, f] = -(\Delta f) - 2(\boldsymbol{\nabla} f)\cdot\boldsymbol{\nabla} - f\Delta + f\Delta = -(\Delta f) - 2(\boldsymbol{\nabla} f)\cdot\boldsymbol{\nabla}$. Thus $[f,[H,f]] = [f, -(\Delta f) - 2(\boldsymbol{\nabla} f)\cdot\boldsymbol{\nabla}] = [f, -2(\boldsymbol{\nabla} f)\cdot\boldsymbol{\nabla}] = 2|\boldsymbol{\nabla} f|^2$, so equation (8.9) holds true.

(b) By equation (8.7), $J_aHJ_a = \frac{1}{2}(J_a^2H + HJ_a^2) + |\boldsymbol{\nabla} J_a|^2$, so $\sum_{a\in A} J_aHJ_a = \frac{1}{2}\left(\sum_{a\in A} J_a^2H + H\sum_{a\in A} J_a^2\right) + \sum_{a\in A}|\boldsymbol{\nabla} J_a|^2$. Since $\sum_{a\in A} J_a^2 = 1$, this implies $\sum_{a\in A} J_aHJ_a = H + \sum_{a\in A}|\boldsymbol{\nabla} J_a|^2$.

■

Lemma

There exists a family $(J_k)_{k=0}^N$ of functions $J_k : \mathbb{R}^{3N} \to \mathbb{R}$ with $\forall\, 0 \le |\alpha| \le 2, k \in \{0,\dots,N\}$: $\partial^\alpha J_k \in L^\infty\left(\mathbb{R}^{3N}\right)$ such that

[3] For example, if $\psi(x) = \mathrm{e}^{-|x|^2}$, then $(fH\psi)(x) = f(x)(-\Delta + V(x))\mathrm{e}^{-|x|^2}$.

[4] The idea behind this formula is to decompose the entire operator H into a sum of localized operators J_aHJ_a which are easier to analyze, plus a (hopefully small) error.

1. $\operatorname{supp}(J_0)$ is compact.
2. $\forall k \geq 1 : \operatorname{supp}(J_k) \subseteq \{(x_1, \ldots, x_N) \in \mathbb{R}^{3N} : |x_k| \geq 1\}$.
3. $\displaystyle\sum_{k=0}^{N} J_k^2 = 1$.

Interpretation:

1. Either all electrons are close to nucleus.
2. The k-th electron is far from the nucleus.
3. Possible because either all electrons are close to nucleus or at least one of them is far.

Proof. Let $j \in C^\infty(\mathbb{R};[0,1])$ with $j(r) = 0$ for $r \leq 1$, $j(r) = 1$ for $r \geq 2$. Let $f_0(x) = 1 - j\left(\frac{|x|}{2N}\right)$, $f_k(x) = j(|x_k|)$, $k = 1, \ldots, N$, where $x = (x_1, \ldots, x_N)$. Then $\operatorname{supp}(f_0)$ is compact and $\operatorname{supp}(f_k) \subseteq \{x : |x_k| \geq 1\}$. Moreover, for all $x \in \mathbb{R}^{3N}$ there exists a k such that $f_k(x) = 1$. Thus the functions $J_k := \frac{f_k}{\left(\sum_{n=0}^N f_n^2\right)^{\frac{1}{2}}}$ satisfy the desired properties. ■

Theorem 8.6 (HVZ-Theorem (Hunziker - van Winter - Zhislin))
Let $H_N : H^2(\mathbb{R}^{3N}) \subseteq L^2(\mathbb{R}^{3N}) \to L^2(\mathbb{R}^{3N})$,

$$(H_N\Phi)(x) = \sum_{j=1}^{N}\left(-\Delta_{x_j} - \frac{Z}{|x_j|}\right)\Phi(x) + \sum_{1\leq i<j\leq N}\frac{1}{|x_i - x_j|}\Phi(x), x = (x_1, \ldots, x_N) \in \mathbb{R}^{3N}.$$

(Hamiltonian of an ion with N electrons and Z protons).
Then $\sigma_{\text{ess}}(H_N) = [\inf \sigma(H_{N-1}), \infty)$.

Proof. Let $E_{N-1} = \inf \sigma(H_{N-1}) = \inf\limits_{\substack{\|\psi\|_{L^2}=1\\ \psi\in H^1\left(\mathbb{R}^{3(N-1)}\right)}} \langle \psi, H_{N-1}\psi\rangle$

We will prove:

(i) $[E_{N-1}, \infty) \subseteq \sigma(H_N)$ (Easy direction)

(ii) $\inf \sigma_{\text{ess}}(H_N) \geq E_{N-1}$ (Hard direction, need Theorem 8.5)

As (i) implies $[E_{N-1}, \infty) \subseteq \sigma_{\text{ess}}(H_N)$ directly, Theorem 8.6 follows directly.

(i)

$$H_N = H_{N-1} - \Delta_{x_N} - \frac{Z}{|x_N|} + \sum_{i=1}^{N-1} \frac{1}{|x_i - x_N|}. \tag{8.10}$$

Let $\lambda \geq E_{N-1}$. To show: $\lambda \in \sigma(H_N)$.

$\lambda = E_{N-1} + \delta$, where $E_{N-1} \in \sigma(H_{N-1})$ and $\delta \in [0, \infty) = \sigma(-\Delta_{x_N})$.

Thus by Theorem 7.5 and $\sigma(\Delta_{x_N}) = [0, \infty)$:

$\forall \varepsilon > 0\, \exists \psi_{N-1} \in C_c^\infty\left(\mathbb{R}^{3(N-1)}\right)$ and $\varphi \in C_c^\infty(\mathbb{R}^3)$, $\|\varphi\| = \|\psi_{N-1}\| = 1$ such that

$$\|(H_{N-1} - E_{N-1})\psi_{N-1}\| < \frac{\varepsilon}{3}, \tag{8.11}$$

$$\|(\Delta_{x_N} - \delta)\varphi\| < \frac{\varepsilon}{3}. \tag{8.12}$$

Let $\varphi_h(x) := \varphi(x - h)$.

Then with $(\psi_{N-1} \otimes \varphi_h)(x_1, \ldots, x_N) = \psi_{N-1}(x_1, \ldots, x_{N-1}) \cdot \varphi_h(x_N)$:

$$\begin{aligned}\|(H_N - \lambda)\psi_{N-1} \otimes \varphi_h\| \leq{}& \underbrace{\|(H_{N-1} - E_{N-1})\psi_{N-1} \otimes \varphi_h\|}_{<\frac{\varepsilon}{3}\cdot 1 \text{ by eqn. (8.11)}} + \underbrace{\|(-\Delta_{x_N} - \delta)\psi_{N-1} \otimes \varphi_h\|}_{<1\cdot\frac{\varepsilon}{3} \text{ by eqn. (8.12)}} \\ &+ \underbrace{\left\|\left(-\frac{Z}{|x_N|} + \sum_{i=1}^{N-1} \frac{1}{|x_i - x_N|}\right)\psi_{N-1} \otimes \varphi_h\right\|}_{\to 0, |h| \to \infty \text{ as } \psi_{N-1}, \varphi_h \text{ compact support}}.\end{aligned}$$

Therefore for $|h|$ large enough we have $\|(H_N - \lambda)\psi_{N-1} \otimes \varphi_h\| < \varepsilon$. Thus by Theorem 7.5 we have $\lambda \in \sigma(H_N)$ as $\|\psi_{N-1} \otimes \varphi_h\| = 1$ and $\|(H_N - \lambda)\psi_{N-1} \otimes \varphi_h\| \to 0$.

(ii) Let $J_{k,R} = J_k\left(\frac{x}{R}\right)$ for J_k as in the Lemma before Theorem 8.6. Then:

$$\begin{aligned}&\operatorname{supp}(J_{0,R}) \text{ compact}, \\ &\forall k \geq 1 : \operatorname{supp}(J_{k,R}) \subseteq \{(x_1, \ldots, x_N) \in \mathbb{R}^{3N} : |x_k| \geq R\}, \\ &\sum_{k=0}^{N} J_{k,R}^2 = 1.\end{aligned} \tag{8.13}$$

By the IMS localization formula (Theorem 8.5) we have

$$H_N = \sum_{k=0}^{N} J_{k,R} H_N J_{k,R} - \sum_{k=0}^{N} |\boldsymbol{\nabla} J_{k,R}|^2. \tag{8.14}$$

As $H_N \geq E_N$:

$$J_{0,R} H_N J_{0,R} \geq E_N J_{0,R}^2 \tag{8.15}$$

$$\begin{aligned}
J_{N,R} H_N J_{N,R} &\overset{\text{eqn. (8.10)}}{=} J_{N,R} \left(H_{N-1} - \underbrace{\Delta_{x_N}}_{\geq 0} - \frac{Z}{|x_N|} - \underbrace{\sum_{i=1}^{N-1} \frac{1}{|x_i - x_N|}}_{\geq 0} \right) J_{N,R} \\
&\geq J_{N,R} \left(H_{N-1} - \frac{Z}{|x_N|} \right) J_{N,R} \overset{|x_N| \geq R \text{ in } \operatorname{supp}(J_{N,R})}{\geq} J_{N,R} \left(H_{N-1} - \frac{Z}{R} \right) J_{N,R} \\
&\geq \left(E_{N-1} - \frac{Z}{R} \right) J_{N,R}^2
\end{aligned}$$

Similarly we get for all $k \geq 1$:

$$J_{k,R} H_N J_{k,R} \geq \left(E_{N-1} - \frac{Z}{R} \right) J_{k,R}^2 \tag{8.16}$$

From equation (8.14), equation (8.15) and equation (8.16) it follows that

$$\begin{aligned}
H_N &\geq E_N J_{0,R}^2 + \sum_{k=1}^{N} \left(E_{N-1} - \frac{Z}{R} \right) J_{k,R}^2 - \sum_{k=0}^{N} \underbrace{|\nabla J_{k,R}|^2}_{\substack{\leq \frac{D}{R^2} \text{ for some } D>0 \\ \text{as } \nabla J \in L^\infty(\mathbb{R}^{3N})}} \\
&\overset{\textit{eqn. } (8.13)}{\geq} (E_N - E_{N-1}) J_{0,R}^2 + \sum_{k=0}^{N} E_{N-1} J_{k,R}^2 - \frac{C}{R}
\end{aligned}$$

Where $-\frac{C}{R}$ comes from $-\frac{Z}{R} - \frac{D}{R^2}$. And so with equation (8.13) we have

$$H_N \geq (E_N - E_{N-1}) J_{0,R}^2 + E_{N-1} - \frac{C}{R} \tag{8.17}$$

Now let $\lambda \in \sigma_{\text{ess}}(H_N)$. By Weyl's criterion (Theorem 8.2) $\exists (\psi_n)_{n\in\mathbb{N}} \subseteq D(H_N)$ with $\|\psi_n\|_{L^2} = 1, \|(H_N - \lambda)\psi_n\| \to 0$ and $\psi_n \rightharpoonup 0$. Thus

$$|\langle \psi_n, (H_N - \lambda)\psi_n \rangle| \leq \|\psi_n\| \|(H_N - \lambda)\psi_n\| \to 0 \tag{8.18}$$

But with equation (8.17) we have $\langle \psi_n, H_N \psi_n \rangle \geq (E_N - E_{N-1}) \left\langle \psi_n, J_{0,R}^2 \psi_n \right\rangle + E_{N-1} - \frac{C}{R}$ and $\left\langle \psi_n, J_{0,R}^2 \psi_n \right\rangle = \|J_{0,R}\psi_n\|^2 \to 0$ in L^2 by Theorem 6.9 for any $R > 0$.

Let $\varepsilon > 0$ and choose R with $\frac{C}{R} < \frac{\varepsilon}{2}$. Then for n large enough we have

$$\langle \psi_n, H_N \psi_n \rangle \geq (E_N - E_{N-1}) \|J_{0,R}\psi_n\|^2 + E_{N-1} - \frac{C}{R} \geq E_{N-1} - \varepsilon \tag{8.19}$$

Together with equation (8.18) we get $\lambda = \lim\limits_{n\to\infty} \langle \psi_n, H_N \psi_n \rangle \geq E_{N-1} - \varepsilon$ for all $\varepsilon > 0$ and therefore $\lambda \geq E_{N-1}$

■

Remark

This can be easily generalized for molecules.

The interval from $E_N = \inf \sigma(H_N)$ to $E_{N-1} = \inf \sigma_{\text{ess}}(H_N)$ is called the *ionization energy*. This is the energy needed to push one electron to infinity.

For E_{N-1} the same happens again, this time for the second electron.

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 $\sigma_{\text{ess}}(A) = \sigma_{\text{ess}}(B)$.

Proof. We have to show that $\sigma_{\text{ess}}(A) \subseteq \sigma_{\text{ess}}(B)$ (the other inclusion follows from exchanging A and B). Let $\lambda \in \sigma_{\text{ess}}(A)$. By Weyl's criterion (Theorem 8.2) there exists a sequence $(\psi_n)_{n\in\mathbb{N}}$ in $D(A) = D(B)$ such that $\|\psi_n\| = 1$, $\|(A - \lambda)\psi_n\| \to 0$, $\psi_n \rightharpoonup 0$. But then $\left[(z - A)^{-1} - (z - \lambda)^{-1}\right]\psi_n = (z - A)^{-1}(z - \lambda)^{-1} \underbrace{(A - \lambda)\psi_n}_{\to 0} \to 0$, since $z - \lambda \neq 0$ ($\lambda \in \mathbb{R}$, $z \in \mathbb{C} \setminus \mathbb{R}$) and because $(z - A)^{-1}$ is bounded ($z \in \rho(A)$). Similarly, $\left[(z - B)^{-1} - (z - \lambda)^{-1}\right]\psi_n = (z - \lambda)^{-1}(B - \lambda)(z - B)^{-1}\psi_n$. But

$$\left[(z - B)^{-1} - (z - \lambda)^{-1}\right]\psi_n = \left[(z - B)^{-1} - (z - A)^{-1}\right]\psi_n + \left[(z - A)^{-1} - (z - \lambda)^{-1}\right]\psi_n \to 0\,. \tag{8.20}$$

The second term goes to zero by the above argument, the first term goes to zero because $\psi_n \rightharpoonup 0$ and $(z - B)^{-1} - (z - A)^{-1}$ is compact. So $(B - \lambda)(z - B)^{-1}\psi_n \to 0$. But by Equation (8.20) $\lim\limits_{n\to\infty} \left\|(z - B)^{-1}\psi_n\right\| = \left|(z - \lambda)^{-1}\right| \neq 0$. Thus $\varphi_n = \dfrac{(z - B)^{-1}\psi_n}{\|(z - B)^{-1}\psi_n\|}$ is normalized. But $\varphi_n \rightharpoonup 0$ because $(z - B)^{-1}\psi_n \rightharpoonup 0$ and because $\lim\limits_{n\to\infty} \left\|(z - B)^{-1}\psi_n\right\| \neq 0$. So $(B - \lambda)(z - B)^{-1}\psi_n \to 0 \Rightarrow (B - \lambda)\dfrac{(z - B)^{-1}\psi_n}{\|(z - B)^{-1}\psi_n\|} \to 0 \Rightarrow (B - \lambda)\varphi_n \to 0$. ■

Corollary 8.8

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

Proof. $(z - B)^{-1} - (z - A)^{-1} = -(z - B)^{-1}(B - A)(z - A)^{-1}$. But $(z - B)^{-1}$ is bounded and $(B-A)(z-A)^{-1}$ is compact, so $(z-B)^{-1}-(z-A)^{-1}$ is compact, so we can apply Theorem 8.7. ■

Let E_H, E_{H^+}, E_{H^-} be the ground-state energy of the hydrogen atom (resp. +1 ion, resp. −1 ion). Then $E_H + E_H < E_{H^+} + E_{H^-}$ (this can be shown using the HVZ theorem).

Definition 8.9

Let $H = H^*$ be a self-adjoint operator acting on $L^2(\mathbb{R}^n)$ that is bounded from below $\left(\inf_{\varphi \in D(H)} \langle \varphi, H\varphi\rangle > -\infty\right)$ which satisfies the IMS localization formula (Theorem 8.5). For $R > 0$ let $\Sigma_R = \inf_{\substack{\psi \in D(H) \\ \|\psi\|=1 \\ \operatorname{supp}(\psi) \subseteq (B(R,0))^c}} \langle \psi, H\psi\rangle$ (the IMS localization formula guarantees that the infimum is assumed over a non-empty set). Σ_R is the least possible energy for ψ supported outside the ball of radius R and center at 0. The *ionization threshold* of H is defined by $\Sigma := \lim_{R\to\infty} \Sigma_R$.

Interpretation: Σ is the energy that the system should reach so that at least one particle goes to infinity.

Remark

For $H_{N,Z}$, $\Sigma = \inf \sigma(H_{N-1,Z}) \overset{\text{HVZ}}{=} \inf \sigma_{\text{ess}}(H_{N,Z})$. So in this case $\Sigma - \underbrace{\inf \sigma(H_{N,Z})}_{=:E_{N,Z}} = E_{N-1,Z} - E_{N,Z}$ is the ionization energy for $H_{N,Z}$. For an atom with atomic number Z, $E_{Z-1,Z} - E_{Z,Z}$ is called the *first ionization energy*. $r_k := E_{Z-k,Z} - E_{Z-(k-1),Z}$ is called the *k-th ionization energy* of the atom. In mathematics, it is still an open problem whether $r_1 < r_2 < \ldots < r_k < r_{k+1}$, whereas this ordering is trivial from the physical point of view since the electron-electron repulsion forces increase with the number of electrons in the atom/ion.

Exercise: Prove that the last ionization energy is larger than the second-last ionization energy.

8.1 Exponential decay of eigenfunctions

Let $\varphi \in L^2(\mathbb{R})$ be a C^2 solution of the one-dimensional (stationary) Schrödinger equation

$$-\varphi'' + V\varphi = E\varphi\,, \tag{8.21}$$

where $V(x) > E$ for $|x| > R$. In this case φ'' and φ have the same sign ($\varphi'' = a\varphi$ for some $a > 0$). A solution to Equation (8.21) is $\varphi(x) = C_1 \mathrm{e}^{\sqrt{a}x} + C_2 \mathrm{e}^{-\sqrt{a}x}$. So we expect that φ is either exponentially growing or decaying with $|x|$. Since $\varphi \in L^2(\mathbb{R})$, in particular $\int_{\mathbb{R}} |\psi(x)|^2 \, \mathrm{d}x < \infty$, it can only exponentially decay.

Note: If $\lim_{|x|\to\infty} V(x)$ exists then $\lim_{|x|\to\infty} V(x) = \Sigma$.

Theorem 8.10 (Exponential decay of eigenfunctions to eigenvalues below Σ)
Let H be as in Definition 8.9 ($H = H^*$, $\inf_{\substack{\|\psi\|=1 \\ \psi \in D(H)}} \langle \psi, H\psi \rangle > -\infty$ and if $f \in C^2$ with $\partial^\alpha f \in L^\infty$, $0 \le |\alpha| \le 2$, then $fD(H) \subseteq D(H)$ and $fHf = \frac{1}{2}\left(f^2 H + Hf^2\right) + |\boldsymbol{\nabla} f|^2)$, e.g. $H = -\Delta + V$. If

$$H\psi = E\psi\,, \tag{8.22}$$

where $E < \Sigma$, then $\mathrm{e}^{\beta x}\psi \in L^2(\mathbb{R}^n)$ $\forall \beta > 0$ with $\beta^2 > \Sigma - E$.

Proof. Let $\chi : \mathbb{R}^n \to [0,1]$, $\chi \in C^\infty$ with $\chi(x) := \begin{cases} 1, |x| \ge 2 \\ 0, |x| \le 1 \end{cases}$ and $\chi_R(x) := \chi\left(\frac{x}{R}\right)$. For $0 < \varepsilon < 1$ we define $f_\varepsilon(x) := \frac{\beta |x|}{1 + \varepsilon |x|}$ and $G_\varepsilon := \chi_R \, \mathrm{e}^{f_\varepsilon}$. Our goal is to show that

$$\|G_\varepsilon \psi\| \le D_R \|\psi\| \tag{8.23}$$

for some suitable $R > 0$, where D_R is independent of ε. Once we have equation (8.23) it follows that $\int_{|x|\ge 2R} \mathrm{e}^{2\beta|x|} |\psi(x)|^2 \, \mathrm{d}x = \int_{|x|\ge 2R} \lim_{\varepsilon\to 0} \mathrm{e}^{2 f_\varepsilon(x)} |\psi(x)|^2 \, \mathrm{d}x \overset{\substack{\text{monotone} \\ \text{conv.}}}{=} \lim_{\varepsilon \to 0} \int_{|x|\ge 2R} \mathrm{e}^{2 f_\varepsilon(x)} |\psi(x)|^2 \, \mathrm{d}x$. Since

$$\begin{aligned} \int_{|x|\ge 2R} \mathrm{e}^{2 f_\varepsilon(x)} |\psi(x)|^2 \, \mathrm{d}x &\le \int \chi_R^2(x) \mathrm{e}^{2 f_\varepsilon(x)} |\psi(x)|^2 \, \mathrm{d}x = \int G_\varepsilon(x) |\psi(x)|^2 \, \mathrm{d}x \\ &= \|G_\varepsilon \psi\|^2 \overset{\text{eqn. (8.23)}}{\le} D_R^2 < \infty \end{aligned} \tag{8.24}$$

and

$$\int_{|x|\le 2R} \mathrm{e}^{2\beta|x|} |\psi(x)|^2 \, \mathrm{d}x \le \mathrm{e}^{4\beta R} \int_{|x|\le 2R} |\psi(x)|^2 \, \mathrm{d}x < \infty\,, \tag{8.25}$$

it follows that $\mathrm{e}^{\beta|x|} \in L^2(\mathbb{R}^n)$. We now show equation (8.23): we have

$$|\boldsymbol{\nabla} f_\varepsilon(x)| = \left| \frac{\beta \frac{x}{|x|}}{1 + \varepsilon|x|} - \frac{\beta |x| \varepsilon \frac{x}{|x|}}{(1+\varepsilon|x|)^2} \right| = \left| \frac{\beta \frac{x}{|x|}(1+\varepsilon|x|) - \beta\varepsilon x}{(1+\varepsilon|x|)^2} \right| = \left| \frac{\beta \frac{x}{|x|}}{(1+\varepsilon|x|)^2} \right| \le \beta\,. \tag{8.26}$$

Now $\boldsymbol{\nabla} G_\varepsilon = (\boldsymbol{\nabla}\chi_R)\, \mathrm{e}^{f_\varepsilon} + \chi_R \, \mathrm{e}^{f_\varepsilon} (\boldsymbol{\nabla} f_\varepsilon) = (\boldsymbol{\nabla}\chi_R)\, \mathrm{e}^{f_\varepsilon} + G_\varepsilon (\boldsymbol{\nabla} f_\varepsilon)$, so

$$|\boldsymbol{\nabla} G_\varepsilon|^2 = \underbrace{|(\boldsymbol{\nabla}\chi_r)|^2 \mathrm{e}^{2 f_\varepsilon} + 2(\boldsymbol{\nabla}\chi_R) \mathrm{e}^{f_\varepsilon} G_\varepsilon (\boldsymbol{\nabla} f_\varepsilon)}_{\le C_R \ (\varepsilon-\text{independent because } \operatorname{supp}(\boldsymbol{\nabla}\chi_R) \subseteq \{|x| \le 2R\}} + G_\varepsilon^2 |\boldsymbol{\nabla} f_\varepsilon|^2\,. \tag{8.27}$$

By the IMS localization formula (Theorem 8.5) we have $G_\varepsilon H G_\varepsilon = \frac{1}{2}\left(G_\varepsilon^2 H + H G_\varepsilon^2\right) + |\nabla G_\varepsilon|^2$, so $\langle \psi, G_\varepsilon (H-E) G_\varepsilon \psi\rangle = \frac{1}{2}\left\langle \psi, G_\varepsilon^2 \underbrace{(H-E)\psi}_{=0}\right\rangle + \frac{1}{2}\left\langle \underbrace{(H-E)\psi}_{=0}, G_\varepsilon^2 \psi\right\rangle + \left\langle \psi, |\nabla G_\varepsilon|^2 \psi\right\rangle$
$= \left\langle \psi, |\nabla G_\varepsilon|^2 \psi\right\rangle$. Hence

$$\left\langle G_\varepsilon \psi, \left(H - E - |\nabla f_\varepsilon|^2\right) G_\varepsilon \psi\right\rangle \le C_R \|\psi\|^2 . \tag{8.28}$$

But

$$\begin{aligned}\left\langle G_\varepsilon \psi, \left(H - E - |\nabla f_\varepsilon|^2\right) G_\varepsilon \psi\right\rangle &\overset{\text{eqn. (8.26)}}{\ge} \left\langle G_\varepsilon \psi, \left(\Sigma_R - E - \beta^2\right) G_\varepsilon \psi\right\rangle \\ &= \|G_\varepsilon \psi\|^2 \left(\Sigma_R - E - \beta^2\right) .\end{aligned} \tag{8.29}$$

From equation (8.28) and equation (8.29) if follows that $\left(\Sigma_R - E - \beta^2\right)\|G_\varepsilon\psi\|^2 \le C_R \|\psi\|^2$. Since $\Sigma - E - \beta^2 > 0$, choosing R large enough we find $\Sigma_R - E - \beta^2 > 0$. Thus $\|G_\varepsilon \psi\|^2 \le \frac{C_R}{\Sigma_R - E - \beta^2}\|\psi\|^2 < \infty$ (ε-independent). ■

Remark

If E is the ground-state energy of a molecule, $\frac{1}{\beta}$ is interpreted as the radius of the molecule.

9 Spectral theorem for self-adjoint operators

Theorem 9.1 (Spectral theorem in multiplication-operator form)
Let $\mathcal{H}$ be a separable Hilbert space and A a self-adjoint operator on $\mathcal{H}$ with domain $D(A) \subseteq \mathcal{H}$. Then there exists a measure space (M, μ) with a finite measure, a unitary operator $U : \mathcal{H} \to L^2(M, \mathrm{d}\mu)$ (where $\mathrm{d}\mu$ denotes the integration with respect to μ), and a real-valued function f finite almost everywhere such that

(a) $\psi \in D(A) \Leftrightarrow f(U\psi) \in L^2(M, \mathrm{d}\mu)$

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

Example 9.1
Let $A \in \mathbb{C}^{n\times n}$ be self-adjoint, $\vec{v_1}, \dots, \vec{v_n}$ be a basis of $\mathbb{C}^n$ with $A\vec{v_i} = \lambda\vec{v_i}$ for all $i \in \{1, \dots, n\}$. Let $U : \mathbb{C}^n \to L^2(\{1, \dots, n\}, \mu)$ with μ being a counting measure, so $\mu(B) = \#B$ for all $B \subseteq \{1, \dots, n\}$, and $\underbrace{[U(c_1\vec{v_1} + \dots + c_n\vec{v_n})]}_{=:\varphi}(j) = c_j$ for all $j \in \{1, \dots, n\}$.
Then $UAU^{-1}\varphi = UA(c_1\vec{v_1} + \dots + c_n\vec{v_n}) = U(c_1\lambda_1\vec{v_1} + \dots + c_n\lambda_n\vec{v_n})$.
So $(UAU^{-1}\varphi)(j) = c_j\lambda_j = \lambda_j\phi(j) = f(j)\varphi(j)$ where $f : \{1, \dots, n\} \to \mathbb{R}, f(j) = \lambda(j)$.

Example 9.2

- This is the same idea as what we did earlier: If $A = -\Delta \Rightarrow A = F^{-1}|\xi|F$ with F being the Fourier transformation.
- The conclusion of Theorem 9.1 can also be written as $UAU^{-1} = T_f$ with T_f being the multiplication operator of f.
- For matrices Theorem 9.1 $\Leftrightarrow$ Matrix is diagonalizable.

Theorem 9.2 (Spectral theorem in 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 $\psi \in \mathcal{H}$.

Those four properties determine ϕ uniquely. Additionally we have:

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

(f) If $h \geq 0$ then $\phi(h) \geq 0$, namely $\langle\psi, \phi(h)\psi\rangle \geq 0$ for all $\psi \in \mathcal{H}$.

Part of idea of proof: By Theorem 9.1 we have that $UAU^{-1} = T_f \Rightarrow A = U^{-1}T_fU$. Define $\phi(h) = U^{-1}T_{h\circ f}U$. Then ϕ satisfies $(a) - (f)$.

Step 1: Prove functional calculus form for continuous functions if A is bounded (first for polynomials, then by approximation for continuous functions).

Step 2: Multiplication-operator form for bounded self-adjoint operators using step 1 (needs Zorn's Lemma).

Step 3: Prove Theorem 9.1 using boundedness of $A(A - z)^{-1}$ for some $z \in \rho(A)$.

Step 4: Theorem 9.1 $\Rightarrow$ Theorem 9.2 as above.

■

Example 9.3

Let $h_t(x) = e^{itx}$. Then $\phi(h_t) = \mathrm{e}^{\mathrm{i}tA}$. This can be proven using our knowledge that $\mathrm{e}^{\mathrm{i}tA}$ is a strongly continuous unitary group as well as:

$$\phi(h_t)^*\phi(h_t) \overset{\text{Thm. 9.2}}{=} \phi(\overline{h_t})\phi(h_t) \overset{\text{Thm. 9.2}}{=} \phi(\overline{h_t}h_t) = \phi(|h_t|^2) \overset{\text{Def of } h_t}{=} \phi(1) = I$$

Similarly we get $\phi(h_t)\phi(h_t)^* = I$. Thus $\phi(h_t)$ is unitary. Now prove with Theorem 9.2 that $\phi(h_t)$ is a strongly continuous unitary group. Uniqueness gives $\phi(h_t) = \mathrm{e}^{\mathrm{i}tA}$.

Theorem 9.3

Let $\Omega \subseteq \mathbb{R}$ be Borel and $P(\Omega) := \phi(\chi_\Omega)$. From Theorem 9.2 it follows that the family $\{P(\Omega)\}$ satisfies:

(i) (a) Each $P(\Omega)$ is an orthogonal projection.

(b) $P(\emptyset) = 0, P((-\infty,\infty)) = I$.

(c) If $\Omega = \bigcup_{n=1}^{N} \Omega_n$ ($N \in \mathbb{N} \cup \infty$) with $\forall n \neq m : \Omega_n \cap \Omega_m = \emptyset$ then $P(\Omega)\psi = \sum_{n=1}^{N} P(\Omega_n)\psi$.

(d) $P(\Omega_1) P(\Omega_2) = P(\Omega_1 \cap \Omega_2)$.

Every such family is called a *projection-valued measure*.

(ii) For all Borel subsets $\Omega \subseteq \mathbb{R}$ we have that $P(\Omega) A \subseteq AP(\Omega)$. If Ω is open then

$$\sigma(A) \cap \Omega \subseteq \sigma\left(A|_{\mathrm{Ran}(P(\Omega))}\right) \subseteq \overline{\sigma(A) \cap \Omega}\,. \tag{9.1}$$

Proof. (i) Proven in Exercise 40

(ii) As we need Theorem 9.9 this will be proven in Section 9.1.

■

Remark

If Ω is compact and $\sigma(A) \cap \Omega$ is isolated from $\sigma(A) \cap \Omega^c$ then $P(\Omega)$ is just $\frac{1}{2\pi \mathrm{i}} \oint_\gamma (z - A)^{-1}\,\mathrm{d}z$ where as in Theorem 7.4 γ is positively oriented and $\sigma(A) \cap \Omega$ is inside γ while $\sigma(A) \cap \Omega^c$ is outside γ.

Remark

If A is an observable and ψ is a state then $\langle \psi, P(\Omega)\psi \rangle$ is the probability that the measurement of A in the state ψ yields a value in Ω.

Theorem 9.4 (Application: the minimax principle)

Let $H : D(H) \subseteq \mathcal{H} \to \mathcal{H}$ be self-adjoint and bounded from below ($\inf_{\substack{\varphi \in D(H),\\ \|\varphi\|=1}} \langle \varphi, H\varphi \rangle > -\infty$).

Let $\mu_n(H) := \inf_{\substack{M \subseteq D(H),\\ \dim M = n}} (\sup_{\substack{\varphi \in M,\\ \|\varphi\|=1}} \langle \varphi, H\varphi \rangle)$.

Then for all $n \in \mathbb{N}$ we have either (exclusive):

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

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

Here counting multiplicity means that for example if -3 is a double eigenvalue, -2 is a single eigenvalue and $0 = \inf \sigma_{\text{ess}}(H)$, then $\mu_1(H) = -3 = \mu_2(H), \mu_3(H) = -2$ and $0 = \mu_4(H) = \mu_5(H) = \dots$.

Proof. If H has at least n eigenvalues below $\inf \sigma_{\text{ess}}(H)$ let E_n be the n-th eigenvalue from below (counting multiplicity), otherwise let $E_n := \inf \sigma_{\text{ess}}(H)$. We have to show that $\mu_n(H) = E_n$ for all $n \in \mathbb{N}$.

"$\leq$": We show that $\mu_n(H) \leq E_n + \varepsilon$ for all $\varepsilon > 0$.

Let $P(\Omega) := \phi(\chi_\Omega)$ be the functional calculus of $H : D(H) \subseteq \mathcal{H} \to \mathcal{H}$. If E_n is the n-th eigenvalue then

$$\sigma\left(H|_{\text{Ran}(P((-\infty, E_n+\varepsilon)))}\right) \overset{\text{eqn. (9.1)}}{\supseteq} \sigma(H) \cap (-\infty, E_n + \varepsilon) \supseteq \{E_1, \dots, E_n\} \tag{9.2}$$

If $E_n = \inf \sigma_{\text{ess}}(H)$ then

$$E_n \notin \sigma(H) \cap (E_n + \varepsilon, \infty) \supseteq \sigma\left(H|_{\text{Ran}(P((E_n+\varepsilon, \infty)))}\right) \tag{9.3}$$

and so $E_n \in \sigma_{\text{ess}}\left(H|_{\text{Ran}(P((-\infty, E_n+\varepsilon)))}\right)$ and thus $\dim \text{Ran}\,(P((-\infty, E_n + \varepsilon))) = \infty$. So in any case we have $\dim \text{Ran}\,(P((-\infty, E_n + \varepsilon))) \geq n$.

If $M \subseteq \text{Ran}\,(P((-\infty, E_n + \varepsilon)))$ has dimension n and is invariant under H then

$$\mu_n(H) \overset{\text{smaller subset}}{\leq} \sup_{\substack{\varphi \in M, \\ \|\varphi\|=1}} \langle \varphi, H\varphi \rangle = \max\{\text{ eigenvalues of } H|_M\} \overset{\text{eqn. (9.1)}}{\leq} E_n + \varepsilon.$$

"$\geq$": By equation (9.1) we have that $\dim \text{Ran}\,(P((-\infty, E_n))) < n$ because

$$\sigma\left(H|_{\text{Ran}(P((-\infty, E_n)))}\right) \subseteq \overline{\sigma(H) \cap (-\infty, E_n)}.$$

So if M has dimension n then there exists a $\varphi \in M \cap \text{Ran}\,(P((-\infty, E_n)))^\perp$. Therefore $\sup_{\substack{\psi \in M, \\ \|\psi\|=1}} \langle \psi, H\psi \rangle \geq \langle \varphi, H\varphi \rangle \geq E_n$ because φ is orthogonal to all eigenspaces to eigenvectors below E_n.

■

An elementary proof in a special case can be constructed rather explicitly:

An elementary proof of **Theorem 9.4** *in a special case.* Simplifying assumptions: We assume $n=2$ and that H has an orthonormal basis of eigenfunctions $(v_m)_{m\in\mathbb{N}}$ to eigenvalues $(E_m)_{m\in\mathbb{N}}$ with $E_1 \le E_2 \le \ldots \le E_m \le \ldots$, i.e. $Hv_m = E_m v_m$. Thus we have to prove that

$$\inf_{\substack{M\subseteq D(H)\\ \dim M=2}} \sup_{\substack{\varphi\in M\\ \|\varphi\|=1}} \langle \varphi, H\varphi\rangle \le E_2 \tag{9.4}$$

and

$$\inf_{\substack{M\subseteq D(H)\\ \dim M=2}} \sup_{\substack{\varphi\in M\\ \|\varphi\|=1}} \langle \varphi, H\varphi\rangle \ge E_2\,. \tag{9.5}$$

To prove equation (9.4) let $\varphi \in \operatorname{span}\{v_1, v_2\}$ with $\|\varphi\| = 1$, i.e. $\varphi = c_1v_1 + c_2v_2$ with $|c_1|^2 + |c_2|^2 = 1$. Thus $\langle \varphi, H\varphi\rangle = \langle c_1v_1 + c_2v_2, H(c_1v_1 + c_2v_2)\rangle \overset{v_1\perp v_2}{=} |c_1|^2 \langle v_1, Hv_1\rangle + |c_2|^2 \langle v_2, Hv_2\rangle = |c_1|^2E_1 + |c_2|^2E_2 \le E_2$ since $E_1 \le E_2$ and $|c_1|^2 + |c_2|^2 = 1$. Hence $\sup\limits_{\substack{\varphi\in M\\ \|\varphi\|=1}} \langle \varphi, H\varphi\rangle \ge E_2$ and also $\inf\limits_{\substack{M\subseteq D(H)\\ \dim M=2}} \sup\limits_{\substack{\varphi\in M\\ \|\varphi\|=1}} \langle \varphi, H\varphi\rangle \le E_2$. Thus equation (9.4) holds.

Now we prove equation (9.5). Let $M \subseteq D(H)$ with $\dim M = 2$. Then $M = \operatorname{span}\{u, w\}$ with u, w orthonormal. We can write u as

$$u = \sum_{j=1}^{N_1} c_{n_j} v_{n_j}, n_1 \le n_2 \le \ldots, n_j \ne 0\, \forall j, \sum_{j=1}^{N_1} \left|c_{n_j}\right|^2 = 1 \tag{9.6}$$

and w as

$$w = \sum_{i=1}^{N_2} d_{m_i} v_{m_i}, m_1 \le m_2 \le \ldots, m_i \ne 0\, \forall i, \sum_{i=1}^{N_2} |d_{m_i}|^2 = 1\,, \tag{9.7}$$

where $N_1, N_2 \in \mathbb{N} \cup \{+\infty\}$. Thus

$$\langle u, Hu\rangle = \sum_{j=1}^{N_1} \left|c_{n_j}\right|^2 E_{n_j}\,, \tag{9.8}$$

since the v_n form a basis of eigenfunctions for H, and similarly $\langle w, Hw\rangle = \sum\limits_{i=1}^{N_2} |d_{m_i}|^2 E_{m_i}$. Now we have to distinguish between two cases:

(1) (i) $n_1 > 1$: In this case $2 \le n_1 \le n_2 \le \ldots$, so $\langle u, Hu\rangle \ge E_2$.

(ii) $m_1 > 1$: In this case $2 \le m_1 \le m_2 \le \ldots$, so $\langle w, Hw\rangle \ge E_s$.

(2) $n_1 = m_1 = 1$: In this case $d_1u - c_1w \in M$ is nonzero (because $u \perp w$) and orthogonal to v_1. So $\dfrac{d_1u - c_1w}{\|d_1u - c_1w\|}$ can be written in the form of equation (9.6), where all $n_j > 1$. Thus, arguing as for equation (9.8), we find $\left\langle \dfrac{d_1u - c_1w}{\|d_1u - c_1w\|}, H\dfrac{d_1u - c_1w}{\|d_1u - c_1w\|}\right\rangle \ge E_2$.

Thus, in both cases $\sup_{\substack{\varphi\in M\\ \|\varphi\|=1}} \langle \varphi, H\varphi\rangle \geq E_2$. Since $M \subseteq D(H)$ was arbitrary we find $\inf_{\substack{M\subseteq D(H)\\ \dim M=2}} \sup_{\substack{\varphi\in M\\ \|\varphi\|=1}} \langle \varphi, H\varphi\rangle \geq E_2$, so equation (9.5) holds as well. ∎

There is another proof using the spectral theorem in projection-valued measure form in Section 9.1.

Remark (for **Theorem 9.4**)

For example $\mu_1(H) = \inf_{\substack{\varphi\in D(H),\\ \|\varphi\|=1}} \langle \varphi, H\varphi\rangle$ = ground state energy of H as $\dim \mu = 1$ means that $M = \operatorname{span}(\varphi)$.

If A is observable, ϕ is its functional calculus, ψ is a state and $P(\Omega) = \phi(\chi_\Omega)$, then $\langle \psi, P(\Omega)\psi\rangle$ = probability that a measurement of A is in Ω.

Corollary 9.5

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

Proof. From Theorem 9.4 one of

a) $\mu_1(H) < \inf \sigma_{\text{ess}}(H)$ and it is the lowest eigenvalue of H. Then $\mu_1(H) \in \sigma(H)$

b) $\mu_1(H) = \inf \sigma_{\text{ess}}(H)$ so $\mu_1(H) \in \sigma(H)$ because $\sigma(H)$ is closed by Theorem 2.4.

has to hold. ∎

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

(ii) If there exists a subspace $M \subseteq D(H)$ of dimension $N \in \mathbb{N}\cup\{\infty\}$ with $\langle \psi, H\psi\rangle < \inf \sigma_{\text{ess}}(H)$ for all $\psi \in M$ with $\|\psi\| = 1$ then there are at least N eigenvalues below $\inf \sigma_{\text{ess}}(H)$ (counting multiplicity).

Proof. (i) $\mu_1(H) = \inf_{\substack{\|\phi\|=1\\ \phi\in D(H)}} \langle \phi, H\phi\rangle \leq \langle \varphi, H\varphi\rangle < \inf \sigma_{\text{ess}}(H)$. Thus for $\mu_1(H)$ case b) of Theorem 9.4 cannot happen and thus by a) $\mu_1(H)$ is the lowest eigenvalue of H and it is below $\inf \sigma_{\text{ess}}(H)$.

(ii) If $N \in \mathbb{N}$ then $\mu_N(H) \leq \sup\limits_{\substack{\phi \in M, \\ \|\phi\|=1}} \langle \phi, H\phi \rangle = \max\limits_{\substack{\phi \in M, \\ \|\phi\|=1}} \langle \phi, H\phi \rangle < \inf \sigma_{\text{ess}}(H)$ $(\dim M < \infty)$.

So for $\mu_N(H)$ case b) is eliminated again, therefore a) holds and so there are at least N eigenvalues below $\inf \sigma_{\text{ess}}(H)$.

If $N = \infty$ there are at least n eigenvalues below $\inf \sigma_{\text{ess}}(H)$ for all $n \in \mathbb{N}$. Therefore there are infinitely many eigenvalues below $\inf \sigma_{\text{ess}}(H)$.

■

Example 9.4

The operator $H : H^2(\mathbb{R}^3) \subseteq L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3), H = -\Delta - \frac{1}{|x|}$ (hydrogen atom) has infinitely many eigenvalues below $\inf \sigma_{\text{ess}}(H)$.

Proof. We have $\sigma_{\text{ess}}(H) = [0, \infty)$ so $\inf \sigma_{\text{ess}}(H) = 0$. Therefore by Corollary 9.6 it suffices to find $M \subseteq H^2(\mathbb{R}^3)$ with $\dim M = \infty$ and $\langle \psi, H\psi \rangle < 0$ for all $\psi \in M \setminus \{0\}$.
Let $\psi \in C_c^\infty(\mathbb{R}^3)$ with $\operatorname{supp}(\psi) \subseteq \{x \in \mathbb{R}^3 \mid 1 < |x| < 2\}$. Define $\psi_n(x) := 2^{-3n/2}\psi(2^{-n}x)$. To show:

(i) $\operatorname{supp}(\psi_n) \cap \operatorname{supp}(\psi_m) = \emptyset$ if $n \neq m$ and $\|\psi\| = 1$ for all $n \in \mathbb{N}$.

(ii) $\exists N_0 \in \mathbb{N} : \forall n \geq N_0 : \langle \psi_n, H\psi_n \rangle < 0$

(iii) If $M = \operatorname{span}\{\psi_n \mid n \geq N_0\}$ then $\dim M = \infty$ and $\langle \varphi, H\varphi \rangle < 0$ for all $\varphi \in M \setminus \{0\}$.

(i) $\operatorname{supp}(\psi_m) \subseteq \{x \in \mathbb{R}^3 \mid 1 < |2^{-n}x| < 2\} = \{x \in \mathbb{R}^3 \mid 2^n < |x| < 2^{n+1}\}$.

Thus $\operatorname{supp}(\psi_n) \cap \operatorname{supp}(\psi_m) = \emptyset$ for all $m \neq n$.

Moreover $\psi_n = U_{2^{-n}}\psi$ where U_λ as in Exercise 33. As U_λ is unitary $\|\psi_n\| = 1$.

(ii) We have

$$\begin{aligned}
\langle \psi_n, H\psi_n \rangle &= \langle \psi_n, -\Delta\psi_n \rangle - \left\langle \psi_n, \frac{1}{|x|}\psi_n \right\rangle \\
&= \langle U_{2^{-n}}\psi, -\Delta U_{2^{-n}}\psi \rangle - \left\langle U_{2^{-n}}\psi, \frac{1}{|x|}U_{2^{-n}}\psi \right\rangle \\
&\overset{U_\lambda^* = U_\lambda^{-1} = U_{\lambda^{-1}}}{=} \langle \psi, U_{2^n}(-\Delta)U_{2^{-n}}\psi \rangle - \left\langle \psi, U_{2^n}\frac{1}{|x|}U_{2^{-n}}\psi \right\rangle \\
&\overset{\text{Exercise 33}}{=} \frac{1}{4^n}\langle \psi, -\Delta\psi \rangle - \left\langle \psi, \frac{1}{|2^n x|}\psi \right\rangle = \frac{1}{2^n}\left(\frac{1}{2^n}\langle \psi, -\Delta\psi \rangle - \left\langle \psi, \frac{1}{|x|}\psi \right\rangle \right) < 0
\end{aligned}$$

for all $n \geq n_0$ for some $n_0 \in \mathbb{N}$ since the first term vanishes as $n \to \infty$.

(iii) Let $\varphi \in M\backslash\{0\}$. Then $\varphi = c_{n_1}\psi_{n_1}+\ldots+c_{n_k}\psi_{n_k}$ for some $n_1,\ldots,n_k \in \mathbb{N}$ with $c_{n_1},\ldots,c_{n_k} \neq 0$. Thus $\langle\varphi, H\varphi\rangle = \left\langle \sum_{m=1}^{n} c_{n_m}\psi_{n_m}, H\sum_{l=1}^{k} c_{n_l}\psi_{n_l} \right\rangle = \sum_{m=1}^{k}\sum_{l=1}^{k} \overline{c_{n_m}} c_{n_l} \langle\psi_{n_m}, H\psi_{n_l}\rangle$. Since $\operatorname{supp}(\psi_i) \cap \operatorname{supp}(\psi_j) = \emptyset$ for all $i \neq j$, the functions ψ_{n_m} and ψ_{n_l} are orthogonal if $n_m \neq n_l$, so we have $\langle\varphi, H\varphi\rangle = \sum_{l=1}^{k} |c_{n_l}|^2 \langle\psi_{n_l}, H\psi_{n_l}\rangle < 0 = \inf\sigma_{\text{ess}}(H)$ because of (ii). We have $\dim M = \infty$ since M is the span of infinitely many orthonormal (thus linearly independent) ψ_n. Thus, by Corollary 9.6 there are infinitely many eigenvalues below $\inf\sigma_{\text{ess}}(H)$.

■

Definition 9.7

Let $A : D(A) \subseteq \mathcal{H} \to \mathcal{H}$ be self-adjoint with functional calculus ϕ from Theorem 9.2. The map

$$P : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H}), \quad P(\Omega) := P_\Omega := \phi(\chi_\Omega) = \chi_\Omega(A)$$

is called the *spectral measure of* A, where $\mathcal{B}(\mathbb{R})$ are the Borel subsets of $\mathbb{R}$. Here

$$\operatorname{supp}(P) := \{x \in \mathbb{R} \mid P(U) \neq 0 \text{ for all neighbourhoods } U \text{ of } x\}.$$

Theorem 9.8

Let A be self-adjoint with spectral measure P. Then

1.) $S = \operatorname{supp}(P)$ is closed.

2.) $P(S) = I, P(\mathbb{R} \setminus S) = 0$.

3.) $\forall f \in \mathcal{B}(\mathbb{R}) \cap C(\mathbb{R}) : \|f(A)\| = \|\phi(F)\| = \sup_{x\in S} |f(x)|$.

4.) $\forall z \in \rho(A) : \left\|(z-A)^{-1}\right\| = \operatorname{dist}(z, \sigma(A))^{-1}$.

5.) $S = \sigma(A)$.

Proof. 1.) Let $x \in \mathbb{R} \setminus S$. Then by definition of S there exists a neighborhood U_x of x with $P(U_x) = 0$. But then there exists an $\varepsilon > 0$ such that $(x-\varepsilon, x+\varepsilon) \subseteq U_x$. For all $y \in (x-\varepsilon, x+\varepsilon)$ U_x is a neighborhood of y as well. Thus $y \in \mathbb{R} \setminus S$ and $\mathbb{R} \setminus S$ is open.

2.) We will prove that $P(\mathbb{R}\setminus S)=0$. Then by Theorem 9.3(i) we have $P(S)=P(\mathbb{R})-P(\mathbb{R}\setminus S)=I-0=I$. First we prove $P(K)=0$ for all compact subsets $K\subseteq\mathbb{R}\setminus S$: for each $x\in K\subseteq\mathbb{R}\setminus S$ there exists a neighborhood U_x of x such that $P(U_x)=0$. But $K\subseteq\bigcup_{x\in K}U_x$. Since K is compact, there exist $x_1,\dots,x_n\in K$ such that $K\subseteq U_{x_1}\cup U_{x_2}\cup\ldots\cup U_{x_n}$. But $P\left(U_{x_j}\right)=0$ by 1.). Therefore $\sum_{j=1}^{n}P\left(U_{x_j}\right)=0$. Since $\emptyset\subseteq K\subseteq U_{x_1}\cup\ldots\cup U_{x_n}$ we find $P(\emptyset)\le P(K)\le\sum_{j=1}^{n}P\left(U_{x_j}\right)=0$, so $0\le P(K)\le 0$. Hence $P(K)=0$.

Let now $K_n:=\left\{x\in\mathbb{R}\setminus S:\operatorname{dist}(x,S)\ge\frac{1}{n},|x|\le n\right\}$. Then $K_n\subseteq\mathbb{R}\setminus S$ is compact. Thus $P(K_n)=0$. But $\mathbb{R}\setminus S=\bigcup_{n\in\mathbb{N}}K_n$ because $\mathbb{R}\setminus S$ is open, and since $\sum_{n\in\mathbb{N}}P(K_n)=0$ we obtain similarly as before that $P(\mathbb{R}\setminus S)=0$.

3.) Since $\phi(\chi_S)=P(S)=I$ by Theorem 9.2(a) we have $\phi(\chi_S f)=\phi(\chi_S)\phi(f)=\phi(f)$. Thus $\|\phi(f)\|=\|\phi(\chi_S f)\|\overset{\text{Thm. 9.2(b)}}{\le}\|\chi_S f\|_{L^\infty}=\sup_{x\in S}|f(x)|$. Now let $x\in S$. We will prove that $\|\phi(f)\|\ge|f(x)|$: if $|f(x)|=0$ there is nothing to be shown since the norm is always non-negative. So assume $|f(x)|>0$. We will prove that $\|\phi(f)\|\ge f(x)-\varepsilon$ for all $\varepsilon\in(0,|f(x)|)$. Since f is continuous there exists a neighborhood U_x of x such that $|f(y)-\varepsilon|>0$ for all $y\in U_x$. But $x\in S\Leftrightarrow P(U_x)\neq 0$. So there exists a $\psi\in\operatorname{Ran}(P(U_x))$ with $\|\psi\|\neq 0$. Thus $\|\phi(f)\psi\|\overset{\psi\in\operatorname{Ran}(P(U_x))}{=}\|\phi(f)P(U_x)\psi\|\|\phi(f)\phi(\chi_{U_x})\psi\|\overset{\text{Thm. 9.2(a)}}{=}\|\phi(f\chi_{U_x})\psi\|$. Hence $\|\phi(f)\psi\|^2=\|\phi(f\chi_{U_x})\psi\|^2=\langle\psi,\phi^*(f\chi_{U_x})\phi(f\chi_{U_x})\psi\rangle\overset{\text{Thm. 9.2(a)}}{=}\left\langle\psi,\phi(|f|^2\chi_{U_x})\psi\right\rangle$ $\overset{\text{Thm. 9.2(f)}}{\ge}\left\langle\psi,\phi\left((|f(x)|-\varepsilon)^2\chi_{U_x}\right)\psi\right\rangle\overset{\substack{\text{Thm. 9.2(a)}\\ x\text{ fixed}}}{=}(|f(x)|-\varepsilon)^2\langle\psi,\phi(\chi_{U_x})\psi\rangle$ $\overset{\psi\in\operatorname{Ran}(P(U_x))}{=}(|f(x)|-\varepsilon)^2\|\psi\|^2$. So $\|\phi(f)\|\ge f(x)-\varepsilon$.

4.) $$\underbrace{\left\|(z-A)^{-1}\right\|_{\mathcal{L}(\mathcal{H})}}_{=\|f(A)\|_{\mathcal{L}(\mathcal{H})}}\overset{3.)}{=}\sup_{x\in S}\left|(z-x)^{-1}\right|=\frac{1}{\inf_{x\in S}|z-x|}=\frac{1}{\operatorname{dist}(z,S)}.$$

5.) We have $$\lambda\in\sigma(A)\overset{\text{Thm. 2.4}}{\Leftrightarrow}\left\|\left(A-\lambda+\frac{\mathrm{i}}{n}\right)^{-1}\right\|\overset{n\to\infty}{\to}\infty\overset{4.)}{\Leftrightarrow}\operatorname{dist}\left(\lambda+\frac{\mathrm{i}}{n},S\right)\overset{n\to\infty}{\to}0$$ $$\Leftrightarrow\lambda\in\overline{S}\overset{S\text{ closed}}{=}S.$$

■

Corollary

(1) $\lambda\in\sigma(A)\Leftrightarrow\lambda\in S\Leftrightarrow P((\lambda-\varepsilon,\lambda+\varepsilon))\neq 0$ for all $\varepsilon>0$.

(2) For all $f \in \mathcal{B}(\mathbb{R}) \cap C(\mathbb{R})$ we have $\|f(A)\| = \sup_{x\in\sigma(A)} |f(x)|$.

We now tend towards a third version of the spectral theorem. For this we need to introduce some notations first.
For each $\varphi \in \mathcal{H}$ the map μ defined by $\mu(\Omega) := \langle \varphi, P(\Omega)\psi\rangle$ is a well defined Borel measure, namely $\mu(\emptyset) = 0$, for all $\Omega \subseteq \mathbb{R} : \mu(\Omega) \geq 0$ and if $\Omega_n \cap \Omega_m = \emptyset \, \forall n \neq m$ we have $\mu\left(\bigcup_{n\in\mathbb{N}} \Omega_n\right) = \sum_{n\in\mathbb{N}} \mu(\Omega_n)$.
Moreover $\mu(B) = \sup\{\mu(D) \mid D \subseteq B, D \text{ compact}\} = \inf\{\mu(O) \mid B \subseteq O, O \text{ open}\}$.
Thus we can define integration with respect to the measure with the notation $\mathrm{d}\langle\varphi, P(\lambda)\varphi\rangle$.

Bounded case: If g is bounded Borel we define

$$\langle \varphi, g(A)\varphi\rangle := \int_{-\infty}^{\infty} g(\lambda)\,\mathrm{d}\langle\varphi, P(\lambda)\varphi\rangle\,,$$

where

$$\int_{\Omega} \mathrm{d}\langle\varphi, P(\lambda)\varphi\rangle = \langle\varphi, P(\Omega)\varphi\rangle\,.$$

Then the functional calculus $g(A)$ satisfies the properties $(a) - (d)$ of Theorem 9.2 and thus $g(A) = \phi(g)$.
With Exercise 2 one can also define $\langle\varphi, g(A)\psi\rangle$, $\langle\varphi, P(\lambda)\psi\rangle$ and

$$\langle\varphi, g(A)\psi\rangle = \int_{-\infty}^{\infty} g(\lambda)\,\mathrm{d}\langle\varphi, P(\lambda)\varphi\rangle\,. \tag{9.9}$$

Unbounded Borel case: If g is an unbounded Borel function and

$$D_g := \left\{\varphi \in \mathcal{H} \mid \int_{-\infty}^{\infty} |g(\lambda)|^2\,\mathrm{d}\langle\varphi, P(\lambda)\varphi\rangle < \infty\right\}$$

where $\int_{-\infty}^{\infty} |g(\lambda)|^2\,\mathrm{d}\langle\varphi, P(\lambda)\varphi\rangle$ is supposed to be $\|g(A)\varphi\|^2$.
Then $g(A)$ is defined on D_g as in equation (9.9).
Symbolically $g(A) = \int_{-\infty}^{\infty} g(\lambda)\,\mathrm{d}P(\lambda) \overset{\mathrm{supp}(P)=\sigma(A)}{=} \int_{\sigma(A)} g(\lambda)\,\mathrm{d}P(\lambda)$.

Comparison to measure theory: If μ is a Lebesgue measure on $\mathbb{R}$:

$$\int_{\mathbb{R}} \chi_\Omega \,\mathrm{d}\mu := \mu(\Omega), \qquad \int_{\mathbb{R}} \sum_{k=1}^{n} a_k \chi_{\Omega_k} \,\mathrm{d}\mu := \sum_{k=1}^{n} a_k \mu(\Omega_k)$$

Then we approximate general functions f with simple functions.

Here:

$$\int_{\mathbb{R}} \chi_\Omega \,\mathrm{d}P(\lambda) := P(\Omega), \qquad \int_{\mathbb{R}} \sum_{k=1}^{n} a_k \chi_{\Omega_k} \,\mathrm{d}P(\lambda) := \sum_{k=1}^{n} a_k P(\Omega_k)$$

If f is Borel and bounded it can be uniformly approximated by simple functions as well, so $\int_{\mathbb{R}} f(\lambda)\,\mathrm{d}P(\lambda)$ can be defined.

Theorem 9.9 (Spectral theorem in projection-valued measure form)

There is a $1-1$ correspondence between self-adjoint operators A and projection-valued measures P with the correspondence given by

$$A = \int_{-\infty}^{\infty} \lambda \,\mathrm{d}P(\lambda) = \int_{\sigma(A)} \lambda \,\mathrm{d}P(\lambda) \tag{9.10}$$

If g is a real-valued Borel function on $\mathbb{R}$ then $g(A) := \int g(\lambda)\,\mathrm{d}P(\lambda)$ is self-adjoint on D_g.

If g is bounded then $g(A) = \phi(g)$ with ϕ being the functional calculus of A

If P has discrete support $P(\mathbb{R}) = \sum_{n=1}^{\infty} P(\{\lambda_n\})$ then the spectral theorem becomes:

$$A = \int_{\sigma(A)} \lambda \,\mathrm{d}P(\lambda) = \sum_{n=1}^{\infty} \lambda_n P(\{\lambda_n\})$$

where $P(\{\lambda_n\})$ is the projection onto the eigenspace to eigenvalue λ_n.

9.1 Proofs using spectral theorem in projection-valued measure form

Proof for **Theorem 9.3** (ii). Let $\mu \in \sigma(A) \cap \Omega$. Then by Exercise 42 we have for all $n \in \mathbb{N}$: $P\left((\mu - \frac{1}{n}, \mu + \frac{1}{n})\right) \neq 0$.

Thus there exists $\varphi_n \in \operatorname{Ran}\left(P\left((\mu-\frac{1}{n},\mu+\frac{1}{n})\right)\right)$ with $\|\varphi_n\| = 1$. Then

$$\begin{aligned}
\|(A-\mu)\varphi_n\|^2 &= \langle \varphi, (A-\mu)^2\varphi_n\rangle = \int_{\lambda\in\sigma(A)} (\lambda-\mu)^2 \,\mathrm{d}\langle\varphi_n, P(\lambda)\varphi_n\rangle \\
&\overset{P((\mu-1/n,\mu+1/n)^c)\varphi_n=0}{=} \int_{\lambda\in\sigma(A)\cap(\mu-1/n,\mu+1/n)} \underbrace{(\lambda-\mu)^2}_{\le 1/n^2} \mathrm{d}\langle\varphi_n, P(\lambda)\varphi_n\rangle \\
&\le \frac{1}{n^2}\int_{\lambda\in\sigma(A)\cap(\mu-1/n,\mu+1/n)} \mathrm{d}\langle\varphi_n, P(\lambda)\varphi_n\rangle \overset{P(\lambda)\ge 0}{\le} \frac{1}{n^2}\int_{\mathbb{R}} \mathrm{d}\langle\varphi_n, P(\lambda)\varphi_n\rangle \\
&= \frac{1}{n^2}\,\mathrm{d}\langle\varphi_n, P(\mathbb{R})\varphi_n\rangle = \frac{1}{n^2}\|\varphi_n\| = \frac{1}{n^2}
\end{aligned}$$

Therefore $\|(A-\mu)\varphi_n\|^2 \le \frac{1}{n^2} \to 0$ and $\|\varphi_n\| = 1$. Also $\varphi_n \in \operatorname{Ran}\left(P\left((\mu-\frac{1}{n},\mu+\frac{1}{n})\right)\right) \subseteq \operatorname{Ran}(P(\Omega)) =: \mathcal{H}_\Omega$ for n large enough because $\mu \in \Omega$ and Ω open. Therefore by Theorem 7.5 $\mu \in \sigma(A\,|_{\mathcal{H}_\Omega})$.
Suppose that $\mu \in \overline{\sigma(A)\cap\Omega}$. Then $\operatorname{dist}\left(\mu, \overline{\sigma(A)\cap\Omega}\right) =: \delta > 0$. Thus as before $\forall f \in P(\Omega)\,D(A)$:

$$\begin{aligned}
\|(A-\mu)\varphi\|^2 &= \int_{\lambda\in\sigma(A)\cap\Omega} \underbrace{(\lambda-\mu)^2}_{\ge\delta^2} \mathrm{d}\langle\varphi, P(\lambda)\varphi\rangle \ge \delta^2 \int_{\lambda\in\sigma(A)\cap\Omega} \mathrm{d}\langle\varphi, P(\lambda)\varphi\rangle \\
&= \delta^2\langle\varphi, P(\Omega)\varphi\rangle = \delta^2\|\varphi\|^2.
\end{aligned}$$

Therefore $\nexists$ a set of approximate eigenfunctions to μ. So by Theorem 7.5 $\mu \notin \sigma(A\,|_{\mathcal{H}_\Omega})$. ■

Alternative proof of **Theorem 9.4** *using* **Theorem 9.9**.
If H has at least n eigenvalues below $\inf\sigma_{\text{ess}}(H)$ let E_n be the n-th eigenvalue from below (counting multiplicity), otherwise let $E_n := \inf\sigma_{\text{ess}}(H)$. We have to show that $\mu_n(H) = E_n$ for all $n \in \mathbb{N}$.

"$\le$": We show that $\mu_n(H) \le E_n + \varepsilon$ for all $\varepsilon > 0$. If $E_n = \inf\sigma_{\text{ess}}(H)$ then $E_n \in \sigma_{\text{ess}}(H)$ (exercise) and thus by Exercise 42:

$$\dim\operatorname{Ran}(P((-\infty, E_n+\varepsilon))) = \infty.$$

If $E_n < \inf\sigma_{\text{ess}}(H)$ then we have $E_1 \le \cdots \le E_n < \inf\sigma_{\text{ess}}(H)$ and let $\vec{v_i}$ be orthonormal with $A\vec{v_i} = E_i\vec{v_i}$, then $\vec{v_1},\ldots,\vec{v_n} \in \operatorname{Ran}(P((-\infty, E_n+\varepsilon)))$ because $\sigma\left(A\,|_{(-\infty,E_n+\varepsilon)^c}\right) \subseteq [E_n+\varepsilon, \infty]$.

So in any case we have $\dim\operatorname{Ran}(P((-\infty, E_n+\varepsilon))) \ge n$.

If $M \subseteq \operatorname{Ran}(P((-\infty, E_n + \varepsilon)))$ has dimension n and is invariant under H then

$$\mu_n(H) \overset{\text{smaller subset}}{\leq} \sup_{\substack{\varphi \in M, \\ \|\varphi\|=1}} \langle \varphi, H\varphi \rangle \leq E_n + \varepsilon.$$

because

$$\langle \varphi, H\varphi \rangle = \int_{-\infty}^{E_n+\varepsilon} \lambda \, \mathrm{d} \langle \varphi, P(\lambda) \varphi \rangle \leq (E_n + \varepsilon) \langle \varphi, \varphi \rangle .$$

Thus $\forall \varepsilon > 0 : \mu_n(H) \leq E_n + \varepsilon$ and so $\mu_n(H) \leq E_n$.

"$\geq$": By equation (9.1) we have that $\dim \operatorname{Ran}(P((-\infty, E_n))) < n$ because

$$\sigma\left(H|_{\operatorname{Ran}(P((-\infty,E_n)))}\right) \subseteq \overline{\sigma(H) \cap (-\infty, E_n)}.$$

So if M has dimension n then there exists a $\varphi \in M \cap \operatorname{Ran}(P((-\infty, E_n)))^{\perp}$.

Thus

$$\langle \varphi, H\varphi \rangle \overset{\varphi \in P([E_n,\infty])}{=} \int_{E_n}^{\infty} \lambda \, \mathrm{d} \langle \varphi, P(\lambda) \varphi \rangle \geq E_n \int_{E_n}^{\infty} \mathrm{d} \langle \varphi, P(\lambda) \varphi \rangle \overset{\|\varphi\|=1}{=} E_n.$$

So $\sup_{\substack{\varphi \in M, \\ \|\varphi\|=1}} \langle \varphi, H\varphi \rangle \geq E_n$ and since M was arbirtary we have $\mu_n \geq E_n$.

■

10 Newton's theorem and Zhislin's theorem

Theorem 10.1 (Newton's theorem)

We consider a spherically symmetric function $\rho : \mathbb{R}^3 \to \mathbb{R}$ and assume that for all $x \in \mathbb{R}^3$ the function $g(y) := \dfrac{\rho(y)}{|x-y|}$ is in $L^1(\mathbb{R}^3)$. Then $\displaystyle\int_{\mathbb{R}^3} \frac{\rho(y)}{|x-y|}\,\mathrm{d}y = \int_{\mathbb{R}^3} \frac{\rho(y)}{\max\{|x|,|y|\}}\,\mathrm{d}y = \frac{1}{|x|}\int_{|y|\leq|x|} \rho(y)\,\mathrm{d}y + \int_{|y|\geq|x|} \frac{\rho(y)}{|y|}\,\mathrm{d}y.$

Proof. The second equality follows immediately after splitting the integral over $\mathbb{R}^3$ into an integral where $|y| \leq |x|$ and an integral where $|y| \geq |x|$. So it suffices to prove the first equality. Since $\rho(y) =: f(|y|)$ we have

$$\begin{aligned}
\int_{\mathbb{R}^3} \frac{\rho(y)}{|x-y|}\,\mathrm{d}y &= \int_0^\infty f(r)\left[\int_{\partial B(0,r)} \frac{1}{|x-y|}\,\mathrm{d}\sigma(y)\right]\mathrm{d}r \overset{\text{Exercise 36}}{=} \int_0^\infty f(r)\frac{4\pi r^2}{\max\{r,|x|\}}\,\mathrm{d}r \\
&= \int_0^\infty \frac{f(r)}{\max\{r,|x|\}}\left(\int_{\partial B(0,r)} 1\,\mathrm{d}\sigma(y)\right)\mathrm{d}r \\
&= \int_0^\infty \int_{\partial B(0,r)} \frac{f(r)}{\max\{r,|x|\}}\,\mathrm{d}\sigma(y)\,\mathrm{d}r \\
&= \int_{\mathbb{R}^3} \frac{\rho(y)}{\max\{|x|,|y|\}}\,\mathrm{d}y\,.
\end{aligned}$$

■

Remark

In particular, if $\operatorname{supp}(\rho) \subseteq B(0,|x|)$, then we have $\displaystyle\int_{\mathbb{R}^3} \frac{\rho(y)}{|x-y|}\,\mathrm{d}y = \frac{1}{|x|}\int_{|y|\leq|x|} \rho(y)\,\mathrm{d}y$.

Interpretation: Recall that $\dfrac{1}{|x|}$ is the potential created by a charge $+1$ located at position $y = 0$; mathematically $\dfrac{1}{|x|}$ is (up to a constant $-\dfrac{1}{4\pi}$) the fundamental solution (Green's function) of the equation $\Delta\phi(x) = \delta(x)$, where $\delta(x)$ is the Dirac delta (distribution). We can use the Poisson equation to interpret $\phi(x) = \dfrac{q}{|x-y|}$ as the potential of a charge q at

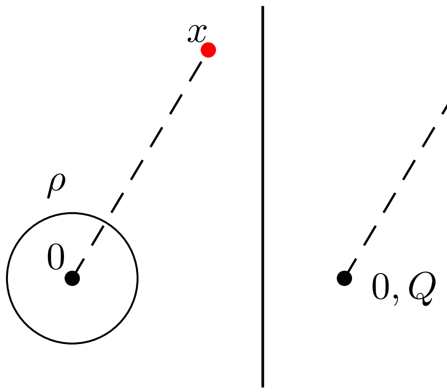

Figure 10.1: Outside of supp (ρ) (with spherically symmetric ρ) the potential is the same as the potential of a single charge $Q = \int_{\mathbb{R}^3} \rho(y)\,\mathrm{d}y$ located at 0; created with MGA-TeX 2.4 by K. Fritzsche [4].

position y, measured at position x. By the superposition principle, and taking the charge to be a (smeared out) distribution, we can interpret $\int_{\mathbb{R}^3} \frac{\rho(y)}{|x-y|}\,\mathrm{d}y$ as the potential of the charge distribution measured at x.
On the other hand $\int_{\mathbb{R}^3} \rho(y)\,\mathrm{d}y$ just gives the total charge Q and $\frac{1}{|x|}\int_{\mathbb{R}^3} \rho(y)\,\mathrm{d}y$ is therefore the potential of a charge Q located at 0.
Thus, outside of supp (ρ) it is irrelevant whether the charge is distributed or located at a single point, as long as ρ is spherically symmetric. This holds not only for electric charges and their potentials, but e.g. also for gravitational "charge distributions" (i.e. mass distributions) and the gravitational potential. Assuming that the earth is spherically symmetric it creates a potential $\frac{M}{|x|}$ outside of its support, where M is the total mass of the earth.

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

$$(H_{N,Z}\Phi)(x) = \sum_{j=1}^{N} \left(-\Delta_{x_j} - \frac{Z}{|x_j|}\right)\Phi(x) + \sum_{1\leq i<j\leq N} \frac{1}{|x_i - x_j|}\Phi(x), x = (x_1, \dots, x_N) \in \mathbb{R}^{3N}.$$

If $Z > N-1$ then $H_{N,Z}$ has infinitely many eigenvalues below $\sigma_{\text{ess}}(H_{N,Z})$.

Proof. We will prove the statement for $N < Z + 1$ by induction on N.
$\mathbf{N = 1}$: proved in Example 9.4 for $Z = 1$ and for $Z > 0$ the proof remains the same

Induction step: If the statement holds for $N-1$ then $H_{N-1,Z}$ has infinitely many eigenvalues below $\inf \sigma_{\text{ess}}(H_{N-1,Z})$. In particular it has a ground state

$$\varphi_{N-1} \in L^2\left(\mathbb{R}^{3(N-1)}\right) \text{ with } \|\varphi_{N-1}\| = 1 \tag{10.1}$$

Let $\psi \in C_c^\infty\left(\mathbb{R}^3\right), \|\psi\| = 1, \operatorname{supp}(\psi) \subseteq \{x \in \mathbb{R}^3 \mid 1 < |x| < 2\}$ and ψ spherically symmetric.
Let $\psi_n = U_{2^{-n}}\psi$ where $U_\lambda \psi = \lambda^{3/2}\psi(\lambda x)$. Then like in Example 9.4 we have

$$\|\psi_n\| = 1 \tag{10.2}$$

and $\operatorname{supp}(\psi_n) \cap \operatorname{supp}(\psi_m) = \emptyset$ if $m \neq n$. Thus by Corollary 9.6 it is enough to prove that for infinitely many n:

$$\begin{aligned}\langle \varphi_{N-1} \otimes \psi_n, H_{N,Z}\varphi_{N-1} \otimes \psi_n\rangle < \underbrace{\langle \varphi_{N-1}, H_{N-1,Z}\varphi_{N-1}\rangle}_{=:a} &= E_{N-1,Z} = \inf \sigma\left(H_{N-1,z}\right) \\ &\overset{\text{HVZ}}{=} \inf \sigma_{\text{ess}}\left(H_{N,Z}\right)\end{aligned} \tag{10.3}$$

where $\varphi_{N-1} \otimes \psi_n(x) = \varphi_{N-1}(x_1, \ldots, x_{N-1})\psi_n(x_N)$.
Since

$$H_{N,Z} = H_{N-1,Z} - \Delta_{x_N} - \frac{Z}{|x_N|} + \sum_{i=1}^{N-1} \frac{1}{|x_i - x_N|} \tag{10.4}$$

we have

$$\begin{aligned}
&\langle \varphi_{N-1} \otimes \psi_n, H_{N,Z}\varphi_{N-1} \otimes \psi_n\rangle \\
&\overset{\text{eqn. (10.4)}}{=} \left\langle \varphi_{N-1} \otimes \psi_n, \left(H_{N-1,Z} - \Delta_{x_N} - \frac{Z}{|x_N|} + \sum_{i=1}^{N-1} \frac{1}{|x_i - x_N|}\right)(\varphi_{N-1} \otimes \psi_n)\right\rangle \\
&= \langle \varphi_{N-1} \otimes \psi_n, H_{N-1,Z}(\varphi_{N-1} \otimes \psi_n)\rangle + \left\langle \varphi_{N-1} \otimes \psi_n, \left(-\Delta_{x_N} - \frac{Z}{|x_N|}\right)(\varphi_{N-1} \otimes \psi_n)\right\rangle \\
&+ \sum_{i=1}^{N-1} \left\langle \varphi_{N-1} \otimes \psi_n, \frac{1}{|x_i - x_N|}(\varphi_{N-1} \otimes \psi_n)\right\rangle.
\end{aligned}$$

Because $H_{N-1,Z}$ only acts on $x_1, \ldots, x_{N-1}$ and equation (10.2) we have:

$$\langle \varphi_{N-1} \otimes \psi_n, H_{N-1,Z}(\varphi_{N-1} \otimes \psi_n)\rangle = \langle \varphi_{N-1}, H_{N-1,Z}\varphi_{N-1}\rangle = a.$$

Because $\Delta_{x_N} - \dfrac{Z}{|x_N|}$ only acts on x_N and equation (10.1) we have

$$\left\langle \varphi_{N-1} \otimes \psi_n, \left(-\Delta_{x_N} - \frac{Z}{|x_N|}\right)(\varphi_{N-1} \otimes \psi_n)\right\rangle = \left\langle \psi_n, \left(-\Delta_{x_N} - \frac{Z}{|x_N|}\right)\psi_n\right\rangle.$$

Last but not least we have with Fubini:

$$\begin{aligned}
&\sum_{i=1}^{N-1}\left\langle \varphi_{N-1}\otimes\psi_n, \frac{1}{|x_i-x_N|}(\varphi_{N-1}\otimes\psi_n)\right\rangle \\
&= \sum_{i=1}^{N-1}\int |\varphi_{N-1}(x_1,\dots,x_{N-1})|^2\left(\int \frac{|\psi_n(x_N)|^2}{|x_i-x_N|}\,\mathrm{d}x_N\right)\mathrm{d}x_1\dots\mathrm{d}x_{N-1} \\
&\underset{\psi\text{ symmetric}}{\overset{\text{Thm. 10.1}}{\leq}} \sum_{i=1}^{N-1}\int |\varphi_{N-1}(x_1,\dots,x_{N-1})|^2\left(\int \frac{|\psi_n(x_N)|^2}{|x_N|}\,\mathrm{d}x_N\right)\mathrm{d}x_1\dots\mathrm{d}x_{N-1}
\end{aligned}$$

So putting those three equations together and using equation (10.1) again we get:

$$\begin{aligned}
&\langle \varphi_{N-1}\otimes\psi_n, H_{N,Z}\varphi_{N-1}\otimes\psi_n\rangle \leq a + \left\langle \psi_n, \left(-\Delta_{x_N} - \frac{Z-(N-1)}{|x_N|}\right)\psi_n\right\rangle \\
&= a + \langle \psi_n, -\Delta_{x_N}\psi_n\rangle - (Z-(N-1))\left\langle \psi_n, \frac{1}{|x_N|}\psi_n\right\rangle < a
\end{aligned}$$

for all $n \geq n_0$ for some n_0 for the same reason as in Example 9.4, concluding the proof. ■

Remark

Theorem 10.2 shows that it costs energy to send an electron at infinity, so the ion with a nucleus with Z protons and N electrons exists as it is stable.
In the physical case we have $U \in \mathbb{N}$ and so $Z > N-1 \Leftrightarrow Z \geq N$ which means that atoms and positive ions exist.

Open problems:

1. Do negative ions exist? So is $\inf\sigma(H_{N+1,N}) < \inf\sigma(H_{N,N})$?
2. Does $\inf\sigma(H_{N,Z}) < \inf\sigma(H_{N-1,Z})$ imply $\inf\sigma(H_{N-1,Z}) < \inf\sigma(H_{N-2,Z})$? Or in other words, if an ion with N electrons exist, does the ion with $N-1$ electrons exist? (Only for negative ions, for positive ions see Theorem 10.2).

11 Pure point spectrum, continuous spectrum, RAGE theorem

Definition 11.1

Let $H : D(H) \subset \mathcal{H} \to \mathcal{H}$ be a self-adjoint operator. We define $\mathcal{H}_{\text{pp}} := \overline{\text{span}\{\psi \in H\psi : \psi \text{ eigenfunction of } H\}}$ and $\mathcal{H}_c := \mathcal{H}_{\text{pp}}^{\perp}$.
Then $\sigma_{\text{pp}}(H) := \{\lambda : \lambda \text{ is eigenvalue of } H\}$ and we have $\overline{\sigma_{\text{pp}}(H)} = \sigma\left(H|_{\mathcal{H}_{\text{pp}}}\right)$ is called the *pure point spectrum* of H and $\sigma_c(H) := \sigma\left(H|_{\mathcal{H}_c}\right)$ is called the *continuous spectrum* of H.

Remark

It can occur that $\mathcal{H}_{\text{pp}} = \emptyset$, e.g. the Laplace operator $-\Delta$ does not have eigenfunctions in L^2. To see this, assume that $-\Delta u = \lambda u$ for some function $u \neq 0$ and $\lambda \in \mathbb{R}$, i.e. that there is an eigenfunction. Then by Fourier transformation $\left(|\xi|^2 - \lambda\right)\hat{u}(\xi) = 0$ and hence $\hat{u}(\xi) = 0$ if $|\xi|^2 \neq \lambda$. So $\hat{u} = 0$ almost everywhere, and by Fourier transforming again, we have that $u = 0$ almost everywhere, so u is not an eigenfunction of $-\Delta$.

Remark 11.2

We have $\sigma(H) = \overline{\sigma_{\text{pp}}(H)} \cup \sigma_c(H)$; this union is not necessarily disjoint. If $H\varphi = E\varphi$ then $\langle\varphi, P(\Omega)\varphi\rangle = \begin{cases} 1, E \in \Omega \\ 0, E \notin \Omega \end{cases}$, so $\langle\varphi, P(\Omega)\varphi\rangle$ is a Dirac measure supported in one point. If $\varphi \in \mathcal{H}_{\text{pp}}$ then $\Omega \mapsto \langle\varphi, P(\Omega)\varphi\rangle$ is a measure with discrete support (pure point measure). If $\varphi \in \mathcal{H}_c$ then $\Omega \mapsto \langle\varphi, P(\Omega)\varphi\rangle$ is a continuous measure, i.e. $\langle\varphi, P(\{\lambda\})\varphi\rangle = 0$ for all $\lambda \in \mathbb{R}$.

Theorem 11.3 (RAGE-Theorem: Ruelle, Amrein, Georgescu, Enss)

Let H be a self-adjoint operator on $L^2\left(\mathbb{R}^d\right)$. Assume that $\chi_{B(0,R)}(H + \mathrm{i})^{-1}$ is compact for all $R > 0$. Then

(i)

$$\varphi \in \mathcal{H}_{\text{pp}} \Leftrightarrow \lim_{R\to\infty} \sup_{t\geq 0} \left\|\left(1 - \chi_{B(0,R)}\right) \mathrm{e}^{-\mathrm{i}tH}\varphi\right\| = 0\,. \tag{11.1}$$

(ii)

$$\varphi \in \mathcal{H}_c \Leftrightarrow \lim_{T\to\infty} \frac{1}{T} \int_0^T \left\| \chi_{B(0,R)} \mathrm{e}^{-\mathrm{i}tH} \varphi \right\|^2 \mathrm{d}t = 0 \text{ for all } R > 0 \,. \tag{11.2}$$

Remark

If e.g.

$$\left\{ \begin{array}{l} \mathrm{i}\dfrac{\mathrm{d}}{\mathrm{d}t}\varphi_t = H\varphi_t \\ \varphi_t|_{t=0} = \varphi \end{array} \right\}, \tag{11.3}$$

then $\varphi_t = \mathrm{e}^{-\mathrm{i}Ht}\varphi$ is the solution of the Schrödinger equation. If φ_t describes the evolution of a particle, then equation (11.1) means that the particle remains localized. In the case of equation (11.2), the particle escapes the ball $B(0, R)$ for all $R > 0$ and comes back to it only rarely in time (on average it is outside the ball).

Before we prove Theorem 11.3, we discuss two prominent examples.

Example

(1) If $H = -\Delta$ then $\chi_R(H+\mathrm{i})^{-1}$ is compact for all $R > 0$ since $(H+\mathrm{i})^{-1} : L^2\left(\mathbb{R}^d\right) \to H^1\left(\mathbb{R}^d\right)$ is bounded and $\chi_R : H^1\left(\mathbb{R}^d\right) \to L^2\left(\mathbb{R}^d\right)$ (acting as a multiplication operator) is compact by Theorem 6.10. Then $\mathcal{H} = \mathcal{H}_c$ (there is no pure point spectrum, as explained in the remark above). Therefore equation (11.2) holds for all $\varphi \in \mathcal{H} = \mathcal{H}_c$.

(2) Let $H = -\Delta + V$, where V is a real-valued function such that $V\psi \in L^2$ and such that there exist $c > 0$ and $a \in (0, 1)$ with $\|V\psi\| \leq a\|-\Delta\psi\| + c\|\psi\|$ (in some sense, V is considered as a small perturbation to the free Hamilton operator $H = -\Delta$). Then V is called $-\Delta$-bounded with relative bound a. By Kato's theorem (Theorem 3.8) H is self-adjoint. Moreover $\chi_R(H+\mathrm{i})^{-1}$ is compact for all $R > 0$ since $\chi_R(H+\mathrm{i})^{-1} = \underbrace{\chi_R(-\Delta+\mathrm{i})^{-1}}_{\text{compact by Thm. 6.10}} (-\Delta+\mathrm{i})(H+\mathrm{i})^{-1}$, so it is enough to show that $(-\Delta+\mathrm{i})(H+\mathrm{i})^{-1}$ is bounded. We have $(-\Delta+\mathrm{i})(H+\mathrm{i})^{-1} = (-\Delta+\mathrm{i})(H+\mu\mathrm{i})^{-1} \underbrace{(H+\mu\mathrm{i})(H+\mathrm{i})^{-1}}_{=(H+\mathrm{i})(H+\mathrm{i})^{-1}+(\mu-1)\mathrm{i}(H+\mathrm{i})^{-1} \Rightarrow \text{bounded}}$, so suffices to show that $(-\Delta+\mathrm{i})(H+\mu\mathrm{i})^{-1}$ is bounded. Indeed, $(-\Delta+\mathrm{i})(H+\mu\mathrm{i})^{-1} = (-\Delta+\mathrm{i})(-\Delta+V+\mu\mathrm{i})^{-1} = (-\Delta+\mathrm{i})\left[\left(I+V(-\Delta+\mu\mathrm{i})^{-1}\right)(-\Delta+\mu\mathrm{i})\right]^{-1}$. Since $\left\|V(-\Delta+\mu\mathrm{i})^{-1}\right\| < 1$ for $|\mu|$ large enough (see the proof of Theorem 3.8), $\left(I+V(-\Delta+\mu\mathrm{i})^{-1}\right)$ is invertible by Exercise 7

and we obtain $(-\Delta+\mathrm{i})(H+\mu\mathrm{i})^{-1} = (-\Delta+\mathrm{i})(-\Delta+\mu\mathrm{i})^{-1}\underbrace{\left[I+V+(-\Delta+\mu\mathrm{i})^{-1}\right]^{-1}}_{\text{bounded}}$, so $(-\Delta+\mathrm{i})(H+\mu\mathrm{i})^{-1}$ is bounded.

Lemma 11.4

Let μ be a complex-valued finite measure on $\mathbb{R}$. We define $\hat{\mu}(t) := \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}t\lambda}\,\mathrm{d}\mu(\lambda)$. Then $\lim_{T\to\infty}\frac{1}{T}\int_0^T \left|\hat{\mu(t)}\right|^2 \mathrm{d}t = \sum_{y\in\mathbb{R}} |\mu(\{y\})|^2$. In particular, if μ is continuous (i.e. $\mu(\{y\})=0$ for all $y\in\mathbb{R}$), then $\lim_{T\to\infty}\frac{1}{T}\int_0^T |\hat{\mu}(t)|^2\,\mathrm{d}t = 0$.

Proof. $|\hat{\mu}(t)|^2 = \hat{\mu}(t)\overline{\hat{\mu}(t)} = \int_{\mathbb{R}} \mathrm{e}^{-\mathrm{i}tx}\,\mathrm{d}\mu(x)\int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}ty}\overline{\mathrm{d}\mu(y)}$. Applying Fubini's theorem, $\frac{1}{T}\int_0^T |\hat{\mu}(t)|^2\,\mathrm{d}t = \int_{\mathbb{R}}\int_{\mathbb{R}}\left(\frac{1}{T}\int_0^T \mathrm{e}^{\mathrm{i}t(y-x)}\,\mathrm{d}t\right)\mathrm{d}\mu(x)\,\overline{\mathrm{d}\mu(y)}$. But $\left|\frac{1}{T}\int_0^T \mathrm{e}^{\mathrm{i}t(y-x)}\,\mathrm{d}t\right| \leq 1$ for all $T\in\mathbb{R}$ and $\lim_{T\to\infty}\frac{1}{T}\int_0^T \mathrm{e}^{\mathrm{i}t(y-x)}\,\mathrm{d}t = \chi_{\{y\}}(x) = \begin{cases} 1, x=y \\ 0, x\neq y\end{cases}$. Using $\left|\frac{1}{T}\int_0^T \mathrm{e}^{\mathrm{i}t(y-x)}\,\mathrm{d}t\right| \leq 1$ and the fact that the measure is finite, we can apply the theorem of dominated convergence to obtain $\lim_{T\to\infty}\frac{1}{T}\int_0^T |\hat{\mu}(t)|^2\,\mathrm{d}t = \int_{\mathbb{R}}\underbrace{\int_R \chi_{\{y\}}(x)\,\mathrm{d}\mu(x)}_{=\mu(\{y\})}\overline{\mathrm{d}\mu(y)} = \int_{\mathbb{R}}\mu(\{y\})\,\overline{\mathrm{d}\mu(y)} = \sum_{y\in\mathbb{R}}|\mu(\{y\})|^2$. ■

Lemma 11.5

Let $H : D(H)\subseteq\mathcal{H}\to\mathcal{H}$ be a self-adjoint operator. If $\varphi\in\mathcal{H}$ and $\psi\in\mathcal{H}_c$ then $\lim_{T\to\infty}\frac{1}{T}\int_0^T \left|\langle\varphi, \mathrm{e}^{-\mathrm{i}Ht}\psi\rangle\right|^2\mathrm{d}t = 0$.

Proof. We may assume without loss of generality that $\varphi\in\mathcal{H}_c$ as well[1]. Since $\varphi,\psi\in\mathcal{H}_c$ the measure $\mu:\mathcal{B}\to\mathbb{C}$, $\mu(\Omega) := \langle\varphi, P(\Omega)\psi\rangle$ is (finite, complex and) continuous (because of Exercise 2 and since $\langle\varphi, P(\Omega)\varphi\rangle$ is continuous for all $\varphi\in\mathcal{H}_c$). Thus $\left\langle\varphi, \mathrm{e}^{-\mathrm{i}Ht}\psi\right\rangle \overset{\text{Thm. 9.9}}{=} \left\langle\varphi, \int \mathrm{e}^{-\mathrm{i}\lambda t}\,\mathrm{d}P(\Omega)\psi\right\rangle = \int \mathrm{e}^{-\mathrm{i}\lambda t}\,\mathrm{d}\langle\varphi, P(\Omega)\psi\rangle = \int \mathrm{e}^{-\mathrm{i}\lambda t}\,\mathrm{d}\mu(\lambda) = \hat{\mu}(t)$. Hence $\lim_{T\to\infty}\frac{1}{T}\int_0^T \left|\langle\varphi, \mathrm{e}^{-\mathrm{i}Ht}\psi\rangle\right|^2\mathrm{d}t = \lim_{T\to\infty}\frac{1}{T}\int_0^T |\hat{\mu}(t)|^2\,\mathrm{d}t \overset{\text{Lemma 11.4}}{=} 0$, since μ is continuous. ■

We are now finally ready to prove Theorem 11.3.

[1] If g is an eigenfunction of H ($Hg = Eg$ for some $E\in\mathbb{R}$, $g\neq 0$), then $\left\langle g, \mathrm{e}^{-\mathrm{i}Ht}\psi\right\rangle = \left\langle \mathrm{e}^{\mathrm{i}Ht}g, \psi\right\rangle = \mathrm{e}^{\mathrm{i}Et}\langle g,\psi\rangle = 0$, because $g\in\mathcal{H}_{\mathrm{pp}}\perp\mathcal{H}_c\ni\psi$. Thus if $\varphi = \varphi_{\mathrm{pp}}+\varphi_c$ with $\varphi_{\mathrm{pp}}\in\mathcal{H}_{\mathrm{pp}}$, $\varphi_c\in\mathcal{H}_c$, then $\left\langle\varphi, \mathrm{e}^{-\mathrm{i}Ht}\psi\right\rangle = \left\langle\varphi_c, \mathrm{e}^{-\mathrm{i}Ht}\psi\right\rangle$.

Proof of **Theorem 11.3**. Let $\mathcal{H}_{\text{bound}} := \left\{\psi \in L^2\left(\mathbb{R}^d\right) : \lim_{R\to\infty} \sup_{t\geq 0} \left\|(1-\chi_R)\,\mathrm{e}^{-\mathrm{i}Ht}\psi\right\| = 0\right\}$ and $\mathcal{H}_{\text{leaving}} := \left\{\psi \in L^2\left(\mathbb{R}^d\right) : \lim_{T\to\infty} \frac{1}{T}\int_0^T \left\|\chi_R \mathrm{e}^{-\mathrm{i}tH}\psi\right\|^2 \mathrm{d}t = 0 \text{ for all } R > 0\right\}$. By the triangle inequality, $\mathcal{H}_{\text{bound}}$ and $\mathcal{H}_{\text{leaving}}$ are subspaces of $\mathcal{H} = L^2\left(\mathbb{R}^d\right)$. The proof will proceed in four steps:

1.) $\mathcal{H}_{\text{bound}}$ is closed

2.) $\mathcal{H}_{\text{pp}} \subseteq \mathcal{H}_{\text{bound}}$

3.) $\mathcal{H}_{\text{bound}} \perp \mathcal{H}_{\text{leaving}}$

4.) $\mathcal{H}_c \subseteq \mathcal{H}_{\text{leaving}}$

The other direction is simple: to show that $\mathcal{H}_{\text{bound}} \subseteq \mathcal{H}_{\text{pp}}$, assume that $\varphi \in \mathcal{H}_{\text{bound}}$, but $\varphi \notin \mathcal{H}_{\text{pp}}$. Then $\varphi \in (\mathcal{H}_{\text{pp}})^c = \mathcal{H}_c \subseteq \mathcal{H}_{\text{leaving}}$, so $\varphi \in \mathcal{H}_{\text{leaving}}$. But $\mathcal{H}_{\text{leaving}} \perp \mathcal{H}_{\text{bound}}$, so $\varphi \in \mathcal{H}_{\text{bound}}$ and $\varphi \notin \mathcal{H}_{\text{bound}}$, a contradiction. So if $\varphi \in \mathcal{H}_{\text{bound}}$ then automatically $\varphi \in \mathcal{H}_{\text{pp}}$, i.e. $\mathcal{H}_{\text{bound}} \subseteq \mathcal{H}_{\text{pp}}$. In the same manner one shows that $\mathcal{H}_{\text{leaving}} \subseteq \mathcal{H}_c$, i.e. we have $\mathcal{H}_{\text{bound}} = \mathcal{H}_{\text{pp}}$ and $\mathcal{H}_{\text{leaving}} = \mathcal{H}_c$ which then concludes the proof of Theorem 11.3.

1.) Let $\psi \in \overline{\mathcal{H}_{\text{bound}}}$ and $\varepsilon > 0$. Then there exists $\psi_\varepsilon \in \mathcal{H}_{\text{bound}} : \|\psi - \psi_\varepsilon\| < \frac{\varepsilon}{2}$. As $\psi_\varepsilon \in \mathcal{H}_{\text{bound}}$ there exists $R_0 > 0$ such that

$$\sup_{t\in\mathbb{R}} \left\|(1-\chi_R)e^{-\mathrm{i}tH}\psi_\varepsilon\right\| < \frac{\varepsilon}{2} \tag{11.4}$$

for all $R > R_0$. Therefore we have for all $R > R_0$:

$$\begin{aligned}\sup_{t\geq 0}\left\|(1-\chi_R)e^{-\mathrm{i}tH}\psi\right\| &\overset{\Delta-\text{ineq.}}{\leq} \sup_{t\geq 0}\left\|(1-\chi_R)e^{-\mathrm{i}tH}\psi_\varepsilon\right\| + \sup_{t\geq 0}\left\|(1-\chi_R)e^{-\mathrm{i}tH}(\psi-\psi_\varepsilon)\right\| \\ &\overset{\text{eqn. (11.4)}}{\leq} \frac{\varepsilon}{2} + \sup_{t\geq 0}\left\|e^{-\mathrm{i}tH}(\psi-\psi_\varepsilon)\right\| = \frac{\varepsilon}{2} + \sup_{t\geq 0}\|(\psi-\psi_\varepsilon)\| < \frac{\varepsilon}{2} + \frac{\varepsilon}{2} = \varepsilon\end{aligned}$$

2.) Since by step 1 $\mathcal{H}_{\text{bound}}$ is a closed subspace it suffices to prove $H\psi = \lambda\psi \Rightarrow \psi \in \mathcal{H}_{\text{bound}}$. $H\psi = \lambda\psi \overset{\text{Thm. 9.2 f)}}{=} e^{\mathrm{i}tH}\psi = e^{\mathrm{i}\lambda t}\psi$. Thus

$$\lim_{R\to\infty}\sup_{t\geq 0}\left\|(1-\chi_R)e^{-\mathrm{i}tH}\psi\right\| = \lim_{R\to\infty}\sup_{t\geq 0}\left\|(1-\chi_R)e^{-\mathrm{i}t\lambda}\psi\right\| \leq \lim_{R\to\infty}\|(1-\chi_R)\psi\| = 0$$

3.) Let $\varphi \in \mathcal{H}_{\text{bound}}, \psi \in \mathcal{H}_{\text{leaving}}, \|\varphi\| = \|\psi\| = 1$. To show: $\forall\varepsilon > 0 : |\langle\varphi,\psi\rangle| < \varepsilon$.

$$\langle\varphi,\psi\rangle \overset{\text{unitary}}{=} \left\langle e^{-\mathrm{i}t\lambda}\varphi, e^{-\mathrm{i}t\lambda}\psi\right\rangle = \left\langle(1-\chi_R)e^{-\mathrm{i}t\lambda}\varphi, e^{-\mathrm{i}t\lambda}\psi\right\rangle + \left\langle e^{-\mathrm{i}t\lambda}\varphi, \chi_R e^{-\mathrm{i}t\lambda}\psi\right\rangle.$$

Thus for all R and all $t \geq 0$:

$$|\langle \varphi, \psi \rangle| \overset{CS}{\leq} \left\|(1-\chi_R)e^{-\mathrm{i}tH}\varphi\right\| + \left\|\chi_R e^{-\mathrm{i}tH}\psi\right\|$$

$$\Rightarrow |\langle \varphi, \psi \rangle|^2 \overset{CS}{\leq} 2 \cdot \left\|(1-\chi_R)e^{-\mathrm{i}tH}\varphi\right\|^2 + 2 \cdot \left\|\chi_R e^{-\mathrm{i}tH}\psi\right\|^2.$$

We therefore have

$$\frac{1}{T}\int_0^T |\langle \varphi, \psi \rangle|^2 \,\mathrm{d}t \leq \sup_{t\geq 0} 2 \cdot \left\|(1-\chi_R)e^{-\mathrm{i}tH}\varphi\right\|^2 + 2 \cdot \frac{1}{T}\int_0^T \left\|\chi_R e^{-\mathrm{i}tH}\psi\right\|^2 \mathrm{d}t < \varepsilon$$

because by the definition of $\mathcal{H}_{\text{pp}}$ the first addend is less than $\frac{\varepsilon}{2}$ for some $R = R_0 > 0$ and for the same R_0 there exists a $T_0 > 0$ such that the second addend is also less than $\frac{\varepsilon}{2}$.

4.) By Lemma 11.5 and the Riesz representation theorem we have for all $f : \mathcal{H} \to \mathbb{C}$ linear and bounded:

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \left\|f(e^{-\mathrm{i}tH}\psi)\right\|^2 \mathrm{d}t = 0 \tag{11.5}$$

It follows that for all linear, bounded and finite rank $g : \mathcal{H} \to \mathcal{H}$:

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \left\|g(e^{-\mathrm{i}tH}\psi)\right\|^2 \mathrm{d}t = 0 \tag{11.6}$$

because $g(h) = g_1(h)h_1 + \cdots + g_n(h)h_n$ where each $g_i : \mathcal{H} \to \mathbb{C}$ is linear and bounded. Then we use equation (11.5).

Since compact operators $K : \mathcal{H} \to \mathcal{H}$ can be approximated with finite rank operators (without proof) it follows from equation (11.6) that for all compact oeprators K:

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \left\|K(e^{-\mathrm{i}tH}\psi)\right\|^2 \mathrm{d}t = 0 \tag{11.7}$$

Let $\psi \in D(H) \cap \mathcal{H}_c$. Then there exists $\varphi \in \mathcal{H} : \psi = (H + \mathrm{i})^{-1}\varphi$ because $\mathrm{i} \in \rho(H)$ (H is self-adjoint).

Then $\varphi \in \mathcal{H}_c$ because if $Hu = Eu$ we have:

$$0 = \langle \psi, u \rangle = \left\langle (H+\mathrm{i})^{-1}\varphi, u \right\rangle = \left\langle \varphi, (H-\mathrm{i})^{-1}u \right\rangle = (\lambda - i)^{-1} \langle \varphi, u \rangle$$
$$\Rightarrow \langle \varphi, u \rangle = 0$$

Thus for all $R > 0$:

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \left\|\chi_R e^{-\mathrm{i}tH}\psi\right\|^2 \mathrm{d}t = \lim_{T\to\infty} \frac{1}{T}\int_0^T \left\|\chi_R e^{-\mathrm{i}tH}(H+\mathrm{i})^{-1}\varphi\right\|^2 \mathrm{d}t$$
$$= \lim_{T\to\infty} \frac{1}{T}\int_0^T \left\|\chi_R (H+\mathrm{i})^{-1} e^{-\mathrm{i}tH}\varphi\right\|^2 \mathrm{d}t \overset{\text{eqn. (11.7)}}{\to} 0$$

As $D(H) \cap \mathcal{H}_c$ is dense in $\mathcal{H}_c$ we thus finished our proof. ■

12 Exercises

Here the statements from the exercise session used in the lecture will be restated.

Exercise 2

Let $A : \mathcal{D}(A) \subset X \to X$ be a linear operator such that $\langle \psi, A\psi \rangle = \langle A\psi, \psi \rangle$ for all $\psi \in \mathcal{D}(X)$. Then

$$\langle \varphi, A\psi \rangle = \langle A\varphi, \psi \rangle$$

for all $\varphi, \psi \in \mathcal{D}(X)$.

Hint: Use the polarization identity.

Exercise 4

Let X be a Banach space. Let $A : \mathcal{D}(A) \subseteq X \to X$ be a closed linear operator and $z, w \in \rho(A)$. Then

1. $R_A(z) - R_A(w) = (w - z)R_A(z)R_A(w)$.
2. $R_A(z)R_A(w) = R_A(w)R_A(z)$.
3. $R_A(z)A \subseteq AR_A(z) = zR_A(z) - I$.

Exercise 5

1. Let $(X, \| \cdot \|)$ be a Banach space, let $A : \mathcal{D}(A) \subseteq X \to X$ be a closed operator and $g : [0, T] \to (\mathcal{D}(A), \| \cdot \|_A)$ be continuous where $\| \cdot \|_A$ is a graph norm. Then

$$A \int_0^T g(t) \mathrm{d}t = \int_0^T Ag(t) \mathrm{d}t \,.$$

Hint: Integrals can be understood as Riemannian integrals.

2. Let $g : [0, T] \to H^2(\mathbb{R}^3)$ be continuous. Then

$$-\Delta_x \int_0^T g(t) \mathrm{d}t = \int_0^T -\Delta_x g(t) \mathrm{d}t \,.$$

Exercise 7

Show the following: Let X be a Banach space, $K : X \to X$ be linear operator s.t. $\|K\| < 1$. Then $I + K$ is invertible and $(I+K)^{-1} = \sum_{n=0}^{\infty} (-1)^n K^n$.

Exercise 8

Define $X := (\{\varphi \in L^2(\mathbb{R}) | \varphi \in C^1(\mathbb{R}), \nabla\varphi \in L^2(\mathbb{R})\}, \|\cdot\|_2 + \|\nabla \cdot\|_2)$. Show that

$$f_n = \exp\left[-\left(\frac{1}{n} + |x|^2\right)^{\frac{1}{2}}\right].$$

is a Cauchy sequence in X but f_n does not converge in X. Furthermore show that $f_n \to f$ in $H^1(\mathbb{R})$.

Exercise 9

Let $V \in C(\mathbb{R}^n, \mathbb{C})$. Then we define $M_V : \mathcal{D}(M_V) \subseteq L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ as

$$M_V f(x) = V(x) f(x)$$

where $D(M_V) := \{f \in L^2(\mathbb{R}^n) \mid V \times f \in L^2(\mathbb{R}^n)\}$. Show that

$$\overline{\mathrm{Ran}(V)} \subseteq \sigma(M_V).$$

Exercise 10

Let A, B be densely defined linear operators on a Hilbert space $\mathcal{H}$. Show the following

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

Exercise 11

Let $\mathcal{H} = L^2(\mathbb{R})$ and $g \in \mathcal{H}$ with $\|g\| = 1$. Let $A : C_c(\mathbb{R}) \subset \mathcal{H} \to \mathcal{H}, Af = f(0)g$. Show that

$$\langle \varphi, g \rangle \neq 0, \varphi \in \mathcal{H} \Rightarrow \varphi \notin \mathcal{D}(A^*).$$

Exercise 12

Let V and T be densely defined linear operators on a Hilbert space $\mathcal{H}$ with $\mathcal{D}(T) \subset \mathcal{D}(V)$. Consider two assumptions:

1. For some $a, b \in \mathbb{R}$ and all $\psi \in \mathcal{D}(T)$
$$\|V\psi\| \leq a\|T\psi\| + b\|\psi\|. \tag{12.1}$$

2. For some $\tilde{a}, \tilde{b} \in \mathbb{R}$ and all $\psi \in \mathcal{D}(T)$

$$\|V\psi\|^2 \leq \tilde{a}^2\|T\psi\|^2 + \tilde{b}^2\|\psi\|^2 \,. \tag{12.2}$$

Show the following statements:

1. If (12.2) holds, then (12.1) holds with $a = \tilde{a}$ and $b = \tilde{b}$.
2. If (12.1) holds, then (12.2) holds for $\tilde{a}^2 = (1+\varepsilon)a^2$ and $\tilde{b}^2 = (1+\varepsilon^{-1})b^2$ for each $\varepsilon > 0$. Thus the infimum of all a in (12.1) is the same as the infimum of all $\tilde{a}$ in (12.1).

Exercise 13

Consider a Hamiltonian describing n electron atom in Born-Oppenheimer approximation. Let $\mathcal{H} = H^2(\mathbb{R}^{3n})$,

$$T = \sum_{j=1}^{n} -\Delta_j \ , \ \mathcal{D}(T) = \mathcal{H}$$

where $-\Delta_j$ is a kinetic energy operator of j-th electron and V is a multiplication operator defined using the function

$$v(x) = -\sum_{j=1}^{n} \frac{Z}{|x_j|} + \sum_{k>j=1}^{n} \frac{1}{|x_j - x_k|}$$

where $|x_j|$ is a coordinate of the j-th electron.
Show the following:

1. V is bounded w.r.t. T with $a < 1$, i.e. there exists $0 \leq a < 1$ and $b \in \mathbb{R}_0^+$ s.t. (12.1) holds
2. $T + V$ is lower semibounded, i.e. there exists $a \in \mathbb{R}$ s.t. $\forall \varphi \in \mathcal{H}$: $\langle \varphi, (T+V)\varphi \rangle \geq a\|\varphi\|^2$,
3. $T + V$ is self-adjoint.

Exercise 14

Let $H_0^1(\mathbb{R}^+) = \overline{C_c^\infty(\mathbb{R}^+)}$. Then we define "momentum operator" $P : H_0^1(\mathbb{R}^+) \to L^2(\mathbb{R}^+)$ as

$$Pf(x) = -i\frac{\mathrm{d}}{\mathrm{d}x}f(x)\,.$$

Show the following:

1. P is symmetric and P^* is not symmetric,
2. P is closed and

3. P is not essentially self-adjoint.

Exercise 17

Let $\psi \in H^1(\mathbb{R}^3)$. Prove that

$$\int_{\mathbb{R}^3} \frac{|\psi(x)|^2}{|x|} \mathrm{d}x \leq \|\nabla\psi\|_2 \|\psi\|_2 \,.$$

Equality holds only if

$$\psi(x) \sim e^{-c|x|}$$

for some constant $c > 0$.
Hint: Use that $\frac{1}{|x|} = \frac{1}{2}\nabla\left(\frac{x}{|x|}\right)$.

Exercise 23

Let $\mathcal{H} \neq \{0\}$ be a Hilbert space and $A \in \mathcal{L}(H)$. Show that the spectrum of A is not empty.

Exercise 24

Let $\mathcal{H}$ be a Hilbert space and $A \in \mathcal{L}(H)$. Assume that for all $|s| < r$ the function $f(s) := (1 - sA)^{-1}$ exists and is bounded. Prove that $f(s)$ has a series expansion in s and that for all $\varepsilon > 0$ the series converges uniformly in $|s| < r - \varepsilon$.

Exercise 30

Let $\psi \in H^1(\mathbb{R}^3)$. Show that

$$\lim_{h\to\infty} \left\| \frac{\psi(x-h)}{x} \right\| = 0 \,.$$

Exercise 31

Let $f \in \{\psi \in C(\mathbb{R}^d) | \lim_{|x|\to\infty} \psi = 0\}$ and $M_f : H^1(\mathbb{R}^d) \to L^2(\mathbb{R}^d), M_f\varphi := f\varphi$. Show that M_f is compact.

Exercise 33

Let $\lambda > 0$ then the operator $U_\lambda : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ is defined as

$$[U_\lambda\phi](x) := \lambda^{n/2}\phi(\lambda x) \,.$$

Show that:

1. U_λ is unitary, $U_\lambda^{-1} = U_{\lambda^{-1}}$ and U_λ leaves $H^s(\mathbb{R}^n)$ invariant,

2. On $\mathcal{S}(\mathbb{R}^n)$ the following holds

$$U_\lambda \Delta U_\lambda^{-1} = \frac{1}{\lambda^2}\Delta\,, \quad U_\lambda V(x) U_\lambda^{-1} = V(\lambda x)\,,$$

with V being multiplication operator satisfying $V\mathcal{S}(\mathbb{R}^n) \subset L^2(\mathbb{R}^n)$.

Exercise 36

Prove that the following equality holds

$$\int_{|x|=r} \frac{d\sigma(x)}{|x-R|} = \frac{4\pi r^2}{\max\{r, |R|\}}$$

where $d\sigma(x)$ is a surface measure on a sphere and $R \in \mathbb{R}^3$.
This is known as *Newton's Shell Theorem.*

Exercise 40

Let A be a self-adjoint operator on $\mathcal{H}$. Let $P_\Omega := \chi_\Omega(A)$ where χ_Ω is a characteristic function of the measurable set $\Omega \subset \mathbb{R}$. Show that the family of operators $\{P_\Omega\}$ has the following properties:

1. Each P_Ω is an orthogonal projection.
2. $P_\emptyset = 0$, $P_\mathbb{R} = I$.
3. Let $N \in \mathbb{N} \cup \{0\}$. If $\Omega = \bigcup_{n=1}^{N} \Omega_n$ with $\Omega_n \cap \Omega_m = \emptyset$ if $n \neq m$, then $P_\Omega \psi = \sum_{n=1}^{N} P_{\Omega_n}\psi$, $\forall \psi \in \mathcal{H}$.
4. $P_{\Omega_1} P_{\Omega_2} = P_{\Omega_1 \cap \Omega_2}$.

Exercise 42

Let A be a self-adjoint operator and let $P_\Omega := \chi_\Omega(A)$. Prove the following

1. $\lambda \in \sigma(A)$ if and only if for all $\varepsilon > 0 : P_{(\lambda-\varepsilon,\lambda+\varepsilon)} \neq 0$.
2. $\lambda \in \sigma_d(A)$ if and only if $\lambda \in \sigma(A)$ and there exists $\varepsilon > 0$ s.t. $P_{(\lambda-\varepsilon,\lambda+\varepsilon)}\mathcal{H} < \infty$.
3. $\lambda \in \sigma_{\text{ess}}(A)$ if and only if $\dim(P_{(\lambda-\varepsilon,\lambda+\varepsilon)}\mathcal{H}) = \infty$ for all $\varepsilon > 0$.

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