Mathematical Quantum Mechanics

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Official Lecture Notes

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Contents

Outline

1) Review of Basic Concepts of Analysis

2) Principles of Quantum Mechanics

3) Spectral Theorem

4) Quantum Dynamics

5) Scattering Theory

6) Many-Body Quantum Mechanics

7) Density Functional Theory

8) Entropy

9) Stability and Instability of Matter

Chapter 1

Review of Analysis

1.1 Measure Theory

In measure theory the basic object is a measure space (Ω, Σ, μ) consisting of a (measure) space Ω, a Sigma-algebra Σ, and a measure μ.

Definition 1.1 (Sigma-Algebra). A Sigma-algebra Σ is a collection of subsets of Ω such that

1) $\emptyset, \Omega \in \Sigma$,
2) if $A \in \Sigma$ then $A^C := \Omega \setminus A \in \Sigma$,
3) if $(A_n)_{n=1}^{\infty} \subset \Sigma$ then $\bigcup_{n=1}^{\infty} A_n \in \Sigma$.

If $A \in \Sigma$, A is called ***measurable***. $\square$

Definition 1.2 (Measure). A measure μ is a function $\Sigma \to [0, \infty]$ such that

1) $\mu(A) \geqslant 0$ for all $A \in \Sigma$,
2) if $(A_n)_{n=1}^{\infty} \subset \Sigma$, such that $A_n \cap A_m = \emptyset$ if $n \neq m$, then

$$\mu\left(\bigcup_{n=1}^{\infty} A_n\right) = \sum_{n=1}^{\infty} \mu(A_n).$$

$\square$

Example 1.3. The most common example of a measure space is $\Omega = \mathbb{R}^d$, Σ being the Lebesgue measurable sets, and μ being the Lebesgue measure.
The properties characterising this measure space are:

1) Σ contains all open and closed sets,

2) For all $A \in \Sigma$ and $\varepsilon > 0$, there exists an open set B such that $A \subset B$ and $\mu(B \setminus A) < \varepsilon$ (***Outer Regularity***).

   For all $A \in \Sigma$, there exists a sequence of closed/compact sets $(B_n)_n$ such that $B_n \subset A$, and
$$\mu\left(A \setminus \bigcup_{n=1}^{\infty} B_n\right) = 0,$$
   i.e. $A = \bigcup_{n=1}^{\infty} B_n$ almost everywhere (a.e.) (***Inner Regularity***).

3) ***Completeness***: If $A \in \Sigma$ and $\mu(A) = 0$, then for all $B \subset A$, $B \in \Sigma$ and $\mu(B) = 0$.

4) For all $x \in \mathbb{R}^d$, and all $A \in \Sigma$, $A + x \in \Sigma$ and $\mu(A + x) = \mu(A)$ (***Translation Invariance***).

   For all $\lambda \in \mathbb{R}$, and all $A \in \Sigma$, $\lambda A \in \Sigma$ and $\mu(\lambda A) = |\lambda|^d \mu(A)$ (***Dilation***).

5) ***Normalisation***: The unit cube has measure 1, i.e. $\mu\big([0,1]^d\big) = 1$.

Definition 1.4 (Measurable Functions)**.** Given a measure space (Ω, Σ, μ), a function $f : \Omega \to [0, \infty]$ is called ***measurable*** iff

- $$f^{-1}((t, \infty]) = \left\{x \in \Omega \,\middle|\, f(x) > t\right\} \in \Sigma$$
  for all $t \geqslant 0$. These sets are called ***level sets***.

Or equivalently

- $f(x) = \lim_{n\to\infty} f_n(x)$, where f_n is a step function, i.e.

$$f_n(x) = \sum_{i=1}^{I} \lambda_i \chi_{A_i}$$

where $\lambda_i \in \mathbb{R}$, $A_i \in \Sigma$ and

$$\chi_{A_i}(x) = \begin{cases} 1, & \text{if } x \in A_i \\ 0, & \text{otherwise} \end{cases},$$

or

- (if $\Omega = \mathbb{R}^d$) $f(x) = \lim_{n\to\infty} f_n(x)$, where f_n is a really simple function, i.e. $f_n(x) = \sum_{i=1}^{I} \lambda_i \chi_{A_i}$ where $\lambda_i \geqslant 0$ and A_i are cubes.

In general a function $f : \Omega \to \mathbb{C}$ can be split into $f = f_1 - f_2 + if_3 - if_4$ with $f_i : \Omega \to [0, \infty]$. Then f is measurable iff all f_i are. □

Remark 1.5 (Reminder of Riemann Integral)**.** The Riemann integral can only be defined for functions that are continuous up to a countable set. □

Definition 1.6 (Integration)**.** For any measurable function $f : \Omega \to [0, \infty]$ we define its Lebesgue integral to be

$$\int_{\Omega} f(x) \mathrm{d}\mu(x) := \int_{0}^{\infty} \mu\big(\{x \in \Sigma \,\big|\, f(x) > t\}\big) \mathrm{d}t$$

where the right-hand-side is interpreted as a Riemann integral. This is well-defined as $t \mapsto \mu\big(\{x \in \Sigma \,\big|\, f(x) > t\}\big)$ is monotone decreasing, and thus it is continuous up to a countable set (Exercise 1.1).
For a measurable function $f : \Omega \to \mathbb{C}$ we define

$$\int_{\Omega} f(x) \mathrm{d}\mu(x) := \int f_1 - \int f_2 + i \int f_3 - i \int f_4$$

which makes sense iff $\int f_i < \infty$ for all $i \in \{1, \dots, 4\}$. In this case we call f ***integrable***.

Equivalently, f is integrable iff $|f|$ is measurable and $\int |f| < \infty$. □

1.2 Fundamental Theorems on Integration

Theorem 1.7 (Monotone Convergence). *If $(f_n)_{n=1}^{\infty}$ is a sequence of measurable, real, and integrable functions, $f_n(x) \uparrow f(x)$ (i.e. $f(x) \geqslant f_{n+1}(x) \geqslant f_n(x)$ for all $n \in \mathbb{N}$) for a.e. x (i.e. up to a set of measure 0), then*

$$\int_{\Omega} f(x) \mathrm{d}\mu(x) = \lim_{n\to\infty} \int_{\Omega} f_n(x) \mathrm{d}\mu(x).$$

(which holds even when both sides are $+\infty$). □

Theorem 1.8 (Dominated Convergence). *If $(f_n)_{n=1}^{\infty}$ is a sequence of measurable and integrable functions ($f_n : \Omega \to \mathbb{C}$), $f_n(x) \xrightarrow{n\to\infty} f(x)$ for a.e. x, and there exists an integrable function G, such that $|f_n(x)| \leqslant G(x)$ for a.e. x. Then*

$$\int_{\Omega} f(x) \mathrm{d}\mu(x) = \lim_{n\to\infty} \int_{\Omega} f_n(x) \mathrm{d}\mu(x)$$

(and both sides are finite). □

Remark 1.9. Under the same conditions as in the Theorem 1.8 we also have

$$\int_{\Omega} \big|f_n(x) - f(x)\big| \mathrm{d}\mu(x) \xrightarrow{n\to\infty} 0.$$

This is stronger than the previous convergence theorem as

$$\left| \int_{\Omega} f(x) \mathrm{d}\mu(x) - \int_{\Omega} f_n(x) \mathrm{d}\mu(x) \right| = \left| \int_{\Omega} \big(f(x) - f_n(x)\big) \mathrm{d}\mu(x) \right| \leqslant \int_{\Omega} \big|f(x) - f_n(x)\big| \mathrm{d}\mu(x).$$

□

Remark 1.10 ("Inverse" of Dominated Convergence)**.** If $(f_n)_{n=1}^{\infty}$ is a sequence of integrable functions, f integrable, and

$$\int_\Omega |f_n - f| \mathrm{d}\mu \xrightarrow{n\to\infty} 0$$

then there exists a subsequence $(f_{n_k})_k$ of $(f_n)_n$ such that

$$\begin{cases} f_{n_k}(x) \xrightarrow{k\to\infty} f(x), & \text{for a.e. } x \\ |f_{n_k}(x)| \leqslant G(x), & \text{for a.e. } x \end{cases}$$

for an integrable function G. □

Theorem 1.11 (Fatou's Lemma)**.** *If $(f_n)_n$ is a sequence of integrable functions, $f_n \geqslant 0$, $f_n(x) \xrightarrow{n\to\infty} f(x)$ for a.e. x. Then*

$$\liminf_{n\to\infty} \int_\Omega f_n(x)\mathrm{d}\mu(x) \geqslant \int_\Omega f(x)\mathrm{d}\mu(x)$$

□

Remark 1.12 (Notation)**.**

$$\lim_{n\to\infty} a_n = a_0 :\iff \forall\varepsilon > 0\, \exists N_\varepsilon \in \mathbb{N}\, \forall n \geqslant N_\varepsilon : |a_n - a_0| < \varepsilon$$

$$\liminf_{n\to\infty} a_n := \lim_{n\to\infty} \inf_{m\geqslant n} a_m$$

$$\limsup_{n\to\infty} a_n := \lim_{n\to\infty} \sup_{m\geqslant n} a_m$$

$$\liminf_{n\to\infty} a_n \geqslant a_0 \iff \forall\varepsilon > 0\, \exists N_\varepsilon \in \mathbb{N}\, \forall n \geqslant N_\varepsilon : a_n - a_0 \geqslant -\varepsilon$$

$$\limsup_{n\to\infty} a_n \leqslant a_0 \iff \forall\varepsilon > 0\, \exists N_\varepsilon \in \mathbb{N}\, \forall n \geqslant N_\varepsilon : a_n - a_0 \leqslant \varepsilon$$

□

Theorem 1.13 (Brezis-Lieb Refinement of Fatou's Lemma)**.** *Assume that $(f_n)_n$ is a sequence of integrable functions, $f_n \to f$ for a.e. x, f integrable. Then*

$$\int \big||f_n| - |f| - |f_n - f|\big| \mathrm{d}\mu \xrightarrow{n\to\infty} 0$$

Consequently,

$$\int |f_n| - \int |f| - \int |f_n - f| \xrightarrow{n\to\infty} 0.$$

and if $f_n \to f$ a.e. and $\int |f_n| \to \int |f|$ then $\int |f_n - f| \to 0$. □

Proof. $|f_n| - |f_n - f| \xrightarrow{n\to\infty} |f|$ a.e. and

$$\big||f_n| - |f_n - f|\big| \leqslant |f|$$

with $|f|$ being integrable. The assertion then follows from the dominated convergence Theorem 1.8. *q.e.d.*

Theorem 1.14 (Approximation by Continuous Functions)**.** *If $f : \mathbb{R}^d \to \mathbb{C}$ is an integrable function, then there exists a sequence of continuous functions with compact support (i.e. $f_n\big|_{K^C} \equiv 0$ for some compact set K) $(f_n)_n \subset \mathscr{C}_c\big(\mathbb{R}^d\big)$ such that*

$$\int_{\mathbb{R}^d} |f_n - f| \mathrm{d}x \xrightarrow{n\to\infty} 0.$$

□

1.3 L^p Spaces

Definition 1.15 (L^p Space)**.** Let (Ω, Σ, μ) be a measure space. For all $1 \leqslant p \leqslant \infty$ we define

$$L^p(\Omega) := \big\{ f : \Omega \to \mathbb{C} \,\big|\, f \text{ is measurable}, \|f\|_{L^p} < \infty \big\}$$

where

$$\|f\|_{L^p} := \begin{cases} \left(\int\limits_\Omega |f|^p \mathrm{d}\mu\right)^{1/p}, & \text{if } p < \infty \\ \operatorname{ess\,sup}_{x\in\Omega} |f(x)|, & \text{if } p = \infty. \end{cases}$$

Here

$$\operatorname*{ess\,sup}_{x\in\Omega} |f(x)| := \inf\{\lambda \in \mathbb{R} \,\big|\, |f(x)| \leqslant \lambda \text{ for a.e. } x\}.$$

Convergence with respect to the topology generated by $\|\cdot\|_{L^p}$ is called norm convergence or strong convergence.

□

Remark 1.16 (Fundamental Results for L^p)**.** All fundamental results for L^1 extend to L^p for all $1 \leqslant p < \infty$.

1) (Monotone Convergence for L^p) If $(f_n)_n \subset L^p(\Omega)$ is a sequence of a.e. increasing functions, converging a.e. to f then

$$\int |f_n|^p \xrightarrow{n\to\infty} \int |f|^p.$$

2) (Dominated Convergence) If $(f_n)_n \subset L^p(\Omega)$ is a sequence functions converging a.e. to f and for all $n \in \mathbb{N}$ $|f_n| \leqslant G \in L^p(\Omega)$, then

$$\int |f_n|^p \xrightarrow{n\to\infty} \int |f|^p \quad \text{and} \quad \int |f_n - f|^p \xrightarrow{n\to\infty} 0.$$

Sketch of Proof. $|f_n - f|^p \xrightarrow{n\to\infty} 0$ a.e. and

$$|f_n - f|^p \leqslant (|f_n| + |f|)^p \leqslant 2^p G^p \in L^1.$$

Then the assertion follows from the standard dominated convergence Theorem 1.8.

□

3) (Fatou) If $(f_n)_n \subset L^p(\Omega)$ is a sequence of non-negative functions, converging a.e. to f, then

$$\int |f|^p \leqslant \liminf_{n\to\infty} \int |f_n|^p$$

4) If $(f_n)_n \subset L^p(\Omega)$ is a sequence functions converging a.e. to f and for all $n \in \mathbb{N}$ $\int |f_n|^p \leqslant C$, then

$$\int \big||f_n|^p - |f|^p - |f_n - f|^p\big| \xrightarrow{n\to\infty} 0.$$

$\square$

Definition 1.17 (Dual Space)**.** For any Banach Space X its dual space is

$$X^* := \big\{\mathcal{L} : X \longrightarrow \mathbb{C} \,\big|\, \mathcal{L} \text{ is linear and continuous}\big\}.$$

This is a Banach space with norm

$$\|\mathcal{L}\|_{X^*} := \sup_{\|f\|_X \leqslant 1} |\mathcal{L}(f)|$$

$\square$

Remark 1.18 (Properties of $L^p(\Omega)$)**.** 1) $L^p(\Omega)$ is a Banach space with norm $\|\cdot\|_{L^p}$ for all $1 \leqslant p \leqslant \infty$, i.e.

- $\|f\|_{L^p} \geqslant 0$ for all $f \in L^p(\Omega)$ and $\|f\|_{L^p} = 0 \iff f = 0$ (a.e. x),
- $\|\lambda f\|_{L^p} = |\lambda| \|f\|_{L^p}$ for all $\lambda \in \mathbb{C}$,
- $\|f + g\|_{L^p} \leqslant \|f\|_{L^p} + \|g\|_{L^p}$ (***triangle inequality***),

and it is ***complete***, i.e. if $(f_n)_n \subset L^p(\Omega)$ is a Cauchy sequence, i.e. $\lim_{n,m\to\infty} \|f_n - f_m\|_{L^p} = 0$, then there exists a $f \in L^p(\Omega)$ such that

$$\|f - f_n\|_{L^p} \xrightarrow{n\to\infty} 0.$$

2) (Hölder's Inequality) If $p, q \in [1, \infty]$ and $\frac{1}{p} + \frac{1}{q} = 1$ (such p, q are called ***dual powers***) then

$$\|fg\|_{L^1} \leqslant \|f\|_{L^p} \|g\|_{L^q}$$

for all $f \in L^p$ and $g \in L^q$. More generally if $\frac{1}{p_1} + \frac{1}{p_2} + \cdots \frac{1}{p_n} = 1$, then

$$\|f_1 f_2 \cdots f_n\|_{L^1} \leqslant \|f_1\|_{L^{p_1}} \|f_2\|_{L^{p_2}} \cdots \|f_n\|_{L^{p_n}}.$$

3) (Dual of L^p)

$$(L^p(\Omega))^* = L^q(\Omega)$$

where $\frac{1}{p} + \frac{1}{q} = 1$ for all $1 \leqslant p < \infty$. Note that $(L^\infty(\Omega))^* \supsetneq L^1(\Omega)$.

This means that for all $\mathcal{L} \in (L^p(\Omega))^*$ there exists a unique $g \in L^q(\Omega)$ such that for all $f \in L^p(\Omega)$

$$\mathcal{L}(f) = \int fg.$$

Moreover,

$$\|\mathcal{L}\|_{(L^p)^*} = \sup_{\|f\|_{L^p} \leqslant 1} \left| \int fg \right| = \|g\|_{L^q}.$$

□

Sketch of Proof of (2) & (3). By Young's inequality for all $a, b \geqslant 0$, $\frac{1}{p} + \frac{1}{q} = 1$ with $1 < p < \infty$

$$ab \leqslant \frac{a^p}{p} + \frac{b^q}{q}.$$

A stronger version of this inequality asserts that

$$ab = \inf_{\varepsilon > 0} \left\{ \frac{(\varepsilon a)^p}{p} + \frac{(\varepsilon^{-1} b)^q}{q} \right\}.$$

In particular, we have

$$|fg| \leqslant \frac{|\varepsilon f|^p}{p} + \frac{|\varepsilon^{-1} g|^q}{q}$$

pointwise. Thus,

$$\int |fg| \leqslant \frac{(\varepsilon \|f\|_{L^p})^p}{p} + \frac{(\varepsilon^{-1} \|g\|_{L^q})^q}{q}$$

for all $\varepsilon > 0$. The infimum of the right-hand-side is equal to $\|f\|_{L^p} \|g\|_{L^q}$. This yields Hölder's inequality.

Consequently,

$$\sup_{\|f\|_{L^p} \leqslant 1} \left| \int fg \right| \leqslant \|g\|_{L^q}$$

On the other hand, for all $g \in L^q$, $g \neq 0$ we can define

$$f := \frac{\overline{g} |g|^{q-2}}{\left(\int |g|^q \right)^{1/p}}$$

then $\|f\|_{L^p} = 1$ and

$$\int fg = \left(\int |g|^q\right)^{1/q} = \|g\|_{L^q}.$$

q.e.d.

Definition 1.19 (Weak Convergence)**.** Let $1 < p < \infty$. Then a sequence $(f_n)_n \subset L^p(\Omega)$ is said to converge weakly in L^p

$$f_n \xrightharpoonup{n\to\infty} f$$

iff for all $g \in L^q(\Omega)$, with $\frac{1}{p} + \frac{1}{q} = 1$,

$$\int f_n g \xrightarrow{n\to\infty} \int fg.$$

□

Theorem 1.20 (Banach-Alaoglu)**.** *Let $1 < p < \infty$. If $(f_n)_n$ is a bounded sequence in L^p (i.e. $\|f_n\|_{L^p} \leqslant C$ for all $n \in \mathbb{N}$), then there exists a subsequence $(f_{n_k})_k$ such that $f_{n_k} \xrightharpoonup{k\to\infty} f$ in L^p.* □

Theorem 1.21 (Banach-Steinhaus, Uniform Boundedness Principle)**.** *If $f_n \xrightharpoonup{n\to\infty} f$ in L^p, then $(f_n)_n$ is bounded in L^p.* □

Remark 1.22. Strong convergence (i.e. convergence in norm) implies weak convergence. □

Example 1.23. Let $f, \varphi \in \mathscr{C}_c(\mathbb{R}^d)$. Define

$$f_n(x) := f(x) + \varphi(x + x_n)$$

where $|x_n| \to \infty$. Then for $|x_n|$ large enough

$$\int |f_n|^p = \int |f|^p + \int |\varphi|^p \quad \therefore \quad \|f_n - f\|_{L^p} = \|\varphi\|_{L^p} \neq 0.$$

Thus $f_n \not\to f$ strongly in L^p. But $f_n \rightharpoonup f$ weakly. Indeed, for all $g \in L^q(\Omega)$

$$\int f_n g - \int fg = \int \varphi(x + x_n) g(x) \mathrm{d}\mu(x) \xrightarrow{n\to\infty} 0$$

by the dominated convergence Theorem 1.8 and approximating g by a function $g_\varepsilon \in L^q_c$ with $\|g - g_\varepsilon\|_q < \varepsilon$.

Proof of Theorem 1.20. For all $g \in L^q$, $\left(\int f_n g\right)_n$ is a bounded sequence in $\mathbb{C}$ as

$$\left|\int f_n g\right| \leqslant \|f_n\|_{L^p} \|g\|_{L^q} \leqslant C\|g\|_{L^q}.$$

This means that there exists a subsequence $(f_{n_k})_k$ such that $\int f_{n_k} g$ converges for $k \to \infty$.
Now take a sequence $(g_m)_{m=1}^\infty$ in $L^q(\Omega)$. Then we can choose a subsequence $(f_{n_k})_k$ such that $\int f_{n_k} g_m$ converges as $k \to \infty$ for all $m \in \mathbb{N}$, which can be done by a "Cantor Diagonal Argument".
Taking the subsequence $\left(f_{n_{k_1}}\right)_{k_1}$ constructed for g_1, we may extract a subsequence of this sequence $\left(f_{n_{k_2}}\right)_{k_2}$ converging also for g_2. Doing this for all $m \in \mathbb{N}$ we obtain the double sequence $\left(f_{n_{k_m}}\right)_{(k,m)\in\mathbb{N}^2}$. Then for the sequence $\left(f_{n_{k_k}}\right)_{k\in\mathbb{N}}$, the integrals $\int f_{n_{k_k}} g_m$ converge as $k \to \infty$ for all $m \in \mathbb{N}$, since $\left(f_{n_{k_k}}\right)_{k\geqslant m}$ is a subsequence of the convergent sequence $\left(f_{n_{k_m}}\right)_{k\geqslant m}$, hence it is itself convergent.
Using the fact that $L^q(\Omega)$ is ***separable***, i.e. that there exists a sequence $(g_m)_{m=1}^\infty \subset L^q(\Omega)$ that is dense in $L^q(\Omega)$. (Separability follows from the approximation of L^p functions by step functions or continuous functions with compact support. $L^\infty(\Omega)$ is not separable, hence the assertion fails in that case.)
With this choice of $(g_m)_m$ we can define a linear functional $\mathcal{L} : L^q(\Omega) \to \mathbb{C}$ via

$$\mathcal{L}(g_m) := \lim_{k\to\infty} \int f_{n_{k_k}} g_m.$$

By the above this is well-defined, and as $(g_m)_m$ is dense this functional can be uniquely extended to all of $L^q(\Omega)$ if it is bounded on $(g_m)_m$. This is the case as

$$|\mathcal{L}(g_m)| = \lim_{k\to\infty}\left|\int f_{n_{k_k}} g_m\right| \leqslant \lim_{k\to\infty}\left\|f_{n_{k_k}}\right\|_{L^p} \|g_m\|_{L^q} \leqslant C\|g_m\|_{L^q}.$$

Thus $\mathcal{L} \in (L^q(\Omega))^*$ and there exists a unique $f \in L^p(\Omega)$ such that $\mathcal{L}(g) = \int fg$ for all $g \in L^q$.

By this, we have for all g_m

$$\lim_{k\to\infty} \int f_{n_{k_k}} g_m = \mathcal{L}(g_m) = \int f g_m.$$

For an arbitrary $g \in L^q(\Omega)$ choose a subsequence $(g_{m_l})_l$ converging to g strongly. Then

$$\begin{aligned}
\left|\int f_{n_{k_k}} g - \int f\right| \leqslant{} & \left|\int f_{n_{k_k}} (g - g_{m_l})\right| + \left|\int f_{n_{k_k}} g_{m_l} - \int f g_{m_l}\right| + \left|\int f (g_{m_l} - g)\right| \leqslant \\
& \leqslant \left\| f_{n_{k_k}} \right\|_{L^p} \|g - g_{m_l}\|_{L^q} + \left|\int f_{n_{k_k}} g_{m_l} - \int f g_{m_l}\right| + \left\| f_{n_{k_k}} \right\|_{L^p} \|g - g_{m_l}\|_{L^q} \leqslant \\
& \leqslant C\|g - g_{m_l}\|_{L^q} + \left|\int f_{n_{k_k}} g_{m_l} - \int f g_{m_l}\right| + C\|g - g_{m_l}\|_{L^q} \xrightarrow{k\to\infty} \\
& \longrightarrow 2C\|g - g_{m_l}\|_{L^q}
\end{aligned}$$

The right-hand side can now be made arbitrarily small (by choosing l large enough), hence $\left|\int f_{n_{k_k}} g - \int f g\right| \xrightarrow{k\to\infty} 0$. Thus, indeed

$$f_{n_{k_k}} \xrightarrow{k\to\infty} f.$$

q.e.d.

Definition 1.24. Let $\Omega = \mathbb{R}^d$, f, g measurable and define their convolution for each $x \in \mathbb{R}^d$, if it exists, to be

$$(f * g)(x) = \int_{\mathbb{R}^d} f(x - y) g(y) \mathrm{d}y.$$

□

Remark 1.25. $f * g = g * f$ and $(f * g) * h = f * (g * h)$. □

Theorem 1.26 (Young's Inequality)**.** *Let $1 \leqslant p, q, r \leqslant \infty$. If $f \in L^p, g \in L^q$, then $f * g \in L^r$ with*

$$1 + \frac{1}{r} = \frac{1}{p} + \frac{1}{q}.$$

and $\|f * g\|_{L^r} \leqslant \|f\|_{L^p}\|g\|_{L^q}$. □

Remark 1.27. The Young inequality is equivalent to

$$\left|\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} f(x)g(x-y)h(y)\mathrm{d}x\mathrm{d}y\right| \leqslant \|f\|_{L^p}\|g\|_{L^q}\|h\|_{L^{r'}}$$

where

$$\frac{1}{p}+\frac{1}{q}+\frac{1}{r'}=2$$

and $\frac{1}{r}+\frac{1}{r'}=1$. □

Theorem 1.28 (Approximation by Convolution)**.** *Let* $1 \leqslant p < \infty$ *and* $f \in L^p(\mathbb{R}^d)$. *Let* $g \in L^1(\mathbb{R}^d)$, $\int g = 1$ *and for* $\varepsilon > 0$, $g_\varepsilon = g\left(\frac{x}{\varepsilon}\right)\frac{1}{\varepsilon^d}$, *i.e.* $\int g_\varepsilon = 1$.
Then $g_\varepsilon * f \xrightarrow{\varepsilon\to 0} f$ *strongly in* $L^p(\mathbb{R}^d)$ □

Corollary 1.29. *For all* $L^p(\mathbb{R}^d)$, $1 \leqslant p < \infty$ *there exists a sequence* $(f_n)_n \in \mathscr{C}_c^\infty(\mathbb{R}^d)$, $\|f_n - f\|_{L^p} \to 0$. □

Proof. By approximation, we may assume that $f \in \mathscr{C}_c(\mathbb{R}^d)$ which we shall prove later. For simplicity, we assume that g has compact support. Then

$$\begin{aligned}\big|(g_\varepsilon * f)(x) - f(x)\big| &= \left|\int_{\mathbb{R}^d} g_\varepsilon(y)f(x-y)\mathrm{d}y - \int_{\mathbb{R}^d} g_\varepsilon(y)f(x)\mathrm{d}y\right| = \\ &= \left|\int_{\mathbb{R}^d} g_\varepsilon(y)\big(f(x-y)-f(x)\big)\mathrm{d}y\right| \leqslant \\ &\leqslant \sup_{z\in\operatorname{supp} g_\varepsilon} |f(x-z)-f(x)| \int_{\mathbb{R}^d}|g_\varepsilon(y)|\mathrm{d}y \leqslant \\ &\leqslant \sup_{|z|\leqslant R\varepsilon} |f(x-z)-f(x)|\|g\|_{L^1} \xrightarrow{\varepsilon\to 0} 0\end{aligned}$$

where $\operatorname{supp} g \subset B_R(0)$. Because f has compact support it is uniformly continuous, hence the last limit can be taken uniformly for all $x \in \mathbb{R}^d$.

Thus, $\|g_\varepsilon * f - f\|_\infty \xrightarrow{\varepsilon\to 0} 0$. Since f, g have compact support it follows that $g_\varepsilon * f$ has one as

$$\operatorname{supp}(g_\varepsilon * f) \subset \operatorname{supp} g_\varepsilon + \operatorname{supp} f \subset B_{\varepsilon R}(0) + \operatorname{supp} f \subset B_R(0) + \operatorname{supp}(f).$$

for $\varepsilon \leqslant 1$. Thus, $\|g_\varepsilon * f - f\|_{L^r} \to 0$ for all $1 \leqslant r \leqslant \infty$ as

$$\|f\|_{L^r} \leqslant (\mu(\operatorname{supp} f))^{\frac{1}{r}-\frac{1}{p}} \|f\|_{L^p} \quad \therefore \quad \|f\|_{L^r} \leqslant (\mu(\operatorname{supp} f))^{\frac{1}{r}} \|f\|_{L^\infty}$$

which follows from Hölder's inequality.
To remove the assumption that f and g have compact support we use sequences $(f_n)_n, (g_n)_n \subset \mathscr{C}_c$ such that

$$\|f_n - f\|_{L^p} \xrightarrow{n\to\infty} 0, \qquad \|g_n - g\|_{L^1} \xrightarrow{n\to\infty} 0$$

and utilise Young's inequality $\|f * g\|_{L^p} \leqslant \|f\|_{L^p}\|g\|_{L^1}$ to estimate

$$f * g_\varepsilon - f = (f_n * g_\varepsilon - f_n) + (f - f_n) * g_\varepsilon + (f_n - f),$$

where the third vanishes by assumption and the second term vanishes by both Young's inequality and our assumption as $n \to \infty$, and the first term goes to 0 by the above as $\varepsilon \to 0$.
Concerning g we have the similar estimate

$$f * g_\varepsilon - f = (f * g_{\varepsilon,n} - f) + f * (g_\varepsilon - g_{\varepsilon,n})$$

the second term vanishes by Young's inequality and our assumption as $n \to \infty$ and the first term vanishes as $\varepsilon \to 0$ per our assumption.
For the corollary, we can choose $g \in \mathscr{C}_c^\infty$, $\int g = 1$ and if $f \in \mathscr{C}_c(\mathbb{R}^d)$, then $g_\varepsilon * f \in \mathscr{C}_c^\infty(\mathbb{R}^d)$. *q.e.d.*

Theorem 1.30 (Hardy - Littlewood - Sobolev Inequality)**.**

$$\left| \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{f(x)g(y)}{|x-y|^\lambda} \mathrm{d}x\mathrm{d}y \right| \leqslant C\|f\|_{L^p}\|g\|_{L^q}$$

for $\frac{1}{p} + \frac{1}{q} + \frac{\lambda}{d} = 2$, *for all* $0 < \lambda < d$, *and* $C = C(p, q, \lambda, d)$ *independent of* f, g. $\square$

Remark 1.31. The HLS inequality does not come from Young's inequalty as for $h(z) = \frac{1}{|z|^\lambda}$

$$\int |h(z)|^r = \int |h(z)|^{\frac{d}{\lambda}} = \int_{\mathbb{R}^d} \frac{1}{|z|^d} \mathrm{d}z = +\infty$$

This inequality is also called the "weak Young inequality" as it involves a weak norm of h. □

Proof. We shall use the "Layer-cake" representation

$$\int_{\mathbb{R}^d} |f(x)|^p = p \int_0^\infty h_1(a) a^{p-1} \mathrm{d}a$$

where

$$h_1(a) = \big|\{|f(x)| > a\}\big| = \int_{\mathbb{R}^d} \mathbf{1}_{\{|f(x)|>a\}} \mathrm{d}x$$

and

$$\int_{\mathbb{R}^d} |g(x)|^p = q \int_0^\infty h_2(b) b^{q-1} \mathrm{d}b, \qquad h_2(b) = \int_{\mathbb{R}^d} \mathbf{1}_{\{|g(y)|>b\}} \mathrm{d}y.$$

Without loss of generality we may assume that $\|f\|_{L^p} = \|g\|_{L^q} = 1$ (otherwise rescale the functions). For the left-hand-side, we use

$$|f(x)| = \int_0^\infty \mathbf{1}_{\{|f(x)|>a\}} \mathrm{d}a$$

$$|g(y)| = \int_0^\infty \mathbf{1}_{\{|g(y)|>b\}} \mathrm{d}b$$

$$\frac{1}{|x-y|^\lambda} = \int_0^\infty \mathbf{1}_{\{\frac{1}{|x-y|^\lambda}>c\}} \mathrm{d}c = \lambda \int_0^\infty \mathbf{1}_{\{|x-y|<c\}} \frac{\mathrm{d}c}{c^{\lambda+1}}$$

where the substitution $c \to c^{-\lambda}$ was used for the last equality. Using this, the left-hand-side takes the form

$$\left| \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{f(x)g(y)}{|x-y|^\lambda} \mathrm{d}x \mathrm{d}y \right| = \lambda \int_0^\infty \int_0^\infty \int_0^\infty \left(\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{\mathbf{1}_{\{|f(x)|>a\}} \mathbf{1}_{\{|g(y)|>b\}} \mathbf{1}_{\{|x-y|<c\}}}{c^{\lambda+1}} \mathrm{d}x \mathrm{d}y \right) \mathrm{d}a \mathrm{d}b \mathrm{d}c.$$

We shall denote the function within the parentheses as $I(a,b,c)$. Note that we may arbitrarily exchange by Tonelli's theorem all the integrals in this expression as the integrand is positive.

Now we use a trick: By ignoring one of the three characteristic function we can estimate

$$I(a,b,c) \leqslant \int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} \frac{\mathbf{1}_{\{|f(x)|>a\}}\mathbf{1}_{\{|g(y)|>b\}}}{c^{\lambda+1}}\mathrm{d}x\mathrm{d}y = \frac{h_1(a)h_2(b)}{c^{\lambda+1}}$$

$$I(a,b,c) \leqslant \int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} \frac{\mathbf{1}_{\{|f(x)|>a\}}\mathbf{1}_{\{|x-y|<c\}}}{c^{\lambda+1}}\mathrm{d}x\mathrm{d}y = h_1(a)\int\limits_{\mathbb{R}^d}\frac{\mathbf{1}_{\{|y|<c\}}}{c^{\lambda+1}}\mathrm{d}y = h_1(a)|B_1|\frac{c^d}{c^{\lambda+1}}$$

$$I(a,b,c) \leqslant h_2(b)|B_1|\frac{c^d}{c^{\lambda+1}}$$

where $|B_1|$ is the volume of the unit ball. Thus,

$$I(a,b,c) \leqslant C\frac{\min\{h_1(a)h_2(b), h_1(a)c^d, h_2(b)c^d\}}{c^{\lambda+1}},$$

where C is some constant.

Recalling that

$$\left|\int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d}\frac{f(x)g(y)}{|x-y|^\lambda}\mathrm{d}x\mathrm{d}y\right| \leqslant \lambda\int\limits_0^\infty\int\limits_0^\infty\int\limits_0^\infty I(a,b,c)\mathrm{d}a\mathrm{d}b\mathrm{d}c$$

We have

$$\begin{aligned}
\int\limits_0^\infty I(a,b,c)\mathrm{d}c &= \int\limits_{h_1(a)>c^d} I(a,b,c)\mathrm{d}c + \int\limits_{h_1(a)\leqslant c^d} I(a,b,c)\mathrm{d}c \leqslant \\
&\leqslant \int\limits_{h_1(a)>c^d}\frac{h_2(b)c^d}{c^{\lambda+1}}\mathrm{d}c + \int\limits_{h_1(a)\leqslant c^d}\frac{h_1(a)h_2(b)}{c^{\lambda+1}}\mathrm{d}c = \\
&= h_2(b)\int\limits_{0\leqslant c<h_1(a)^{\frac{1}{d}}} c^{d-\lambda-1}\mathrm{d}c + h_1(a)h_2(b)\int\limits_{h_1(a)^{\frac{1}{d}}\leqslant c}\frac{1}{c^{\lambda+1}}\mathrm{d}c = \\
&= \frac{h_2(b)\left(h_1(a)^{\frac{1}{d}}\right)^{d-\lambda}}{d-\lambda} + \frac{1}{\lambda\left(h_1(a)^{\frac{1}{d}}\right)^\lambda}h_1(a)h_2(b) \leqslant Ch_1(a)^{\frac{d-\lambda}{d}}h_1(b)
\end{aligned}$$

Similarly we have

$$\int\limits_0^\infty I(a,b,c)\mathrm{d}c \leqslant Ch_1(a)h_2(b)^{\frac{d-\lambda}{d}}.$$

Thus

$$\int_0^\infty I(a,b,c)\mathrm{d}c \leqslant C\min\Big\{h_1(a)^{1-\frac{\lambda}{d}}h_2(b), h_1(a)h_2(b)^{1-\frac{\lambda}{d}}\Big\}.$$

We want to estimate the a- and b-integrals in terms of

$$1 = \int_{\mathbb{R}^d} |f(x)|^p \mathrm{d}x = p\int_0^\infty h_1(a)a^{p-1}\mathrm{d}a$$

$$1 = \int_{\mathbb{R}^d} |g(y)|^q \mathrm{d}y = q\int_0^\infty h_2(b)b^{q-1}\mathrm{d}b$$

Using these identities we get

$$\begin{aligned}\int_0^\infty\int_0^\infty\int_0^\infty I(a,b,c)\mathrm{d}a\mathrm{d}b\mathrm{d}c &\leqslant C\int_0^\infty\int_0^\infty \min\Big\{h_1(a)^{1-\frac{\lambda}{d}}h_2(b), h_1(a)h_2(b)^{1-\frac{\lambda}{d}}\Big\}\mathrm{d}a\mathrm{d}b \leqslant\\ &\leqslant C\iint_{a^p\geqslant b^q}\cdots\mathrm{d}a\mathrm{d}b + C\iint_{a^p<b^q}\cdots\mathrm{d}a\mathrm{d}b\leqslant\\ &\leqslant C\iint_{b\leqslant a^{\frac{p}{q}}} h_1(a)h_2(b)^{1-\frac{\lambda}{d}}\mathrm{d}a\mathrm{d}b + C\iint_{a^{\frac{p}{q}}<b} h_1(a)^{1-\frac{\lambda}{d}}h_2(b)\mathrm{d}a\mathrm{d}b\end{aligned}$$

The first term can be estimated by

$$\iint_{b\leqslant a^{\frac{p}{q}}} h_1(a)h_2(b)^{1-\frac{\lambda}{d}}\mathrm{d}a\mathrm{d}b = \iint_{b\leqslant a^{\frac{p}{q}}} h_1(a)a^{p-1}\frac{1}{a^{p-1}}h_2(b)^{1-\frac{\lambda}{d}}\mathrm{d}a\mathrm{d}b$$

We need

$$\int_{b\leqslant a^{\frac{p}{q}}}\frac{1}{a^{p-1}}h_2(b)^{1-\frac{\lambda}{d}}\mathrm{d}b\leqslant C$$

and we conclude. This is done by

$$\int_{b\leqslant a^{\frac{p}{q}}}\frac{1}{a^{p-1}}h_2(b)^{1-\frac{\lambda}{d}}\mathrm{d}b \leqslant a^{1-p}\underbrace{\left(\int_{b\leqslant a^{\frac{p}{q}}} h_2(b)b^{q-1}\mathrm{d}b\right)^{1-\frac{\lambda}{d}}}_{\leqslant 1}\left(\int_0^{a^{\frac{p}{q}}}\frac{1}{b^{\xi}}\mathrm{d}b\right)^{\frac{\lambda}{d}} = \mathrm{const}$$

Here Hölder's inequality was used in the first inequality and

$$(q-1)\left(1-\frac{\lambda}{d}\right)-\xi\frac{\lambda}{d}=0.$$

q.e.d.

Remark 1.32. Another application of the Layer cake representation is the *pqr* theorem, i.e. let $p<q<r$, $(f_n)_n \subset L^p, L^q, L^r$ and $\|f_n\|_{L^p}, \|f_n\|_{L^r} \leqslant C$ and $\|f_n\|_{L^q} \geqslant \varepsilon > 0$ then there exists a subsequence such that $f_n \rightharpoonup f \neq 0$. (Exercise 2.3.) □

1.4 Fourier Transform

For all $f \in L^1(\mathbb{R}^d)$ we may define the Fourier transform to be

$$\hat{f}(k)=\int\limits_{\mathbb{R}^d} f(x)e^{-2\pi ik\cdot x}\mathrm{d}x$$

where $k\cdot x=\sum_{j=1}^d k_j x_j$.

Theorem 1.33 (Plancherl)**.**

- *For all $f \in L^1(\mathbb{R}^d)\cap L^2(\mathbb{R}^d)$, $\|\hat{f}\|_{L^2}=\|f\|_{L^2}$.*
- *We can extend the Fourier transform to $L^2(\mathbb{R}^d)$ as an isometry, i.e. for all $f \in L^2(\mathbb{R}^d)$*

  $$\|f\|_{L^2}=\|\hat{f}\|_{L^2}$$

  and therefore for all $f, g \in L^2(\mathbb{R}^d)$

  $$\int\limits_{\mathbb{R}^d}\overline{\hat{f}}\hat{g}=\int\limits_{\mathbb{R}^d}\overline{f}g.$$

□

Proposition 1.34 (Properties of the Fourier Transform)**.** *1) (Inverse formula) Let $\check{f}(x)=\int\limits_{\mathbb{R}^d} f(k)e^{2\pi ik\cdot x}\mathrm{d}k$, then*

$$f=\check{\hat{f}}=\hat{\check{f}}$$

2) (Convolution) $\widehat{f * g}(k) = \hat{f}(k)\hat{g}(k)$.

3) (Fourier vs. Derivatives) Let $D^\alpha = \partial_{x_1}^{\alpha_1} \cdots \partial_{x_d}^{\alpha_d}$ *where* $(x_1, \dots, x_d) \in \mathbb{R}^d$ *and* $\alpha = (\alpha_1, \dots, \alpha_d) \in \mathbb{N}_0^d$. *Then*

$$\widehat{D^\alpha f}(k) = (2\pi i k)^\alpha \hat{f}(k)$$

where $(2\pi i k)^\alpha = \prod_{j=1}^d (2\pi i k_j)^{\alpha_j}$, *for* $k = (k_1, \dots, k_d) \in \mathbb{R}^d$.

4)

$$\widehat{e^{-\pi|\cdot|^2}}(k) = e^{-\pi|k|^2}$$

$\square$

Proof. 2)

$$\begin{aligned}
\widehat{f * g}(k) &= \int\limits_{\mathbb{R}^d} (f * g)(x) e^{-2\pi i k \cdot x} \mathrm{d}x = \int\limits_{\mathbb{R}^d} \int\limits_{\mathbb{R}^d} f(y) g(x-y) e^{-2\pi i k \cdot x} \mathrm{d}x \mathrm{d}y = \\
&= \int\limits_{\mathbb{R}^d} \int\limits_{\mathbb{R}^d} f(y) e^{-2\pi i k \cdot y} g(x-y) e^{-2\pi i k \cdot (x-y)} \mathrm{d}x \mathrm{d}y = \\
&= \int\limits_{\mathbb{R}^d} f(y) e^{-2\pi i k \cdot y} \mathrm{d}x \int\limits_{\mathbb{R}^d} g(z) e^{-2\pi i k \cdot z} \mathrm{d}z = \hat{f}(k)\hat{g}(k)
\end{aligned}$$

3)

$$\begin{aligned}
\widehat{\partial_{x_1} f}(k) &= \int\limits_{\mathbb{R}^d} (\partial_{x_1} f)(x) e^{-2\pi i k \cdot x} \mathrm{d}x = - \int\limits_{\mathbb{R}^d} f(x) \partial_{x_1} \left(e^{-2\pi i k \cdot x} \right) \mathrm{d}x = \\
&= - \int f(x)(-2\pi i k_1) e^{-2\pi i k \cdot x} \mathrm{d}x = (2\pi i k_1) \hat{f}(k).
\end{aligned}$$

q.e.d.

1.5 Sobolev Space

Definition 1.35. The m^{th} Sobolev Space is defined to be the Banach space

$$H^m := \left\{ f \in L^2(\mathbb{R}^d) \,\middle|\, \forall \alpha \in \mathbb{N}^d : |\alpha| = \sum_{j=1}^{d} \alpha_j \leqslant m \implies D^\alpha f \in L^2(\mathbb{R}^d) \right\} =$$
$$= \left\{ f \in L^2(\mathbb{R}^d) \,\middle|\, (1 + |k|^2)^{\frac{m}{2}} \hat{f}(k) \in L^2(\mathbb{R}^d) \right\}$$

with norm

$$\|f\|_{H^m} = \sqrt{\sum_{|\alpha| \leqslant m} \|D^\alpha f\|_{L^2}^2}.$$

An equivalent norm is given by

$$\sqrt{\sum_{\ell \leqslant m} \left\| (1 + |k|^2)^{\frac{\ell}{2}} \hat{f} \right\|_{L^2}^2}.$$

□

Remark 1.36. The derivatives used in this definition are so-called “distributional derivatives”. They coincide with the normal derivative if the function is differentiable and shall be discussed further in section 3.1. □

1.6 Hilbert Space

Definition 1.37. A complex Hilbert space $\mathscr{H}$ is a Banach space equipped with an inner product $\langle \cdot, \cdot \rangle$ that is anti-linear in its first argument and linear in its second, i.e. $\langle \lambda f, \alpha g \rangle = \overline{\lambda} \alpha \langle f, g \rangle$. The corresponding Banach space norm is given by

$$\|f\|_{\mathscr{H}} = \sqrt{\langle f, f \rangle}.$$

□

Definition 1.38 (Orthogonality)**.** f is said to be ***orthogonal*** to g, $f \perp g$, iff $\langle f, g \rangle = 0$.
An orthonormal family $(f_n)_n$ is a sequence of functions in $\mathscr{H}$ such that $\langle f_n, f_m \rangle = \delta_{nm}$, where δ_{nm} is the Kronecker delta.
An orthonormal basis $(f_n)_n$ is a sequence of function in $\mathscr{H}$ that is an orthonormal

family and is complete, i.e. for all $f \in \mathscr{H}$

$$(\forall n \in \mathbb{N} : f \perp f_n) \iff f = 0.$$

□

Remark 1.39. For all Hilbert spaces there exists an orthonormal basis (by Zorn's lemma). In this lecture, we will always consider separable Hilbert spaces, i.e. Hilbert spaces with a countable basis. □

Theorem 1.40 (Parseval)**.** *If $(u_n)_{n=1}^{\infty}$ is an ONB of $\mathscr{H}$, then for all $u \in \mathscr{H}$*

$$\|u\|_{\mathscr{H}}^2 = \sum_{n=1}^{\infty} |\langle u_n, u\rangle|^2$$

Moreover,

$$u = \sum_{n=1}^{\infty} \langle u_n, u\rangle\, u_n$$

□

Corollary 1.41 (Bessel's Inequality)**.** *If $(u_n)_{n\in\mathbb{N}}$ is an orthonormal family, then for all $u \in \mathscr{H}$*

$$\|u\|^2 \geqslant \sum_{n=1}^{\infty} |\langle u_n, u\rangle|^2$$

□

Theorem 1.42 (Riesz Representation Theorem)**.** *Let $\mathscr{L} \in \mathscr{H}^*$ be a bounded (or continuous) linear functional $\mathscr{L} : \mathscr{H} \to \mathbb{C}$, then there exists a unique $v \in \mathscr{H}$ such that*

$$\mathscr{L}(u) = \langle v, u\rangle$$

for all $u \in \mathscr{H}$. □

Definition 1.43 (Weak Convergence)**.** A sequence $(u_n)_n \subset \mathscr{H}$ converges weakly to u, i.e. $u_n \xrightharpoonup{n\to\infty} u$, iff for all $v \in \mathscr{H}$

$$\langle v, u_n \rangle \xrightarrow{n\to\infty} \langle v, u \rangle .$$

□

Remark 1.44. Any separable Hilbert space is ***isometric*** to $L^2(\mathbb{R})$, i.e. there exists a unitary operator $T : \mathscr{H} \to L^2(\mathbb{R})$, that is T is linear and for all $u, v \in \mathscr{H}$

$$\langle u, v \rangle = \langle Tu, Tv \rangle_{L^2} .$$

As a consequence, we have the Banach-Alaoglu theorem, Theorem 1.20, i.e. if $(u_n)_n$ is bounded in $\mathscr{H}$ then there exists a subsequence such that $u_{n_k} \xrightharpoonup{k\to\infty} u$ weakly in $\mathscr{H}$. The Banach-Steinhaus theorem, Theorem 1.21, also holds for all separable Hilbert spaces by the same argument. □

Physics Introduction

Remark 1.45. For more detailed information on this section see: `http://www.mathematik.uni-muenchen.de/~nam/notes_ws18_19_1.pdf`. □

Postulates of Quantum Mechanics

- (State): Described by an element $\psi \in \mathscr{H}$ of a Hilbert space $\mathscr{H}$.
- (Properties): Given by "Observable" linear operators on $\mathscr{H}$
- (Measurement Value a): Eigenvalues of A
- (Probability for a): $\sum_{|a,i\rangle \in \ker(A-a\mathbb{I})} |\langle a,i\,|\,\psi\rangle|^2$, where $|a,i\rangle$ form an orthonormal basis of the eigenvectors of A corresponding to a, i.e $|a,i\rangle \in \ker(A-a)$. Using this basis the measurement probability can also be written as

  $$\sum_{|a,i\rangle \in \ker(A-a\mathbb{I})} |\langle a,i\,|\,\psi\rangle|^2 = \sum_i = \langle \psi\,|\,a,i\rangle \langle a,i\,|\,\psi\rangle = \sum_i \langle \psi\,|\,P\,|\,\psi\rangle = \sum_i \|P\,|\psi\rangle\,\|^2$$

  where $P := \sum_i |a,i\rangle \langle a,i|$ is the projector onto the subspace of a eigenvectors.
- (Measurement): After the measurement the new state is given by an eigenvector of a
- (Dynamics (I)): $\frac{d}{dt}|\psi\rangle = -iH\psi$,
- (Dynamics (II)): $|\psi,t\rangle = U_t\,|\psi,0\rangle$.

The last two points are equivalent by Stones theorem.

Postulates of Classical Mechanics

In terms of point particles (the classical equivalent of pure states, i.e. wave functions):

- (State): Described by an element $(x, p) \in T^*Q$ in phase space.
- (Properties): Given by observables A, i.e. functions on T^*Q.
- (Measurement Value a): $A(x, p) = a$
- (Probability for a): If $A(x, p) = a$ then probability is 1, and otherwise it is 0.
- (Measurement): After the measurement the system is in the same state.
- (Dynamics): $\frac{d}{dt}(x, p) = X_H$.

In terms of probability distributions (the classical equivalent of mixed states, i.e. density matrices, incorporating classical as well as quantum mechanical lack of knowledge):

- (State): Described by a function $\rho(x, p)$ on T^*Q phase space.
- (Properties): Given by observables A, i.e. functions on T^*Q.
- (Measurement Value a): $A(x, p) = a$
- (Probability for a): $P(a, \rho) = \int_{\{A(x,p)=a\}} \rho(x, p)\mathrm{d}x\mathrm{d}p$.
- (Measurement): After the measurement the new state is given $\frac{\rho(x)\mathbf{1}_{\{A(x,p)=a\}}}{P(a,\rho)}$.
- (Dynamics): $\frac{d}{dt}\rho = \pounds_{X_H}\rho = \{H, \rho\}$.

Strange Observations

Assume that particles only have the properties

- C (colour): red/green (r/g),
- S (status): hard/soft (h/s).

Further assume that we have two apparatuses a colouriser $\hat{C}$ which takes as input a particle of any type and may produce a red or green. Analogously we have the same for the status $\hat{S}$.

Suppose that we our experiments yield the following uniform distributions[1]

$$\mathbb{P}(\to \hat{C}) = \frac{1}{2}, \quad \mathbb{P}(\to \hat{C} \to \hat{S}) = \frac{1}{4}, \quad \mathbb{P}(\to \hat{C} \to \hat{S} \to \hat{C}) = \frac{1}{8}$$

However, we also measure

$$\mathbb{P}(\to \hat{C}) = \frac{1}{2}, \quad \mathbb{P}_{\hat{C}^2}(rr) = \mathbb{P}_{\hat{C}^2}(gg) = \frac{1}{2}, \mathbb{P}_{\hat{C}^2}(rg) = \mathbb{P}_{\hat{C}^2}(gr) = 0,$$
$$\mathbb{P}_{\hat{S}\hat{C}^2}(hrr) = \mathbb{P}_{\hat{S}\hat{C}^2}(srr) = \mathbb{P}_{\hat{S}\hat{C}^2}(hgg) = \mathbb{P}_{\hat{S}\hat{C}^2}(sgg) = \frac{1}{4}.$$

and the other probabilities of the last measurement are 0.

This is the content of the Stern-Gerlach experiment.

EPR - Einstein, Podolski, Rosen (1934)

They made two assumptions of locality and reality and took QM on face value and a system of 2 particles in 1 dimension, i.e.

$$\psi^{(a,b)}(x_1, x_2) \in \mathscr{H}^a \otimes \mathscr{H}^b = L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^3) = L^2(\mathbb{R}^6)$$

Suppose that $\psi = d(x_1 - x_2 - L)d(p_1 + p_2)$, where d is an almost δ function.

If we measure x_1, we know also $x_2 = x_1 - L$ and similarly if we measure p_1 then we know that $p_2 = -p_1$.

Bell Inequality

Suppose that we have reality and locality. Imagine two particles are fully determined by $\boldsymbol{\lambda}$, $\boldsymbol{\mu}$ and measurements a, b, c such that results of the measurement are $a(\boldsymbol{\lambda}), b(\boldsymbol{\lambda}), c(\boldsymbol{\lambda}), a(\boldsymbol{\mu}), \dots,$ are functions of $\boldsymbol{\lambda}, \boldsymbol{\mu}$.

Suppose that we have a source of particles producing $\boldsymbol{\lambda}_j, \boldsymbol{\mu}_j, \dots$.

Say that a, b, c are polarisers in direction $\boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\gamma}$ respectively.

[1] Which is the case if the eigenbases of $\hat{S}$ and $\hat{C}$ are mutually unbiased.

Suppose that our apparatus gives only ± 1. Suppose that we have a source of pair $(\boldsymbol{\lambda}_j, \boldsymbol{\mu}_j)$, such that $c(\boldsymbol{\lambda}_j) = c(\boldsymbol{\mu}_j)$ then

$$1 - b(\boldsymbol{\mu}_j)c(\boldsymbol{\lambda}_j) = a(\boldsymbol{\lambda}_j)(b(\boldsymbol{\mu}_j) - c(\boldsymbol{\mu}_j)), \text{ or } 1 - b(\boldsymbol{\mu}_j)c(\boldsymbol{\lambda}_j) = -a(\boldsymbol{\lambda}_j)(b(\boldsymbol{\mu}_j) - c(\boldsymbol{\mu}_j))$$

Taking the average over many pairs $j = 0, 1, \ldots, N-1$ we get the inequalities

$$1 - \langle bc \rangle \geqslant \max\{\langle a[b-c] \rangle, - \langle a[b-c] \rangle\}$$

i.e.

$$1 - \langle bc \rangle \geqslant |\, \langle ab \rangle - \langle ac \rangle \,|.$$

Quantum mechanics violates this inequality.

Chapter 2

Principles of Quantum Mechanics

Basic Setting of Quantum Mechanics

- A quantum ***state*** is a vector in a Hilbert space $\mathscr{H}$,
- Observables are (bounded or unbounded) operators on $\mathscr{H}$,
- The Hamiltonian H is a self-adjoint operator, with $\langle \psi, H\psi \rangle$ representing the energy of the state ψ,
- The Schrödinger equation:
$$\partial_t \psi(t) = -iH\psi(t)$$
- Mixed states: γ which are trace class operators on $\mathscr{H}$, $\gamma \geqslant 0$, $\operatorname{Tr} \gamma = 1$ which is equivalent to
$$\gamma = \sum_i \lambda_i \left| u_i \right\rangle \left\langle u_i \right|$$
where $(u_i)_i$ is an orthonormal family, $\lambda_i \geqslant 0$ and $\sum_i \lambda_i = 1$.

Remark 2.1 (Dirac "Bra-Ket")**.** By Riesz's representation Theorem 1.42 $\mathscr{H} = \mathscr{H}^*$ with the isomorphism being given by

$$v \longmapsto (\mathscr{L}_v : u \mapsto \langle v, u \rangle)$$

for all $u \in \mathscr{H}$. We say that a state $|u\rangle \in \mathscr{H}$ is a ket, and $\langle u| \in \mathscr{H}^*$ is a bra. In particular the inner product of $u, v \in \mathscr{H}$ is written as

$$\langle u \,|\, v \rangle \,.$$

If $u \in \mathscr{H}$, then $|u\rangle \langle u|$ is the projection onto u, i.e.

$$(|u\rangle \langle u|)\varphi = (|u\rangle \langle u|) \, |\varphi\rangle = \underbrace{\langle u \,|\, \varphi\rangle}_{\in \mathbb{C}} |u\rangle \,.$$

□

Remark 2.2. In classical mechanics we think of particles as being point-like and moving along fixed trajectories in phase/configuration space. In particular their dynamics is determined by the set of equations

$$\begin{aligned} \dot{x}(t) &= v(t) \\ \dot{v}(t) &= F(x(t), v(t)) \end{aligned}$$

with $(x, v) \in \mathbb{R}^d \times \mathbb{R}^d$.
However, within classical mechanics the hydrogen atom is not stable. The ground energy of that system is given by

$$\inf_{(x,v) \in \mathbb{R}^d \times \mathbb{R}^d} \left(\frac{mv^2}{2} - \frac{1}{|x|} \right) = -\infty,$$

which leads to this problem. □

In quantum mechanics a particle is described by a wave function $\psi \in L^2(\mathbb{R}^d)$ with $\|\psi\|_{L^2} = 1$, where $|\psi(x)|^2$ is thought of as the probability distribution of the position of the particle, in particular

$$\mathbb{P}(\text{“}\psi \in \Omega\text{”}) = \int_\Omega |\psi(x)|^2 \mathrm{d}x.$$

Analogously, its Fourier transform $\left|\hat{\psi}(k)\right|^2$ describes a probability distribution for the momentum.

In this case the energy of a particle in the Hydrogen system is given by

$$\langle \psi, H\psi \rangle = \langle \psi, |p|^2\psi \rangle - \left\langle \psi, \frac{1}{|x|}\psi \right\rangle = \int |2\pi k|^2 |\hat{\psi}(k)|^2 \mathrm{d}k - \int \frac{|\psi(x)|^2}{|x|}\mathrm{d}x =$$
$$= \int \left(|\nabla\psi(x)|^2 - \frac{|\psi(x)|^2}{|x|} \right) \mathrm{d}x = \left\langle \psi, \left(-\Delta - \frac{1}{|x|} \right) \psi \right\rangle.$$

Definition 2.3 (Momentum Operator)**.** We define the momentum operator p to be given by

$$p = -i\nabla$$

in x-space, or in k-space

$$p = 2\pi k.$$

□

2.1 Stability of the Hydrogen Atom

Why does

$$\mathcal{E}(u) := \int\limits_{\mathbb{R}^3} \left(|\nabla u|^2 - \frac{|u|^2}{|x|} \right) \mathrm{d}x \geqslant -C$$

hold for all u with $\|u\|_{L^2} = 1$?

We can prove this with the help of so-called uncertainty principles.

Theorem 2.4 (Hardy Uncertainty Principle)**.** *If $u \not\equiv 0$, then $u(x)$ and $\hat{u}(k)$ cannot both have compact support. A stronger version of Hardy's uncertainty principle is given by: If for $\alpha > 0$*

$$|u(x)| \lesssim e^{-\pi\alpha|x|^2}$$

then

$$|\hat{u}(k)| \gtrsim e^{-\frac{\pi|k|^2}{\alpha}}$$

as $|k| \to \infty$.

Note here that

$$\widehat{e^{-\pi\alpha|\cdot|^2}}(k) = e^{-\frac{\pi|k|^2}{\alpha}}$$

□

Theorem 2.5 (Heisenberg Uncertainty Principle)**.** *For all $u \in \mathscr{C}_c^1(\mathbb{R}^d)$, $\|u\|_{L^2} = 1$*

$$\left(\int |\nabla u|^2 \mathrm{d}x\right)\left(\int |x|^2 |u(x)|^2 \mathrm{d}x\right) \geqslant \frac{d^2}{4}.$$

□

Proof. See Exercise 3.4. *q.e.d.*

Remark 2.6. The Heisenberg uncertainty principle is not enough to prove the stability of the Hydrogen atom! □

Theorem 2.7 (Refined Hardy Uncertainty Principle, Hardy's Inequality)**.** *For all $u \in \mathscr{C}_c^1(\mathbb{R}^3)$,*

$$\int_{\mathbb{R}^3} |\nabla u(x)|^2 \mathrm{d}x \geqslant \frac{1}{4} \int_{\mathbb{R}^3} \frac{|u(x)|^2}{|x|^2} \mathrm{d}x$$

□

Proof. Let $g(x) = u(x)|x|^{1/2}$. Then $g(0) = 0$ and

$$\nabla u(x) = \nabla\left(\frac{g(x)}{|x|^{1/2}}\right) = \frac{\nabla g(x)}{|x|^{1/2}} - \frac{1}{2} g(x) \frac{x}{|x|^{5/2}}$$

which implies that

$$|\nabla u(x)|^2 = \frac{|\nabla g(x)|^2}{|x|} + \frac{1}{4} \frac{|g(x)|^2}{|x|^3} - \mathfrak{R}\, \frac{\overline{\nabla g(x)} g(x) x}{|x|^3}.$$

Integrating over this expression yields

$$\int |\nabla u(x)|^2 \mathrm{d}x = \underbrace{\int \frac{|\nabla g(x)|^2}{|x|} \mathrm{d}x}_{\geqslant 0} + \frac{1}{4} \int \frac{|u(x)|^2}{|x|^2} \mathrm{d}x - \int \mathfrak{R}\, \frac{\overline{\nabla g(x)} g(x) x}{|x|^3} \mathrm{d}x.$$

We claim that the last term vanishes which proves the assertion. To see this we integrate by parts

$$\int \Re \frac{\overline{\nabla g(x)} g(x) x}{|x|^3} \mathrm{d}x = -\frac{1}{2} \int_{\mathbb{R}^3} \left(\nabla\left(|g(x)|^2\right)\right) \nabla\left(\frac{1}{|x|}\right) \mathrm{d}x = \frac{1}{2} \int_{\mathbb{R}^3} |g(x)|^2 \Delta\left(\frac{1}{|x|}\right) \mathrm{d}x =$$
$$= -2\pi |g(0)|^2 = 0$$

because $g(0) = 0$ and $-\Delta \frac{1}{|x|} = 4\pi\delta(x)$ (in the distributional sense).

q.e.d.

Remark 2.8 (Comments on the Proof)**.** We proved that

$$\mathcal{E}(u) = \int_{\mathbb{R}^3} \left(|\nabla u|^2 - \frac{1}{4} \frac{|u(x)|^2}{|x|^2} \right) \mathrm{d}x \geqslant 0.$$

If there exists a minimiser for

$$\inf_{u \in \mathscr{C}_c^1} \left(\int \left(|\nabla u(x)|^2 - \frac{1}{4} \frac{|u(x)|^2}{|x|^2} \right) \mathrm{d}x \right)$$

then it would have to solve the Euler-Lagrange equation, i.e. $\frac{d}{dt}\mathcal{E}(u + t\varphi) = 0$ for all $\varphi \in \mathscr{C}_c^\infty$. In this case this is equivalent to

$$\left(-\Delta - \frac{1}{4|x|^2} \right) u(x) = 0 \qquad \Longleftrightarrow \qquad u(x) = \frac{1}{|x|^{1/2}}.$$

However, $\frac{1}{|x|^{1/2}} \notin L^2(\mathbb{R}^3)$ and thus Hardy's inequality is strict, i.e. for all $u \not\equiv 0$

$$\int |\nabla u|^2 > \frac{1}{4} \int \frac{|u(x)|^2}{|x|^2} \mathrm{d}x.$$

Still, we can think of $\frac{1}{|x|^{1/2}}$ as a "ground state". The choice $u(x) = \frac{g(x)}{|x|^{1/2}}$ corresponds to the so-called "ground-state substitution". $\square$

Theorem 2.9 (Stability of the Hydrogen Atom)**.** *There exists $C \geqslant 0$ such that for all $u \in \mathscr{C}_c^1(\mathbb{R}^3)$, $\|u\|_{L^2} = 1$*

$$\int_{\mathbb{R}^3} \left(|\nabla u(x)|^2 - \frac{|u(x)|^2}{|x|} \right) \mathrm{d}x \geqslant -C.$$

□

Proof. We shall combine Hardy's inequality with Hölder's

$$\int_{\mathbb{R}^3} \frac{|u(x)|^2}{|x|} \leqslant \left(\int_{\mathbb{R}^3} \frac{|u(x)|^2}{|x|^2} \right)^{1/2} \left(\int_{\mathbb{R}^3} |u(x)|^2 \right)^{1/2} \leqslant \left(4 \int_{\mathbb{R}^3} |\nabla u(x)|^2 \mathrm{d}x \right)^{1/2}$$

Thus we find that

$$\int \left(|\nabla u(x)|^2 - \frac{|u(x)|^2}{|x|} \right) \geqslant \int |\nabla u|^2 - 2 \left(\int |\nabla u|^2 \right)^{1/2} \geqslant -1$$

where we used that $t^2 - 2t \geqslant -1$. *q.e.d.*

Remark 2.10. In fact one can prove that

$$\int_{\mathbb{R}^3} \left(|\nabla u(x)|^2 - \frac{|u(x)|^2}{|x|} \right) \mathrm{d}x \geqslant -\frac{1}{4}$$

where the constant $-\frac{1}{4}$ is sharp. □

Chapter 3

Sobolev Spaces

3.1 Distribution Theory

Definition 3.1 (Test Functions)**.** We define $\mathscr{D}(\mathbb{R}^d) := \mathscr{C}_c^\infty(\mathbb{R}^d)$ with the very strong topology

$$\varphi_n \xrightarrow{n\to\infty} \varphi \text{ in } \mathscr{D}(\mathbb{R}^d) :\Longleftrightarrow \begin{cases} \|D^\alpha \varphi_n - D^\alpha \varphi\|_{L^\infty} \xrightarrow{n\to\infty} 0, & \text{for all } \alpha \in \mathbb{N}^d \text{ and} \\ \bigcup_{n\in\mathbb{N}} \operatorname{supp} \varphi_n \text{ is compact.} \end{cases}$$

□

Definition 3.2 (Distributions)**.** We define the space of distributions $\mathscr{D}'(\mathbb{R}^d)$ to be the set of continuous linear functionals on $\mathscr{D}(\mathbb{R}^d)$, i.e.

$$T : \mathscr{C}_c^\infty \longrightarrow \mathbb{C}.$$

We equip $\mathscr{D}'(\mathbb{R}^d)$ with the weak topology, i.e.

$$T_n \xrightarrow{n\to\infty} T :\Longleftrightarrow \ \forall u \in \mathscr{D}(\mathbb{R}^d) : T_n(u) \xrightarrow{n\to\infty} T(u).$$

□

Example 3.3. Let $f \in L^1_{\text{loc}}(\mathbb{R}^d)$, i.e. $\mathbf{1}_\Omega f \in L^1(\mathbb{R}^d)$ for any compact set Ω. Then

$$T_f : \begin{aligned} \mathscr{C}_c^\infty(\mathbb{R}^d) &\longrightarrow \mathbb{C} \\ \varphi &\longmapsto \int_{\mathbb{R}^d} f\varphi \end{aligned}.$$

Here T_f is obviously a linear functional and it is continuous. Too see the latter let $(\varphi_n)_n \subset \mathscr{D}(\mathbb{R}^d)$ with $\varphi_n \xrightarrow{n\to\infty} \varphi$ in $\mathscr{D}(\mathbb{R}^d)$. Then $(\|\varphi_n\|_{L^\infty})_n$ is bounded by some constant C and $\Omega := \bigcup_n \operatorname{supp} \varphi_n$ is compact. Thus for all $n \in \mathbb{N}$

$$|f\varphi_n| = |f\mathbf{1}_\Omega \varphi_n| \leqslant C|f|\mathbf{1}_\Omega \in L^1(\mathbb{R}^d)$$

is an integrable majorant independent of $n \in \mathbb{N}$ and we may apply the dominated convergence theorem to conclude

$$\lim_{n\to\infty} T_f(\varphi_n) = \lim_{n\to\infty} \int f\varphi_n = \int f\varphi = T_f(\varphi).$$

Lemma 3.4 (Fundamental Lemma of the Calculus of Variations)**.** *If $f \in L^1_{loc}(\mathbb{R}^d)$ and $\int f\varphi = 0$ for all $\varphi \in \mathscr{C}_c^\infty(\mathbb{R}^d)$, then $f \equiv 0$.* □

Proof. 1) Assume that $f \in L^1(\mathbb{R}^d)$. Then for all $\varphi \in \mathscr{C}_c^\infty$ and all $x \in \mathbb{R}^d$

$$(f * \varphi)(x) = \int_{\mathbb{R}^d} f(y)\varphi(x-y) = 0$$

because $y \mapsto \varphi(x-y) \in \mathscr{C}_c^\infty$. In particular, take $g \in \mathscr{C}_c^\infty$, with $\int g = 1$, $g_\varepsilon(x) := \frac{1}{\varepsilon^d} g\left(\frac{x}{\varepsilon}\right)$. Then $g_\varepsilon * f \xrightarrow{\varepsilon\to 0} f$ in $L^1(\mathbb{R}^d)$. But $g_\varepsilon * f = 0$ by the above argument. Hence $f \equiv 0$.

2) If $f \in L^1_{\text{loc}}(\mathbb{R}^d)$, then taking $g \in \mathscr{C}_c^\infty(\mathbb{R}^d)$, $fg \in L^1(\mathbb{R}^d)$. We have

$$\int_{\mathbb{R}^d} (fg)\varphi = \int_{\mathbb{R}^d} f \underbrace{(g\varphi)}_{\in \mathscr{C}_c^\infty} = 0$$

for all $\varphi \in \mathscr{C}_c^\infty(\mathbb{R}^d)$. Applying the first step to $fg \in L^1(\mathbb{R}^d)$ we conclude that $fg \equiv 0$. Thus $f = 0$ on $\operatorname{supp} g$. But g is arbitrary in $\mathscr{C}_c^\infty$ and therefore $f \equiv 0$.

q.e.d.

Definition 3.5 (Derivatives of Distributions)**.** If $T \in \mathscr{D}'(\mathbb{R}^d)$, we can define $\partial_{x_i} T \in \mathscr{D}'(\mathbb{R}^d)$ via

$$(\partial_{x_i} T)(\varphi) = -T(\partial_{x_i}\varphi)$$

for all $\varphi \in \mathscr{C}_c^\infty(\mathbb{R}^d)$. In general we define for $\alpha \in \mathbb{N}^d$, $D^\alpha T \in \mathscr{D}'(\mathbb{R}^d)$ via

$$(D^\alpha T)(\varphi) = (-1)^{|\alpha|} T(D^\alpha \varphi).$$

□

Remark 3.6. The motivation for this definition is that for $f \in \mathscr{C}^1(\mathbb{R}^d)$

$$\int \partial_{x_i} f \varphi = -\int f \partial_{x_i} \varphi$$

for all $\varphi \in \mathscr{C}_c^\infty(\mathbb{R}^d)$. In this case, $\partial_{x_i} T_f = T_{\partial_{x_i} f}$, i.e. the distributional derivative equals the classical derivative wherever the function is differentiable.
To make sure that this derivative is well-defined, one has to check that $\varphi \mapsto T(D^\alpha \varphi)$ is linear (trivial) and continuous in $\mathscr{D}(\mathbb{R}^d)$. (Exercise) □

Theorem 3.7.

$$\begin{aligned} H^m(\mathbb{R}^d) &= \left\{ f \in L^2(\mathbb{R}^d) \,\middle|\, |k|^m \hat{f}(k) \in L^2(\mathbb{R}^d) \right\} = \\ &= \left\{ f \in L^2(\mathbb{R}^d) \,\middle|\, D^\alpha f \in L^2(\mathbb{R}^d) \textit{ for all } |\alpha| \leqslant m \right\}. \end{aligned}$$

□

Proof. Take $f \in L^2(\mathbb{R}^d)$, with $|k|^m \hat{f}(k) \in L^2(\mathbb{R}^d)$. Take g such that $\hat{g}(k) = (2\pi i k)^\alpha \hat{f}(k)$ which is in $L^2(\mathbb{R}^d)$ for all $|\alpha| \leqslant m$. In particular we also have $g \in L^2(\mathbb{R}^d)$.

Now we prove that $g = D^\alpha f$ in the distributional sense, i.e. for all $\varphi \in \mathscr{C}_c^\infty$

$$\int g\varphi = (-1)^{|\alpha|} \int f(D^\alpha \varphi) \iff \int \overline{\varphi} g = (-1)^{|\alpha|} \int \overline{(D^\alpha \varphi)} f.$$

To prove this we use Placherl's identity to get

$$\int \overline{\varphi} g = \int \overline{\hat{\varphi}} \hat{g} = \int \overline{\hat{\varphi}(k)} (2\pi k i)^{\alpha} \hat{f}(k) \mathrm{d}k = (-1)^{|\alpha|} \int \overline{(2\pi i k)^{\alpha} \hat{\varphi}(k)} \hat{f}(k) \mathrm{d}k =$$
$$= (-1)^{|\alpha|} \int \overline{\widehat{D^{\alpha}\varphi}(k)} f(k) \mathrm{d}k = (-1)^{|\alpha|} \int \overline{D^{\alpha}\varphi} f.$$

The other direction is an easy exercise. *q.e.d.*

Theorem 3.8. *For all $m \geqslant 1$, $\mathscr{C}_c^{\infty}(\mathbb{R}^d)$ is dense in $H^m(\mathbb{R}^d)$.* □

Proof. 1) Take $f \in H^1(\mathbb{R}^d)$. Assume that f has compact support. Take $g \in \mathscr{C}_c^{\infty}$, $\int g = 1$, $g_{\varepsilon}(x) := \frac{1}{\varepsilon^d} g\left(\frac{x}{\varepsilon}\right)$. Then $\mathscr{C}_c^{\infty}(\mathbb{R}^d) \ni g_{\varepsilon} * f \xrightarrow{\varepsilon \to 0} f$ in $L^2(\mathbb{R}^d)$.

Moreover,

$$\partial_{x_i}(g_{\varepsilon} * f) = g_{\varepsilon} * \underbrace{(\partial_{x_i} f)}_{L^2} \xrightarrow{\varepsilon \to 0} \partial_{x_i} f$$

in $L^2(\mathbb{R}^d)$.

2) If $f \in H^1(\mathbb{R}^d)$, take $h \in \mathscr{C}_c^{\infty}(\mathbb{R}^d)$. Then $fh \in H^1(\mathbb{R}^d)$ and

$$\partial_{x_i}(fh) = \underbrace{(\partial_{x_i} f)}_{\in L^2} h + f \underbrace{(\partial_{x_i} h)}_{\mathscr{C}_c^{\infty}},$$

i.e. for all $\varphi \in \mathscr{C}_c^{\infty}$

$$\int fh(\partial_{x_i}\varphi) = \int ((\partial_{x_i} f)h + f(\partial_{x_i} h))\varphi.$$

This is left as an exercise. Thus fh and $\partial_{x_i}(fh)$ have compact support and we can approximate fh by $\mathscr{C}_c^{\infty}(\mathbb{R}^d)$ functions in $H^1(\mathbb{R}^d)$. Finally, we can choose a sequence $(h_n)_n \subset \mathscr{C}_c^{\infty}$ such that

$$fh_n \xrightarrow{n \to \infty} f \text{ in } H^1(\mathbb{R}^d).$$

(e.g. take $h_n = 1$ if $|x| \leqslant n$, $h_n(x) = 0$ if $|x| \geqslant 2n$ and $|\nabla h_n| \leqslant \frac{C}{n}$ (Exercise)).

q.e.d.

3.2 Sobelev Inequalities

Remark 3.9. To see that Hardy's inequality is sharp we may use a so-called scaling argument. Let $u(x) \mapsto \lambda u(\ell x)$ be a dilation. Then for $\lambda = 1$ for example we have

$$\int_{\mathbb{R}^3} |\nabla u(\ell x)|^2 \mathrm{d}x = \int_{\mathbb{R}^3} \ell^2 |\nabla u(x)| \frac{\mathrm{d}x}{\ell^3} = \int_{\mathbb{R}^3} \frac{|\nabla u|^2}{\ell} \mathrm{d}x,$$

$$\int \frac{|u(\ell x)|^2}{|x|^2} \mathrm{d}x = \int \frac{|u(x)^2|}{\left|\frac{x}{\ell}\right|^2} \frac{\mathrm{d}x}{\ell^3} = \int \frac{|u(x)|^2}{\ell |x|^2} \mathrm{d}x.$$

□

Theorem 3.10 (Standard Sobolev Inequality)**.** *If $d \geqslant 3$. Then for all $u \in H^1(\mathbb{R}^d)$*

$$\int_{\mathbb{R}^d} |\nabla u(x)|^2 \mathrm{d}x \geqslant C \left(\int_{\mathbb{R}^d} |u(x)|^p \mathrm{d}x \right)^{\frac{2}{p}}$$

for $p = \frac{2d}{d-2}$. Here the constant $C = C(d)$ is independent of u. In particular we have

$$\|\nabla u\|_{L^2(\mathbb{R}^d)} \geqslant \frac{\sqrt{3}}{2} (2\pi^2)^{\frac{1}{3}} \|u\|_{L^6(\mathbb{R}^6)} \approx 2.34 \|u\|_{L^6(\mathbb{R}^3)}.$$

□

Remark 3.11. The Sobolev inequality is invariant under the dilation

$$u_\ell(x) = \ell^{\frac{d}{2}} u(\ell x)$$

for which we have $\|u_\ell\|_{L^2(\mathbb{R}^d)} = \|u\|_{L^2(\mathbb{R}^d)}$ and

$$\int\limits_{\mathbb{R}^d} |\nabla u_\ell(x)|^2 \mathrm{d}x = \int\limits_{\mathbb{R}^d} \ell^d \ell^2 |(\nabla u)(\ell x)|^2 \mathrm{d}x = \ell^2 \int\limits_{\mathbb{R}^d} |\nabla u(x)|^2 \mathrm{d}x$$

$$\left(\int\limits_{\mathbb{R}^d} |u_\ell(x)|^p \mathrm{d}x\right)^{\frac{2}{p}} = \left(\int\limits_{\mathbb{R}^d} \ell^{\frac{pd}{2}} |u(\ell x)|^p \mathrm{d}x\right)^{\frac{2}{p}} \left(= \ell^{\frac{pd}{2}-d} \int\limits_{\mathbb{R}^d} |u(x)|^p \mathrm{d}x\right)^{\frac{2}{p}} =$$

$$= \ell^{(\frac{pd}{2}-d)\frac{2}{p}} \left(\int\limits_{\mathbb{R}^d} |u(x)|^p \mathrm{d}x\right)^{\frac{2}{p}}$$

If we want

$$\int\limits_{\mathbb{R}^d} |\nabla u_\ell|^2 \geqslant C \left(\int\limits_{\mathbb{R}^d} |u_\ell|^p\right)^{\frac{2}{p}} \iff \ell^2 \int\limits_{\mathbb{R}^d} |\nabla u|^2 \geqslant C \ell^{d-\frac{2d}{p}} \left(\int\limits_{\mathbb{R}^d} |u|^p\right)^{\frac{2}{p}}$$

This holds for all $\ell > 0$ with a universal constant C iff

$$2 = d - \frac{2d}{p} \iff p = \frac{2d}{d-2}.$$

□

Lemma 3.12. *Let $c_s := \pi^{-\frac{s}{2}} \Gamma\left(\frac{s}{2}\right)$, where $\Gamma(s) = \int_0^\infty e^{-t} t^{s-1} \mathrm{d}t$. Then, on $\mathbb{R}^d$*

$$\widehat{\frac{c_s}{|\cdot|^s}}(k) = \frac{c_{d-s}}{|k|^{d-s}}.$$

for all $0 < s < d$. As neither the left nor the right-hand side are integrable this is taken to mean that for all $f \in \mathscr{C}_c^\infty(\mathbb{R}^d)$

$$\widehat{\frac{c_s}{|x|^s} * f} = \frac{c_{d-s}}{|k|^{d-s}} \hat{f}(k).$$

$\square$

Proof. Making the substitution $t = \pi\lambda|x|^2$ we find that

$$\Gamma(s) = \int_0^\infty e^{-t} t^{s-1} \mathrm{d}t = \int_0^\infty e^{-\pi\lambda|x|^2} (\pi\lambda|x|^2)^{s-1} \pi|x|^2 \mathrm{d}\lambda.$$

Therefore

$$\Gamma\left(\frac{s}{2}\right) = \pi^{\frac{s}{2}} |x|^s \int_0^\infty e^{-\pi\lambda|x|^2} \lambda^{\frac{s}{2}-1} \mathrm{d}\lambda.$$

Thus we have for all $x \in \mathbb{R}^d \setminus \{0\}$

$$\frac{c_s}{|x|^s} = \int_0^\infty e^{-\pi\lambda|x|^2} \lambda^{\frac{s}{2}-1} \mathrm{d}\lambda.$$

As we know the Fourier transform of the Gaussian

$$\widehat{e^{-\pi\lambda|\cdot|^2}}(k) = \frac{e^{-\pi\frac{|k|^2}{\lambda}}}{\lambda^{\frac{d}{2}}}.$$

we find

$$\widehat{\frac{c_s}{|\cdot|^s}} = \int_0^\infty \widehat{e^{-\pi\lambda|\cdot|^2}} \lambda^{\frac{s}{2}-1} \mathrm{d}\lambda = \int_0^\infty \frac{e^{-\pi\frac{|k|^2}{\lambda}}}{\lambda^{\frac{d}{2}}} \lambda^{\frac{s}{2}-1} \mathrm{d}\lambda \overset{\lambda \mapsto \lambda^{-1}}{=\!=\!=} \int_0^\infty e^{-\pi\lambda|k|^2} \lambda^{\frac{d}{2}} \lambda^{1-\frac{s}{2}} \frac{\mathrm{d}\lambda}{\lambda^2} =$$
$$= \int_0^\infty e^{-\pi\lambda|k|^2} \lambda^{\frac{d-s}{2}-1} \mathrm{d}\lambda = \frac{c_{d-s}}{|k|^{d-s}}$$

q.e.d.

Proof of Theorem 3.10. Define $\hat{g}(k) = |2\pi k|\hat{u}(k)$, then

$$\|\nabla u\|_{L^2} = \left(\int_{\mathbb{R}^d} |2\pi k|^2 |\hat{u}(k)|^2 \mathrm{d}k\right)^{\frac{1}{2}} = \left(\int_{\mathbb{R}^d} |\hat{g}(k)|^2 \mathrm{d}k\right)^{\frac{1}{2}} = \left(\int_{\mathbb{R}^d} |g(x)|^2 \mathrm{d}x\right)^{\frac{1}{2}} = \|g\|_{L^2(\mathbb{R}^d)}.$$

On the other hand

$$\hat{u}(k) = \frac{1}{|2\pi k|}\hat{g}(k) = \frac{1}{2\pi c_1}\frac{c_1}{|k|}\hat{g}(k) = \frac{1}{2\pi c_1}\widehat{\frac{c_{d-1}}{|x|^{d-1}} * g}(k)$$

by the above lemma. Therefore,

$$u(x) = \frac{c_{d-1}}{2\pi c_1}\left(\frac{1}{|x|^{d-1}} * g\right)(x) = \frac{c_{d-1}}{2\pi c_1}\int\limits_{\mathbb{R}^d} \frac{1}{|x-y|^{d-1}} g(y)\mathrm{d}y.$$

Thus we want to prove that

$$\|g\|_{L^2(\mathbb{R}^d)} \geqslant C\left\|\frac{1}{|x|^{d-1}} * g\right\|_{L^p(\mathbb{R}^d)}.$$

Recall that by the Hardy-Littlewood-Sobolev inequality Theorem 1.30

$$\left|\int\limits_{\mathbb{R}^d} f(x)\left(\frac{1}{|\cdot|^{d-1}} * g\right)(x)\mathrm{d}x\right| = \int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} \frac{|f(x)g(y)|}{|x-y|^{d-1}}\mathrm{d}x\mathrm{d}y \leqslant C\|f\|_{L^q}\|g\|_{L^2}$$

where $\frac{1}{q} + \frac{1}{2} + \frac{d-1}{d} = 2$, i.e. $q = \frac{2d}{d+2}$. Now using that

$$\|h\|_{L^{q'}} = \sup_{f \in L^q(\mathbb{R}^d)\setminus\{0\}} \frac{\left|\int f(x)h(x)\mathrm{d}x\right|}{\|f\|_{L^q}}.$$

we get

$$\left\|\frac{1}{|\cdot|^{d-1}} * g\right\|_{L^{q'}(\mathbb{R}^d)} = \sup_{f \in L^q(\mathbb{R}^d)\setminus\{0\}} \frac{\left|\int f(x)\left(\frac{1}{|\cdot|^{d-1}} * g\right)(x)\mathrm{d}x\right|}{\|f\|_{L^q}} \leqslant C\|g\|_{L^2}$$

where $\frac{1}{q'} + \frac{d+2}{2d} = 1$, i.e. $q' = \frac{2d}{d-2}$.

q.e.d.

Remark 3.13. The proof of the sharp constant is more complicated. It requires so-called "rearrangement inequalities" i.e. for u^* radial

$$\|\nabla u\|_{L^2} \geqslant \|\nabla u^*\|_{L^2}, \qquad \|u\|_{L^p} = \|u^*\|_{L^p}$$

□

Example 3.14 (Using Sobolev's Inequality to prove the Stability of the Hydrogen Atom)**.** We can prove the stability of the hydrogen atom

$$\int_{\mathbb{R}^3} |\nabla u|^2 - \int_{\mathbb{R}^3} \frac{|u(x)|^2}{|x|} \mathrm{d}x \geqslant -C$$

for all $u \in H^1(\mathbb{R}^3)$, with $\|u\|_{L^2} = 1$. We know that

$$\int_{\mathbb{R}^3} |\nabla u|^2 \geqslant \frac{3}{4}(2\pi^2)^{\frac{2}{3}} \|u\|_{L^6}^2$$

and

$$\int_{\mathbb{R}^3} \frac{|u(x)|^2}{|x|} = \int_{|x|\leqslant R} \frac{|u(x)|^2}{|x|} \mathrm{d}x + \int_{|x|\geqslant R} \frac{|u(x)|^2}{|x|} \mathrm{d}x \leqslant$$

$$\leqslant \left(\int_{|x|\leqslant R} |u(x)|^6 \right)^{\frac{1}{3}} \left(\int_{|x|\leqslant R} \frac{1}{|x|^{\frac{3}{2}}} \right)^{\frac{2}{3}} + \int_{|x|\geqslant R} \frac{|u(x)|^2}{R} \mathrm{d}x \leqslant \|u\|_{L^6}^2 4 \left(\frac{\pi}{3}\right)^{\frac{2}{3}} R + \frac{1}{R}$$

Theorem 3.15 (Sobolev Inequality in Lower Dimensions)**.**

$d = 1$: *For all* $2 \leqslant p \leqslant \infty$ *we have*

$$\|u\|_{L^p(\mathbb{R})} \leqslant C \|u\|_{H^1(\mathbb{R})}.$$

Moreover, $H^1(\mathbb{R}) \subset \mathscr{C}(\mathbb{R})$, *with the embedding* $\iota : H^1(\mathbb{R}) \to \mathscr{C}(\mathbb{R})$ *being continuous, and* $\|u\|_{L^\infty}^2 \leqslant \|u'\|_{L^2} \|u\|_{L^2}$ *for all* $u \in H^1(\mathbb{R})$.

$d = 2$: *For all* $2 \leqslant p < \infty$

$$\|u\|_{L^p(\mathbb{R}^2)} \leqslant C \|u\|_{H^1(\mathbb{R}^2)}.$$

□

Proof.

$d = 1$: Take $u \in \mathscr{C}_c^\infty(\mathbb{R})$. Then

$$u(x) = \int_{-\infty}^{x} u'(t)\mathrm{d}t = -\int_{x}^{\infty} u'(t)\mathrm{d}t$$

Thus for all $x \in \mathbb{R}$

$$|u(x)| \leqslant \frac{1}{2}\int_{-\infty}^{\infty} |u'(t)|\mathrm{d}t$$

and therefore

$$|u(x)|^2 = |u(x)^2| \leqslant \frac{1}{2}\int_{-\infty}^{\infty} \left|\frac{d}{dt}\big(u(t)^2\big)\right|\mathrm{d}t = \int_{-\infty}^{\infty} |u'(t)||u(t)|\mathrm{d}t \leqslant \|u'\|_{L^2}\|u\|_{L^2}.$$

Thus

$$\|u\|_{L^\infty}^2 \leqslant \|u'\|_{L^2}\|u\|_{L^2} \leqslant \|u\|_{H^1}^2.$$

Moreover, $\|u\|_{L^2} \leqslant \|u\|_{H^1}$. By interpolation we therefore have for all $2 \leqslant p \leqslant \infty$

$$\|u\|_{L^p} \leqslant \max\{\|u\|_{L^2}, \|u\|_{L^\infty}\} \leqslant \|u\|_{H^1(\mathbb{R})}.$$

Now for $u \in H^1(\mathbb{R})$, then we can find a sequence $(u_n)_n \subset \mathscr{C}_c^\infty$ such that $u_n \xrightarrow{n\to\infty} u$ in $H^1(\mathbb{R})$. Moreover

$$\|u_n - u_m\|_{L^\infty(\mathbb{R})} \leqslant \|u_n - u_m\|_{H^1(\mathbb{R})} \xrightarrow{n,m\to\infty} 0.$$

Thus $(u_n)_n$ is a Cauchy sequence in L^∞, i.e $u_n \to v \in L^\infty$. However, using the implied weak convergence it follows that $u = v$.

We also have for any compact set $\Omega \subset \mathbb{R}$, $(u_n)_n$ is a Cauchy sequence in $\mathscr{C}(\Omega)$ with the supremum-norm for any compact Ω. Thus $u_n \to \varphi$ in $\mathscr{C}(\Omega)$. Thus $u\big|_\Omega = \varphi \in \mathscr{C}(\Omega)$. Since Ω was arbitrary it follows that $u \in \mathscr{C}(\mathbb{R})$.

$d = 2$: We take $u \in \mathscr{C}_c^\infty(\mathbb{R}^2)$. We first prove that

$$\|u\|_{L^2(\mathbb{R}^2)} \leqslant \|\nabla u\|_{L^1(\mathbb{R}^2)}.$$

Indeed

$$|u(x,y)| \leqslant \frac{1}{2}\int\limits_{-\infty}^{\infty} |\partial_x u(z,y)|\mathrm{d}z,$$

$$|u(x,y)| \leqslant \frac{1}{2}\int\limits_{-\infty}^{\infty} |\partial_y u(x,z')|\mathrm{d}z'.$$

Therefore,

$$|u(x,y)|^2 \leqslant \frac{1}{4}\int\limits_{-\infty}^{\infty}\int\limits_{-\infty}^{\infty} |\partial_x u(z,y)||\partial_y(x,z')|\mathrm{d}z\mathrm{d}z'.$$

Taking the x,y integrals we now get

$$\|u\|^2_{L^2(\mathbb{R}^2)} \leqslant \frac{1}{4}\int\limits_{\mathbb{R}}\int\limits_{\mathbb{R}}\int\limits_{\mathbb{R}}\int\limits_{\mathbb{R}} |\partial_x u(z,y)||\partial_y(x,z')|\mathrm{d}x\mathrm{d}y\mathrm{d}z\mathrm{d}z' \leqslant \frac{1}{4}\left(\int\limits_{\mathbb{R}^2} |\nabla u(x,y)|\mathrm{d}x\mathrm{d}y\right)^2$$

and thus

$$\|u\|_{L^2} \leqslant \|\nabla u\|_{L^1}.$$

Using $\|u\|_{L^2} \leqslant \|\nabla u\|_{L^1}$ with u replaced by u^n, $n \in \mathbb{N}$ we get

$$\begin{aligned}\int\limits_{\mathbb{R}^2} |u(\xi)|^{2n}\mathrm{d}\xi \leqslant \left(\int\limits_{\mathbb{R}^2} |\nabla(u(\xi)^n)|\mathrm{d}\xi\right)^2 = \left(\int\limits_{\mathbb{R}^2} n|\nabla u(\xi)|n|u(\xi)^{n-1}|\mathrm{d}\xi\right)^2 \leqslant \\ \leqslant n^2\left(\int |\nabla u|^2\right)\left(\int |u|^{2(n-1)}\right) \leqslant n^2(n-1)^2\left(\int |\nabla u|^2\right)^2\left(\int u^{2(n-2)}\right) \leqslant \\ \leqslant (n!)^2\|u\|^{2n}_{H^1}.\end{aligned}$$

Thus $\|u\|_{L^{2n}}(\mathbb{R}^2) \leqslant \sqrt[n]{n!}\|u\|_{H^1(\mathbb{R})}$ for all $n \in \mathbb{N}$.

For any $2 \leqslant p < \infty$, we can find $n \in \mathbb{N}$ such that $2n \leqslant p \leqslant 2(n+1)$ thus

$$\|u\|_{L^p} \leqslant \max\{\|u\|_{L^{2n}}, \|u\|_{L^{2(n+1)}}\} \leqslant \sqrt[n+1]{(n+1)!}\|u\|_{H^1(\mathbb{R}^2)},$$

i.e. $\|u\|_{L^p} \leqslant C_p\|u\|_{H^1(\mathbb{R}^2)}$. Here we cannot take $p = \infty$ because $C_p \xrightarrow{p\to\infty} \infty$.

For $u \in H^1(\mathbb{R}^2)$ we approximate it by a sequence of $\mathscr{C}_c^\infty$ functions.

q.e.d.

Remark 3.16 (Riesz-Thorin Inequality for L^p spaces)**.** For $p < q < r$ we have

$$\|u\|_{L^q} \leqslant \|u\|_{L^p}^{1-\vartheta(q)} \|u\|_{L^r}^{\vartheta(q)}$$

where $\vartheta(q) = \frac{r(q-p)}{q(r-p)}$ which can be proven using the Hölder inequality. □

Remark 3.17. Recall that weak convergence $u_n \xrightharpoonup{n\to\infty} u$ in $H^1(\mathbb{R}^d)$ means that for all $\varphi \in H^1(\mathbb{R}^d)$

$$\langle u_n, \varphi \rangle_{H^1} \xrightarrow{n\to\infty} \langle u, \varphi \rangle_{H^1}$$

where

$$\langle u, \varphi \rangle_{H^1} = \langle u, \varphi \rangle_{L^2} + \langle \nabla u, \nabla \varphi \rangle_{L^2} = \langle u, \varphi \rangle_{L^2} + \sum_{i=1}^{d} \langle \partial_{x_i} u, \partial_{x_i} \varphi \rangle_{L^2} .$$

□

Lemma 3.18. *Weak convergence $u_n \xrightharpoonup{n\to\infty} u$ in $H^1(\mathbb{R}^d)$ is equivalent to*

$$\begin{cases} u_n \xrightharpoonup{n\to\infty} u, & \text{in } L^2, \\ \partial_{x_i} u_n \xrightharpoonup{n\to\infty} \partial_{x_j} u & \text{in } L^2 \text{ for all } j = 1, \ldots, d. \end{cases}$$

□

Proof. ($\Leftarrow$) Trivial as

$$\langle u_n, \varphi \rangle_{L^2} + \langle \nabla u_n, \nabla \varphi \rangle_{L^2} \xrightarrow{n\to\infty} \langle u, \varphi \rangle_{L^2} + \langle \nabla u, \nabla \varphi \rangle_{L^2} = \langle u, \varphi \rangle_{H^1}$$

($\Rightarrow$) Define for all $\varphi \in L^2$ the functional

$$\mathscr{L}_\varphi : v \longmapsto \langle \varphi, v \rangle_{L^2} .$$

This functional is a linear and continuous map $L^2(\mathbb{R}^d) \to \mathbb{C}$ and $H^1(\mathbb{R}^d) \to \mathbb{C}$ because $\|\varphi\|_{L^2} \leqslant \|\varphi\|_{H^1}$.

Thus $u_n \rightharpoonup u$ in H^1 implies that $\mathscr{L}_\varphi(u_n) \xrightarrow{n\to\infty} \mathscr{L}_\varphi(u)$, i.e. for all $\varphi \in L^2(\mathbb{R}^d)$

$$\langle u_n, \varphi \rangle_{L^2} \xrightarrow{n\to\infty} \langle u, \varphi \rangle_{L^2}$$

Analogously $u_n \rightharpoonup u$ in H^1 implies that $\partial_{x_i} u_n \rightharpoonup \partial_{x_i} u$ in L^2.

q.e.d.

Definition 3.19 (Kernel of Operators)**.** For an operator $K : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$, we call a function $K(x,y)$ the kernel of K if for all $f \in L^2(\mathbb{R}^d)$

$$(Kf)(x) = \int_{\mathbb{R}^d} K(x,y) f(y) \mathrm{d}y.$$

□

Example 3.20.

- ***Green's Function of the Laplacian***: If $K = (-\Delta)^{-1}$ and $d = 3$ then

$$K(x,y) = \frac{1}{4\pi|x-y|}.$$

- ***Heat Kernel***: Let $K = e^{t\Delta}$, i.e.

$$\widehat{e^{t\Delta} f}(k) = e^{-t|2\pi k|^2} \hat{f}(k)$$

then

$$K(x,y) = \frac{1}{(4\pi t)^{\frac{d}{2}}} e^{-\frac{|x-y|^2}{4t}} = G(x-y).$$

This is the case as

$$\widehat{G * f}(k) = \hat{G}(k) \hat{f}(k) = e^{-t|2\pi k|^2} \hat{f}(k).$$

Lemma 3.21 (Heat Kernel)**.** *If $f \in L^2(\mathbb{R}^d)$, then for all $t > 0$*

$$e^{t\Delta} f \in H^m(\mathbb{R}^d)$$

for all $m \geqslant 1$. Moreover, if $f_n \rightharpoonup f$ weakly in $L^2(\mathbb{R}^d)$, then

$$e^{t\Delta} f_n \xrightarrow{n \to \infty} e^{t\Delta} f$$

point-wise and for any bounded set $\Omega \subset \mathbb{R}^d$

$$\mathbf{1}_\Omega e^{t\Delta} f_n \xrightarrow{n\to\infty} \mathbf{1}_\Omega e^{t\Delta} f$$

strongly in $L^2(\mathbb{R}^d)$.

$\square$

Proof. 1) If $f \in L^2$ then

$$\widehat{e^{t\Delta}f}(k) = e^{-t|2\pi k|^2}\hat{f}(k)$$

and thus for all $m \geqslant 1$

$$(1+|k|^2)^{\frac{m}{2}}\widehat{e^{t\Delta}f}(k) = (1+|k|^2)^{\frac{m}{2}}e^{-t|2\pi k|^2}\hat{f}(k) \in L^2(\mathbb{R}^d)$$

because $\hat{f} \in L^2$ and $(1+|k|^2)^{\frac{m}{2}}e^{-t|2\pi k|^2}$ is bounded. Thus $e^{t\Delta}f \in H^m(\mathbb{R}^d)$.

2)

$$\big(e^{t\Delta}f\big)(x) = \frac{1}{(4\pi t)^{\frac{d}{2}}}\int e^{-\frac{|x-y|^2}{4t}} f(y)\mathrm{d}y.$$

For all $x \in \mathbb{R}^d$ we have

$$\big(e^{t\Delta}f_n\big)(x) = \frac{1}{(4\pi t)^{\frac{d}{2}}}\int\limits_{\mathbb{R}^d} e^{-\frac{|x-y|^2}{4t}} f_n(y)\mathrm{d}y \xrightarrow{n\to\infty} \frac{1}{(4\pi t)^{\frac{d}{2}}}\int\limits_{\mathbb{R}^d} e^{-\frac{|x-y|^2}{4t}} f(y)\mathrm{d}y = \big(e^{t\Delta}f\big)(x)$$

because $f_n \rightharpoonup f$ weakly in L^2 and $e^{-\frac{|x-y|^2}{4t}} \in L^2(\mathbb{R}^d)$.

Moreover if $x \in \Omega$, for $\Omega \subset \mathbb{R}^d$ bounded, then

$$\begin{aligned}\big|e^{t\Delta}f_n(x)\big| &= \frac{1}{(4\pi t)^{\frac{d}{2}}}\left|\int\limits_{\mathbb{R}^d} e^{-\frac{|x-y|^2}{4t}} f_n(y)\mathrm{d}y\right| \leqslant \frac{1}{(4\pi t)^{\frac{d}{2}}}\left(\int\limits_{\mathbb{R}^d} e^{-\frac{|x-y|^2}{2t}}\mathrm{d}y\right)^{\frac{1}{2}}\left(\int\limits_{\mathbb{R}^d} |f_n(y)|^2\mathrm{d}y\right)^{\frac{1}{2}} \leqslant \\ &\leqslant \frac{1}{(4\pi t)^{\frac{d}{2}}}\left(\int\limits_{\mathbb{R}^d} e^{-\frac{|y|^2}{2t}}\mathrm{d}y\right)^{\frac{1}{2}} C \leqslant C_t\end{aligned}$$

as $f_n \rightharpoonup f$ and thus $\|f_n\|_{L^2}$ is bounded. Therefore for any bounded set $\mathbf{1}_\Omega$ the function

$$|e^{t\Delta}f_n(x)| \leqslant C_t\mathbf{1}_\Omega$$

is an integrable majorant independent of n. Thus as we have point-wise convergence by dominated convergence it follows that

$$\mathbf{1}_\Omega e^{t\Delta} f_n \xrightarrow{n\to\infty} \mathbf{1}_\Omega e^{t\Delta} f$$

strongly in $L^2(\mathbb{R}^d)$.

q.e.d.

Theorem 3.22 (Sobolev Embedding of $H^1(\mathbb{R}^d)$)**.** *If $u_n \xrightharpoonup{n\to\infty} u$ weakly in $H^1(\mathbb{R}^d)$, then for all $\Omega \subset \mathbb{R}^d$ bounded, $\mathbf{1}_\Omega u_n \xrightarrow{n\to\infty} \mathbf{1}_\Omega u$ strongly in $L^p(\mathbb{R}^d)$ for*

$$\begin{cases} 2 \leqslant p < \frac{2d}{d-2}, & \text{if } d \geqslant 3, \\ 2 \leqslant p < \infty, & \text{if } d = 2, \\ 2 \leqslant p \leqslant \infty & \text{if } d = 1. \end{cases}$$

This means that the embedding $\mathbf{1}_\Omega L^1(\mathbb{R}^d) \subset \mathbf{1}_\Omega L^p(\mathbb{R}^d)$ is compact □

Proof. First we prove that $\mathbf{1}_\Omega u_n \to \mathbf{1}_\Omega u$ strongly in $L^2(\mathbb{R}^d)$ using the heat kernel:

$$\mathbf{1}_\Omega u_n - \mathbf{1}_\Omega u = \mathbf{1}_\Omega\big(u_n - e^{t\Delta}u_n\big) + \mathbf{1}_\Omega\big(e^{t\Delta}u_n - e^{t\Delta}u\big) + \mathbf{1}_\Omega\big(e^{t\Delta}u - u\big)$$

and thus

$$\|\mathbf{1}_\Omega u_n - \mathbf{1}_\Omega u\|_{L^2} \leqslant \big\|\mathbf{1}_\Omega\big(u_n - e^{t\Delta}u_n\big)\big\|_{L^2} + \big\|\mathbf{1}_\Omega\big(e^{t\Delta}u_n - e^{t\Delta}u\big)\big\|_{L^2} + \big\|\mathbf{1}_\Omega\big(e^{t\Delta}u - u\big)\big\|_{L^2}.$$

Note that

$$\big\|\mathbf{1}_\Omega\big(e^{t\Delta}u - u\big)\big\|_{L^2}^2 \leqslant \big\|e^{t\Delta}u - u\big\|_{L^2}^2 = \Big\|\widehat{e^{t\Delta}u} - \hat{u}\Big\|_{L^2}^2 = \int\limits_{\mathbb{R}^d} \Big|1 - e^{-t|2\pi k|^2}\Big| |\hat{u}(k)|^2 \mathrm{d}k$$

and

$$0 \leqslant 1 - e^{-t|2\pi k|^2} \leqslant \min\big\{t|2\pi k|^2, 1\big\} \quad \therefore \quad \Big|1 - e^{-t|2\pi k|^2}\Big| \leqslant \min\big\{t|2\pi k|^2, 1\big\} \leqslant t|2\pi k|^2.$$

Thus

$$\big\|\mathbf{1}_\Omega\big(e^{t\Delta}u - u\big)\big\|_{L^2}^2 \leqslant \int\limits_{\mathbb{R}^d} t|2\pi k|^2 |\hat{u}(k)|^2 \mathrm{d}k = t\|\nabla u\|_{L^2}^2 \leqslant t\|u\|_{H^1}^2.$$

Therefore we have

$$\|\mathbf{1}_\Omega(u_n - u)\|_{L^2} \leqslant C\sqrt{t} + \left\|\mathbf{1}_\Omega\left(e^{t\Delta}u_n - e^{t\Delta}u\right)\right\|_{L^2}.$$

By strong convergence the last term converges to 0 as $n \to \infty$ thus

$$\limsup_{n\to\infty} \|\mathbf{1}_\Omega(u_n - u)\|_{L^2} \leqslant C\sqrt{t} \xrightarrow{t\downarrow 0} 0$$

which proves the strong convergence $\mathbf{1}_\Omega u_n \xrightarrow{n\to\infty} \mathbf{1}_\Omega u$.
The strong convergence in L^p with L^p with $2 \leqslant p < \frac{2d}{d-2} =: p^*$ follows by interpolation. Note that we proved in Exercise 2.4. (i) that if $f_n \to f$ strongly in $L^2(\mathbb{R}^d)$ and $\|f_n\|_{L^{p^*}}$ is bounded for $p^* > 2$ (which follows by the Sobolev inequality, weak convergence and the uniform boundedness principle) then $f_n \to f$ strongly in $L^p(\mathbb{R}^d)$ for all $2 \leqslant p < p^*$.
In the case $d = 1$, we have to prove that

$$\|\mathbf{1}_\Omega u_n - \mathbf{1}_\Omega u\|_{L^\infty} \xrightarrow{n\to\infty} 0.$$

First we prove that $u_n(x) \to u(x)$ pointwise. Since $\mathbf{1}_\Omega u_n \to \mathbf{1}_\Omega u$ in L^2 we can find a subsequence such that this holds. In fact, this is already true for the original sequence because

$$u(y) - u(x) = \int_x^y u'(t)\mathrm{d}t$$

Therefore, if $u_n(x_0) \to u(x_0)$ then

$$u_n(y) - u_n(x_0) = \int_{x_0}^y u_n'(t)\mathrm{d}t \xrightarrow{n\to\infty} \int_{x_0}^y u'(t)\mathrm{d}t = u(y) - u(x_0)$$

as $\mathbf{1}_{[x_0,y]} \in L^2(\mathbb{R}^d)$. Thus for all $u_n(y) \to u(y)$ for all $y \in \mathbb{R}$.
From $u(y) - u(x) = \int_x^y u'(t)\mathrm{d}t$ we have

$$|u(y) - u(x)| \leqslant \left|\int_x^y \mathrm{d}t\right|^{\frac{1}{2}} \left|\int_x^y |u'(t)|\mathrm{d}t\right|^{\frac{1}{2}} \leqslant \sqrt{|x-y|}\|u\|_{H^1}$$

and

$$|u_n(y) - u_n(x)| \leqslant \sqrt{|x-y|}\|u_n\|_{H^1} \leqslant C\sqrt{|x-y|}$$

Now we conclude that $\sup_{x\in\Omega}|u_n(x)-u(x)| \to 0$ for any bounded set $\Omega \subset \mathbb{R}$. Assume that $\sup_{x\in\Omega}|u_n(x)-u(x)| \not\to 0$. Then there exists a $\delta > 0$ and a subsequence $(u_{n_k})_k$ and a sequence $(x_k)_k \subset \Omega$ such that

$$|u_{n_k}(x_k) - u(x_k)| \geqslant \delta > 0$$

for all $k \in \mathbb{N}$. Because $(x_k)_k \subset \Omega$ is bounded, we can descend to a subsequence, and assume that $x_k \xrightarrow{k\to\infty} x_\infty$. Thus

$$\begin{aligned}|u_{n_k}(x_k) - u(x_k)| &\leqslant |u_{n_k}(x_k) - u_k(x_\infty)| + |u_{n_k}(x_\infty) - u(x_\infty)| + |u(x_\infty) - u(x_k)| \leqslant \\ &\leqslant C\sqrt{|x_k - x_\infty|} + |u_n(x_\infty) - u(x_\infty)|\end{aligned}$$

and therefore

$$\lim_{n\to\infty} |u_n(x_n) - u(x_n)| \leqslant 0$$

which is a contradiction. Thus we conclude that

$$\sup_{x\in\Omega} |u_n(x) - u(x)| \xrightarrow{n\to\infty} 0.$$

q.e.d.

Theorem 3.23 (Sobolev Inequality and Embeddings for $H^s(\mathbb{R}^d)$)**.** *For any $s \geqslant 1$*

1)

$$\|f\|_{H^s} \geqslant C\|f\|_{L^p}$$

for all

$$\begin{cases} 2 \leqslant p \leqslant \frac{2d}{d-2s}, & \text{if } 2s < d \\ 2 \leqslant p < \infty, & \text{if } 2s = d \\ 2 \leqslant p \leqslant \infty, & \text{if } 2s > d \end{cases}$$

In particular, if $2s > d$, then $H^s(\mathbb{R}^d) \subset \mathscr{C}(\mathbb{R}^d)$, e.g. $H^2(\mathbb{R}^3) \subset \mathscr{C}(\mathbb{R}^3)$.

2) If $f_n \rightharpoonup f$ weakly in $H^s(\mathbb{R}^d)$, then for all $\Omega \subset \mathbb{R}^d$ bounded

$$\mathbf{1}_\Omega f_n \xrightarrow{n\to\infty} \mathbf{1}_\Omega f$$

strongly in $L^p(\mathbb{R}^d)$ *for all*

$$\begin{cases} 2 \leqslant p < \frac{2d}{d-2s}, & \textit{if } 2s < d \\ 2 \leqslant p < \infty, & \textit{if } 2s = d \\ 2 \leqslant p < \infty, & \textit{if } 2s > d \end{cases}$$

□

Sketch of Proof. 1) The fact that

$$\|f\|_{H^s} \geqslant C\|f\|_{L^p}$$

if $p = \frac{2d}{d-2s}$ if $2s < d$ follows from the Hardy-Littlewood-Sobolev inequality (Exericse).

Now let us focus on $2s > d$. We prove that

$$\|f\|_\infty \leqslant C\|f\|_{H^s(\mathbb{R}^d)}.$$

We can write

$$|f(x)| \leqslant \left|\int e^{2\pi i k\cdot x}\hat{f}(k)\mathrm{d}k\right| \leqslant \left(\int_{\mathbb{R}^d} |\hat{f}(k)|^2\left(1+|k|^2\right)^s \mathrm{d}k\right)^{\frac{1}{2}} \underbrace{\left(\int_{\mathbb{R}^d} \frac{\left|e^{2\pi i k\cdot x}\right|}{(1+|k|^2)^s}\mathrm{d}k\right)^{\frac{1}{2}}}_{\substack{<\infty \\ \text{if } 2s>d}} \leqslant$$

$$\leqslant C\|f\|_{H^s}.$$

Next, we prove that $H^s(\mathbb{R}^d) \subset \mathscr{C}\left(\mathbb{R}^d\right)$. We have

$$|f(x) - f(x')| = \left|\int_{\mathbb{R}^d} \left(e^{2\pi i k\cdot x} - e^{2\pi i k\cdot x'}\right)\hat{f}(k)\mathrm{d}k\right| \leqslant$$

$$\leqslant \left(\int_{\mathbb{R}^d} |\hat{f}(k)|^2\left(1+|k|^2\right)^s \mathrm{d}k\right)^{\frac{1}{2}} \left(\int_{\mathbb{R}^d} \frac{\left|e^{2\pi i k\cdot x} - e^{2\pi i k\cdot x'}\right|}{(1+|k|^2)^s}\mathrm{d}k\right)^{\frac{1}{2}}.$$

Note that

$$\left|e^{2\pi i k\cdot x} - e^{2\pi i k\cdot x'}\right| \leqslant \min\{|2\pi k||x-x'|, 1\}$$

and therefore

$$\left|e^{2\pi ik\cdot x} - e^{2\pi ik\cdot x'}\right|^2 \leqslant C_\varepsilon |k|^\varepsilon |x-x'|^\varepsilon$$

for all $\varepsilon > 0$ small enough. Thus

$$|f(x) - f(x')| \leqslant C_\varepsilon \|f\|_{H^s} \left(\int\limits_{\mathbb{R}^d} \frac{|k|^\varepsilon |x-x'|^\varepsilon}{(1+|k|^2)^s} \mathrm{d}k\right)^{\frac{1}{2}} \leqslant C_\varepsilon |x-x'|^{\frac{\varepsilon}{2}}$$

if $\varepsilon - 2s < -d$ which is equivalent to $\varepsilon < 2s - d$, i.e. for all such ε

$$\sup_{x\neq x'} \frac{|f(x)-f(x')|}{|x-x'|^{\frac{\varepsilon}{2}}} < C_\varepsilon$$

2) For the proof of the embedding $\mathbf{1}_\Omega f_n \to \mathbf{1}_\Omega f$ in L^p, the only difficult part is the L^∞ convergence when $2s > d$.

For the pointwise convergence $f_n \rightharpoonup f$ in $H^s(\mathbb{R}^d)$, then $f_n(x) \to f(x)$ for all $x \in \mathbb{R}^d$.

$$\begin{aligned}
|f_n(x) - f(x)| &= \left|\int\limits_{\mathbb{R}^d} e^{2\pi ik\cdot x}\Big(\hat{f}_n(k) - \hat{f}(k)\Big)\mathrm{d}k\right| \leqslant \\
&\leqslant \left|\int\limits_{|k|\leqslant K} e^{2\pi ik\cdot x}\Big(\hat{f}_n - \hat{f}\Big)\mathrm{d}k\right| + \int\limits_{|k|\geqslant K} |\hat{f}_n(k) - \hat{f}(k)|\mathrm{d}k \leqslant \\
&\leqslant \left|\int\limits_{|k|\leqslant K} \cdots\right| + \left(\int |\hat{f}_n(k) - \hat{f}(k)|^2 \big(1+|k|^2\big)^s \mathrm{d}k\right)^{\frac{1}{2}} \left(\int\limits_{|k|\geqslant K} \frac{1}{(1+|k|^2)^s}\mathrm{d}k\right)^{\frac{1}{2}} \leqslant \\
&\leqslant \left|\int\limits_{|k|\leqslant K} \cdots\right| + \frac{c_\varepsilon}{K^\varepsilon}
\end{aligned}$$

for some $\varepsilon > 0$. Letting $n \to \infty$ the first term vanishes as $\hat{f}_n \rightharpoonup \hat{f}$ weakly and letting $K \to \infty$ the second one does as well.

q.e.d.

Remark 3.24. 1) The kernel $K = (-\Delta)^{-1}$, $K(x,y) = \frac{1}{4\pi|x-y|}$ in $\mathbb{R}^3$ appears in physical applications as the potential $x \mapsto \frac{1}{|x|}$, for example in Coulomb's law

$$\frac{Z_1 Z_2}{|x-y|}$$

and Newton's law of Gravitation

$$\frac{m_1 m_2}{|x-y|}.$$

Recall that $\Delta\left(\frac{1}{|x|}\right) = 0$ for any $x \neq 0$ in $\mathbb{R}^3$. More generally, if $\Delta u = 0$ on $\Omega \subset \mathbb{R}^d$ then we call u a ***harmonic function*** on Ω.

□

Theorem 3.25 (Harmonic Functions). *1) If $\Delta u = 0$ on $\Omega \subset \mathbb{R}^d$ open, then*

$$\frac{1}{|B_r(x)|} \int\limits_{B(x,r)} u(y)\mathrm{d}y = u(x) = \frac{1}{|S(x,r)|} \int\limits_{|x-y|=r} u(y)\mathrm{d}y.$$

for for all balls and spheres such that $B(x,r), S(x,r) \subset \Omega$ This called the ***mean-value theorem*** *for harmonic functions.*

2) On $\mathbb{R}^3$, if f is a radially symmetric function, i.e. $f(Rx) = f(x)$ for all $R \in SO(3)$, then

$$\int\limits_{\mathbb{R}^3} \frac{f(y)}{|x-y|}\mathrm{d}y = \int\limits_{\mathbb{R}^3} \frac{f(y)}{\max\{|x|,|y|\}}\mathrm{d}y.$$

This result is called ***Newton's Theorem****.*

□

Remark 3.26. 1) If u is harmonic on Ω, then $u \in \mathscr{C}^\infty(\Omega)$, which we shall not prove. However, this means that it makes sense to talk about the values of u at a point.

2) Newton's theorem can be used with $f(x)$ replaced by a measure $\mathrm{d}\mu(x)$ as well.

3) It also implies that if $\operatorname{supp} f \subset B_r(0)$ and $|x| > r$ then

$$\int\limits_{\mathbb{R}^3} \frac{f(y)}{|x-y|}\mathrm{d}y = \frac{1}{|x|} \int\limits_{\mathbb{R}^3} f(y)\mathrm{d}y.$$

□

Proof. 1) By Stokes's theorem we have

$$0 = \int\limits_{B(x,r)} \Delta u(y)\mathrm{d}y = \int\limits_{S(x,r)} \nabla u(y)\cdot \boldsymbol{n}\mathrm{d}y$$

where $\boldsymbol{n}$ is the unit normal vector to the point on $y \in S(x,r)$. By a change of variables we have

$$\int\limits_{S(x,r)} \nabla u(y)\cdot \boldsymbol{n}\mathrm{d}y = r^{d-1} \int\limits_{S(0,1)} \nabla u(x+r\omega)\cdot \omega \mathrm{d}\omega \quad \therefore$$

$$\therefore \quad 0 = \int\limits_{S(0,1)} \frac{d}{dr}(u(x+r\omega))\mathrm{d}\omega = \frac{d}{dr}\int\limits_{S(0,1)} u(x+r\omega)\mathrm{d}\omega.$$

This means that the value of the integral is independent of r, and thus

$$\int\limits_{S(x,r)} u(y)\mathrm{d}y = r^{d-1}\int\limits_{S(0,1)} u(x+r\omega)\mathrm{d}\omega = r^{d-1}\int\limits_{S(0,1)} u(x)\mathrm{d}\omega = u(x)r^{d-1}S(0,1) =$$
$$= u(x)S(x,r)$$

which proves the second equality. The first follows immediately from integration over r.

2) Exercise!

q.e.d.

Theorem 3.27. *If $f \in H^1(\mathbb{R}^d)$, then $|f| \in H^1(\mathbb{R}^d)$ and*

$$\nabla|f|(x) = \begin{cases} \frac{\Re f \nabla \Re f + \Im f \nabla \Im f}{|f|}, & \text{if } f(x) \neq 0, \\ 0, & \text{if } f(x) = 0. \end{cases}$$

Consequently we have $|\nabla f(x)| \geqslant |\nabla|f|(x)|$ for a.e. x. □

Proof. Take $f_n \in \mathscr{C}_c^\infty$ such that $f_n \to f$ in $H^1(\mathbb{R}^d)$ and where we assume that f_n and ∇f_n converge also pointwise a.e. x. Write $f_n = u_n + iv_n$, and define $G_n(x) = \sqrt{\frac{1}{n^2} + |u_n(x)|^2 + |v_n(x)|^2} - \frac{1}{n}$. Note that

$$G_n(x) \xrightarrow{n\to\infty} \sqrt{|u(x)|^2 + |v(x)|^2}$$

pointwise. Thus

$$\nabla G_n(x) = \frac{2u_n \nabla u_n + 2v_n \nabla v_n}{2\sqrt{\frac{1}{n^2} + |u_n(x)|^2 + |v_n(x)|^2}} \xrightarrow{n\to\infty} \frac{u(x)\nabla u(x) + v(x)\nabla v(x)}{|f(x)|}$$

pointwise if $f(x) \neq 0$.

????Other case????

We actually have L^2 convergence by dominated convergence as

$$\begin{aligned} |G_n(x)| = \sqrt{\frac{1}{n^2} + |u_n(x)|^2 + |v_n(x)|^2} - \frac{1}{n} &= \frac{|u_n(x)|^2 + |v_n(x)|^2}{\sqrt{\frac{1}{n^2} + |u_n(x)|^2 + |v_n(x)|^2} + \frac{1}{n}} \leqslant \\ &\leqslant \sqrt{|u_n(x)|^2 + |v_n(x)|^2} = |f_n(x)| \leqslant F(x) \in L^2(\mathbb{R}^d). \end{aligned}$$

The existence of F follows from Remark 1.10. Thus $G_n \to |f|$ strongly in $L^2(\mathbb{R}^d)$. Moreover, by the Cauchy-Schwarz inequality we have

$$\begin{aligned} |\nabla G_n(x)| = \left| \frac{u_n \nabla u_n + v_n \nabla v_n}{\sqrt{\frac{1}{n^2} + |u_n|^2 + |v_n|^2}} \right| &\leqslant \frac{\sqrt{|u_n|^2 + |v_n|^2}\sqrt{|\nabla u_n|^2 + |\nabla v_n|^2}}{\sqrt{\frac{1}{n^2} + |u_n|^2 + |v_n|^2}} \leqslant \\ &\leqslant \sqrt{|\nabla u_n|^2 + |\nabla v_n|^2} = |\nabla f_n| \leqslant \widetilde{F}(x) \in L^2(\mathbb{R}^d). \end{aligned}$$

Thus we have

$$\nabla G_n(x) \xrightarrow{n\to\infty} \nabla G = \begin{cases} \frac{\Re f \nabla \Re f + \Im f \nabla \Im f}{|f|}, & \text{if } f(x) \neq 0, \\ 0, & \text{if } f(x) = 0. \end{cases}$$

strongly in $L^2(\mathbb{R}^d)$. Thus $|f| \in H^1(\mathbb{R}^d)$ with $G(x) = \nabla |f|(x)$. *q.e.d.*

Proposition 3.28. *If $(f_n)_n \subset H^1(\mathbb{R}^d)$ s.t. $f_n \to f$ in $L^2(\mathbb{R}^d)$ and $\nabla f_n \to F$ in $L^2(\mathbb{R}^d)$, then $f \in H^1(\mathbb{R}^d)$, and $\nabla f = F$.* □

Proof. Exercise! *q.e.d.*

3.3 Application of Sobolev Embedding

Recall the Hydrogen energy functional

$$\mathcal{E}(u) = \int_{\mathbb{R}^3} |\nabla u|^2 - \int_{\mathbb{R}^3} \frac{|u(x)|}{|x|} \mathrm{d}x$$

for $u \in H^1(\mathbb{R}^3)$, $\|u\|_{L^2} = 1$.

Theorem 3.29. *There exists a minimiser for $\mathcal{E}(u)$ in $H^1(\mathbb{R}^3)$.* □

Proof. Recall that

$$\mathcal{E}(u) = \frac{1}{2}\int_{\mathbb{R}^3} |\nabla u|^2 + \underbrace{\frac{1}{2}\int_{\mathbb{R}^3} |\nabla u|^2 - \int_{\mathbb{R}^3} \frac{|u(x)|}{|x|} \mathrm{d}x}_{\geqslant -C} \geqslant \frac{1}{2}\int_{\mathbb{R}^3} |\nabla u|^2 - C$$

Thus $\mathcal{E}(u)$ is bounded from below, and if $(u_n)_n$ is a minimising sequence

$$\mathcal{E}(u_n) \xrightarrow{n\to\infty} E := \inf\left\{\mathcal{E}(u) \,\middle|\, u \in H^1(\mathbb{R}^3), \|u\|_{L^2} = 1\right\}$$

then $(u_n)_n$ is bounded in $H^1(\mathbb{R}^3)$. By the Sobolev embedding theorem we can pass to a subsequence and assume that $u_n \rightharpoonup u_0$ in $H^1(\mathbb{R}^3)$ and $\mathbf{1}_\Omega u_n \to \mathbf{1}_\Omega u_0$ strongly in $L^p(\mathbb{R}^3)$ for all $2 \leqslant p < 6$.

In particular we have $u_n \rightharpoonup u_0$ and $\nabla u_n \rightharpoonup \nabla u_0$, hence

$$\liminf_{n\to\infty} \int |\nabla u_n|^2 \geqslant \int |\nabla u_0|^2.$$

Using strong convergence on bounded sets we have

$$\int \frac{|u_n(x)|^2}{|x|} \mathrm{d}x \xrightarrow{n\to\infty} \int \frac{|u(x)|^2}{|x|} \mathrm{d}x$$

which is left as an exercise. Thus we have

$$E = \liminf_{n\to\infty} \mathcal{E}(u_n) \geqslant \mathcal{E}(u_0).$$

To say that u_0 is a minimiser for $\mathcal{E}$ it is therefore enough to show that $\|u_0\|_{L^2} = 1$. Here we know that $u_n \rightharpoonup u_0$ in L^2, thus

$$1 = \liminf_{n\to\infty} \|u_n\|_{L^2} \geqslant \|u_0\|_{L^2}$$

Assume that $\|u_0\|_{L^2} = \lambda < 1$. Then we have $E \geqslant 0$ for

($\lambda = 0$) $u_0 = 0$ and thus $E = \mathcal{E}(u_0) = 0$

($\lambda > 0$) Then

$$E = \mathcal{E}(u_0) = \lambda^2 \mathcal{E}\Big(\frac{u_0}{\lambda}\Big) \geqslant \lambda^2 E \quad \therefore \quad E \geqslant 0$$

for $0 < \lambda^2 < 1$. However, we have $E < 0$ which is a contradiction, i.e. $\|u_0\|_{L^2} = 1$ and u_0 is a minimiser for $\mathcal{E}$.

To see this, take $\varphi \in \mathscr{C}_c^\infty(\mathbb{R}^3)$, $\|\varphi\|_{L^2} = 1$, $\varphi_\ell(x) = \ell^{\frac{3}{2}}\varphi(\ell x)$, $\|\varphi_\ell\|_{L^2} = 1$ we have

$$\mathcal{E}(\varphi_\ell) = \int \Big(|\nabla \varphi_\ell(x)|^2 - \frac{|\varphi_\ell(x)|^2}{|x|}\Big) \mathrm{d}x = \ell^2 \underbrace{\int |\nabla\varphi|^2}_{>0} - \ell \underbrace{\int \frac{|\varphi(x)|^2}{|x|} \mathrm{d}x}_{>0} < 0$$

if $\ell > 0$ is small enough.

q.e.d.

Remark 3.30. In general, if V is a “nice enough” potential such that

$$E = \inf\Big\{\int |\nabla u|^2 + \int V(x)|u(x)|^2 \mathrm{d}x \;\Big|\; u \in H^1(\mathbb{R}^d), \|u\|_{L^2} = 1\Big\}$$

satisfies $-\infty < E < 0$, then a minimiser of $\mathcal{E}$ exists. □

Chapter 4

Spectral Theorem

Let $\mathscr{H}$ be a separable Hilbert space.

Definition 4.1.
- A linear operator $A : \mathscr{H} \to \mathscr{H}$ is called bounded if for a bounded set $B \subset \mathscr{H}$, $A(B)$ is bounded.
- A linear operator $A : \mathscr{H} \to \mathscr{H}$ is called compact $\overline{A(B)}$ is compact in $\mathscr{H}$, if B is bounded in $\mathscr{H}$.

$\square$

Example 4.2. The inclusion $H^1(\mathbb{R}^d) \subset L^2(\mathbb{R}^d)$ is trivial a bounded map.
For $\mathbf{1}_\Omega H^1(\mathbb{R}^d) \subset \mathbf{1}_\Omega L^2(\mathbb{R}^d)$ for a bounded Ω, then the inclusion map $H^1 \to L^2$ is even compact.

Lemma 4.3. *Let A be a linear operator $\mathscr{H} \to \mathscr{H}$. Then*

1) *A is bounded iff $x_n \xrightarrow{n\to\infty} x$ strongly implies that $Ax_n \xrightarrow{n\to\infty} Ax$ strongly.*
2) *A is compact iff $x_n \xrightharpoonup{n\to\infty} x$ weakly implies that $Ax_n \xrightarrow{n\to\infty} Ax$ strongly.*

$\square$

Proof. 1) Exercise.

2) Assume that A is a compact operator. If $x \rightharpoonup x$ weakly, then we know that $(x_n)_n$ is bounded in $\mathscr{H}$ by the uniform boundedness principle. By definition $\overline{(Ax_n)_n}$ is compact

in $\mathscr{H}$. This means that there is a subsequence $(Ax_{n_k})_k$ converging to some y in $\mathscr{H}$. We need to show that $y = Ax$. In fact, as A is bounded it follows that $Ax_n \xrightarrow{n\to\infty} Ax$[1], hence it follows that $y = Ax$ and therefore $Ax_{n_k} \xrightarrow{k\to\infty} Ax$ strongly.

The convergence holds actually for the whole sequence. To see this suppose that $Ax_n \not\to Ax$ for the whole sequence. Then there exists a subsequence $(Ax_{n_\ell})_\ell$ such that for some $\varepsilon > 0$ for all $\ell \in \mathbb{N}$

$$\|Ax_{n_\ell} - Ax\| \geqslant \varepsilon > 0.$$

But by the same argument we may find a subsequence of this subsequence that converges to Ax which is a contradiction.

The converse is trivial.

q.e.d.

Definition 4.4. Let A be a bounded operator then

$$\|A\| = \sup_{\|x\|\leqslant 1} \|Ax\| = \sup_{x\neq 0} \frac{\|Ax\|}{\|x\|} < \infty.$$

and there exists a bounded operator $A^* : \mathscr{H} \to \mathscr{H}$ such that for all $x, y \in \mathscr{H}$

$$\langle x, Ay\rangle = \langle A^*x, y\rangle .$$

A^* is called the ***adjoint*** of A. We call A ***self-adjoint*** $A = A^*$ $\square$

Remark 4.5. The existence of A^* follows from the Riesz representation theorem. Since

$$y \longmapsto \langle x, Ay\rangle$$

is a bounded linear functional there exists a unique z such that $\langle z, y\rangle = \langle x, Ay\rangle$ for all $y \in \mathscr{H}$. We define $A^*x =: z$.
From $\langle x, Ay\rangle = \langle A^*x, y\rangle$ for all $x, y \in \mathscr{H}$ we see that A^* is linear. Moreover, A^* is

[1] This is the case as for each $y \in \mathscr{H}$ $\langle y, A\cdot\rangle$ is a bounded functional with norm smaller or equal to $\|y\|\|A\|$. Thus there exists a $\varphi \in \mathscr{H}$ such that $\langle \varphi, \cdot\rangle = \langle y, A\cdot\rangle$ and therefore as $\langle \varphi, x_n\rangle \to \langle \varphi, x\rangle$ the assertion follows.

bounded, in fact

$$\|A^*\| = \sup_{\|x\|\leqslant 1} \|A^*x\| = \sup_{\|x\|\leqslant 1}\sup_{\|y\|\leqslant 1} |\langle x, A^*y\rangle| = \sup_{\|y\|\leqslant 1}\sup_{\|x\|\leqslant 1} |\langle x, Ay\rangle| = \sup_{\|y\|\leqslant 1} \|Ay\| = \|A\|.$$

□

Proposition 4.6. *Let $A : \mathscr{H} \to \mathscr{H}$ be a bounded operator. Then*

$$A = A^* \iff \forall x \in \mathscr{H} : \langle x, Ax\rangle \in \mathbb{R}$$

□

Theorem 4.7 (Spectral Theorem for Compact Operator)**.** *Let $A : \mathscr{H} \to \mathscr{H}$ be a compact operator.*

1) If $A = A^*$, then there exist a sequence of eigenvalues $(\lambda_n)_n \subset \mathbb{R}$ and an orthonormal basis of eigenvectors $(u_n)_n \subset \mathscr{H}$ of A such that

$$A = \sum_{n=1}^{\infty} \lambda_n |u_n\rangle \langle u_n|$$

where $|\lambda_n| \geqslant |\lambda_{n+1}|$ and $\lambda_n \xrightarrow{n\to\infty} 0$.

2) In general, if A is not self-adjoint, then there exists a sequence of eigenvalues $(\lambda_n)_n \subset \mathbb{C}$ and orthonormal bases $(u_n)_n, (v_n)_n \subset \mathscr{H}$ such that

$$A = \sum_{n=1}^{\infty} \lambda_n |u_n\rangle \langle v_n|.$$

In both cases the convergence of the series of operators is taken w.r.t. the operator norm. □

Remark 4.8. If $A = A^*$ is compact, then all non-zero eigenvalues are of finite multiplicity.

If $\mathscr{H}$ is finite dimensional, then A can be regarded as a (finite) matrix. For matrices we know that if $A^* = A$, then there exists a unitary matrix U such that

$$U^*AU = \text{diagonal matrix} = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & & \\ \vdots & & \ddots & \\ 0 & & & \lambda_n \end{pmatrix}$$

with $\{\lambda_1, \dots, \lambda_n\}$ being the eigenvalues of A with "eigenfunctions"

$$U^* \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}.$$

$\square$

Proof. 1) Assume that $A = A^*$.

Step 1 Consider

$$\sup_{\|u\|=1} |\langle u, Au\rangle|.$$

We claim that there exists an optimiser for this supremum. To prove this take an optimising sequence $(\varphi_n)_n$ such that $\|\varphi_n\| = 1$ and

$$|\langle \varphi_n, A\varphi_n\rangle| \xrightarrow{n\to\infty} \sup_{\|u\|=1} |\langle u, Au\rangle|$$

Because $\|\varphi_n\| = 1$ this sequence is bounded, we can descend to a subsequence and assume that $\varphi_n \xrightharpoonup{n\to\infty} u_1$ weakly. Because A is compact, it follows that $A\varphi_n \to Au_1$ strongly. Thus

$$\langle \varphi_n, A\varphi_n\rangle \xrightarrow{n\to\infty} \langle u_1, Au_1\rangle .$$

This holds because, if $x_n \rightharpoonup x$ weakly and $y_n \to y$ strongly, then

$$\langle x_n, y_n\rangle \longrightarrow \langle x, y\rangle .$$

The proof of this is left as an exercise.

Thus $|\langle u_1, Au_1\rangle| = \sup_{\|u\|=1} |\langle u, Au\rangle|$. We only know that $\|u_1\| \leqslant \liminf_{n\to\infty} \|\varphi_n\| = 1$. To prove that $\|u_1\| = 1$ assume that $\|u_1\| < 1$. This would imply that $\langle u, Au\rangle = 0$ for all $u \in \mathscr{H}$. Hence $Au = 0$ for all $u \in \mathscr{H}$, i.e. $A \equiv 0$[2]. In particular this would mean that any $u \in \mathscr{H}$ is an optimiser.

This means that there exists a $u_1 \in \mathscr{H}$ such that $\|u_1\| = 1$ and

$$|\langle u_1, Au_1\rangle| = \sup_{\|u\|=1} |\langle u, Au\rangle|$$

Since $\langle u_1, Au_1\rangle$ may either be positive or negative we have the two cases

$$\begin{cases} \langle u_1, Au_1\rangle = \inf_{\|u\|=1} \langle u, Au\rangle \\ \langle u_1, Au_1\rangle = \sup_{\|u\|=1} \langle u, Au\rangle \end{cases}$$

Thus u_1 is an eigenvector of A, i.e.

$$Au_1 = \lambda u_1, \qquad \lambda_1 = \langle u_1, Au_1\rangle .$$

which is left as an exercise.

Step 2 Define $V_1 = \overline{\operatorname{span}\{u_1\}} = \left\{\lambda u_1 \,\middle|\, \lambda \in \mathbb{C}\right\}$ and write $\mathscr{H} = V_1 \oplus V_1^\perp$.

Because $Au_1 = \lambda u_1$ it follows that $A : V_1 \to V_1$ and $A : V_1^\perp \to V_1^\perp$. In fact, if $\varphi \in V_1^\perp$ then $\langle \varphi, u_1\rangle = 0$ and thus

$$\langle A\varphi, u_1\rangle = \langle \varphi, Au_1\rangle = \lambda_1 \langle \varphi, u_1\rangle = 0 \quad \therefore \quad A\varphi \in V_1^\perp.$$

Now consider the restricted operator $A : V_1^\perp \to V_1^\perp$. Using the previous step with $\mathscr{H}$ replaced by $V_1^\perp$, we can find a $u_2 \in V_1^\perp$ such that $\|u_2\| = 1$ and

$$|\langle u_2, Au_2\rangle| = \sup_{\substack{u\in V_1^\perp \\ \|u\|=1}} |\langle u, Au\rangle|$$

and $Au_2 = \lambda_2 u_2$, $\lambda_2 = \langle u_2, Au_2\rangle$. Further we also have $|\lambda_1| \geqslant |\lambda_2|$.

Next, define $V_2 = \overline{\operatorname{span}\{u_1, u_2\}}$ and write $\mathscr{H} = V_2 \oplus V_2^\perp$. Then we have $A : V_2^\perp \to$

[2] This is the case as otherwise $\frac{|\langle u_1, Au_1\rangle|}{\|u_1\|^2} \leqslant \sup_{\|u\|=1} |\langle u, Au\rangle| = |\langle u_1, Au_1\rangle| < \frac{\langle u_1, Au_1\rangle|}{\|u_1\|^2}$.

$V_2^\perp$ and we can repeat the argument to find a $u_3 \in V_2^\perp$, $\|u_3\| = 1$ such that

$$|\langle u_3, Au_3\rangle| = \sup_{\substack{u \in V_2^\perp \\ \|u\|=1}} |\langle u, Au\rangle|$$

and $Au_3 = \lambda_3 u_3$, $\lambda_3 = \langle u_3, Au_3\rangle$ and $|\lambda_2| \geqslant |\lambda_3|$.

Then by induction there exists a sequence $(u_n)_n \subset \mathscr{H}$ of orthonormal vectors and $(\lambda_n)_n \subset \mathbb{R}$ such that for all $n \in \mathbb{N}$, $Au_n = \lambda_n u_n$ and

$$|\lambda_n| = |\langle u_n, Au_n\rangle| = \sup_{\substack{u \perp u_1, \dots, u_{n-1} \\ \|u\|=1}} |\langle u, Au\rangle|.$$

The sequence $\lambda_n \xrightarrow{n\to\infty} 0$ and as $(u_n)_n$ is an orthonormal family and thus converges weakly to 0. Therefore $Au_n \to 0$ strongly and therefore

$$\lim_{n\to\infty} |\lambda_n| = \lim_{n\to\infty} |\langle u_n, Au_n\rangle| = 0$$

Step 3 We have to prove that $(u_n)_n$ can be extended to be a basis of $\mathscr{H}$. Suppose that $\varphi \perp (u_n)_{n\in\mathbb{N}}$, then $\varphi \in \ker A$, i.e. $A\varphi = 0$. Indeed, for all $n \in \mathbb{N}$

$$|\langle \varphi, A\varphi\rangle| \leqslant |\langle u_n, Au_n\rangle| = |\lambda_n| \xrightarrow{n\to\infty} 0.$$

This means that $\langle \varphi, A\varphi\rangle = 0$ for all $\varphi \in V_\infty^\perp$, where $V_\infty := \overline{\operatorname{span}(u_n)_n}$. Thus $A\varphi = 0$ hence $V_\infty^\perp \subset \ker A$.

Taking an orthonormal basis $(v_n)_n$ of $V_\infty^\perp$, then we can write

$$A = \sum_{n=1}^\infty \lambda_n |u_n\rangle\langle u_n| + \sum_k 0\, |v_k\rangle\langle v_k|.$$

and $(u_n)_n \cup (v_n)_n$ form an orthonormal basis for $\mathscr{H}$.

2) Now consider a general compact operator A. Then AA^* is compact and self-adjoint. Thus

$$AA^* = \sum_{n=1}^\infty \lambda_n^2 |u_n\rangle\langle u_n|$$

where $\lambda_n \to 0$ and $(u_n)_n$ is an orthonormal basis.

Here $\lambda_n^2 \geqslant 0$ as

$$\lambda_n^2 = \langle u_n, AA^* u_n \rangle = \langle A^* u_n, A^* u_n \rangle = \|A^* u_n\| \geqslant 0.$$

Defining $v_n = \frac{A^* v_n}{\lambda_n}$ for $\lambda_n \neq 0$, then $\|v_n\| = 1$ and

$$Av_n = A\frac{A^* v_n}{\lambda_n} = \frac{\lambda_n^2 u_n}{\lambda_n} = \lambda_n u_n.$$

Moreover,

$$\langle v_n, v_m \rangle = \frac{\langle A^* u_n, A^* u_m \rangle}{\lambda_n \lambda_m} = \frac{\langle u_n, AA^* u_m \rangle}{\lambda_n \lambda_m} = \frac{\langle u_n, \lambda_m^2 u_m \rangle}{\lambda_n \lambda_m} = \delta_{nm}$$

Thus $(v_n)_n$ is an orthonormal family and therefore $Av_n \lambda_n u_n$ for all $n \in \mathbb{N}$ where $(v_n)_n$ is an orthonormal family and $(u_n)_n$ is an orthonormal basis. Thus

$$A = \sum \lambda_n \left| u_n \right\rangle \left\langle v_n \right|$$

Here we can compliment $(v_n)_n$ by the basis of $\ker A$ and thus make $(v_n)_n$ an orthonormal basis.

q.e.d.

Remark 4.9 (Motivation)**.** We want to be able to define a "functional calculus", i.e. we are interested in how to define for A, $f(A)$ where f is some function. E.g. if $f(t) = t^2$, then $f(A) = A^2$. But for $f(t) = \sqrt{t}$ how do we define $\sqrt{A}$? □

Definition 4.10 (Spectrum)**.** Let A be a bounded operator in a Hilbert space $\mathscr{H}$, then

- ***Resolvent*** of A

$$\rho(A) := \left\{ \lambda \in \mathbb{C} \,\middle|\, (\lambda - A)^{-1} \text{ is a bounded operator on } \mathscr{H} \right\}$$

- ***Spectrum*** of A

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

□

Example 4.11. If λ is an eigenvalue of A, then $Au = \lambda u$ for some $u \in \mathscr{H}$. Thus

$$\ker(\lambda - A) \supset \overline{\operatorname{span}\{u\}} \neq \{0\}$$

Thus $(\lambda - A)^{-1}$ does not exist and $\lambda \in \sigma(A)$.

Theorem 4.12 (Basic Properties of the Spectrum)**.** *Let A be a self-adjoint bounded operator, then*

- $\sigma(A)$ *is a compact subset of* $\mathbb{R}$
- $\sup|\sigma(A)| = \max|\sigma(A)| = \|A\|$. *Here* $\sup|\sigma(A)| = \sup_{\lambda\in\sigma(A)} |\lambda|$.

□

Proof. 1) Take $\lambda \in \mathbb{C}$ and $|\lambda| > \|A\|$. Then $\lambda \in \rho(A)$. To see this note that $\lambda - A = \lambda(1 - \lambda^{-1}A)$, thus it is enough to prove that $1 - \lambda^{-1}A$ has a bounded inverse. This follows by the first lemma below. This means that $\sigma(A) \subset \overline{B(0, \|A\|)}$ in $\mathbb{C}$.

2) We now prove that $\sigma(A) \subset \mathbb{R}$. Take $\lambda = a + ib$, $a, b \in \mathbb{R}$ and $b \neq 0$. We want to show that $\lambda \in \rho(A)$. Consider $\lambda - A = (a - A) + ib$. Then for all $u \in \mathscr{H}$

$$\|(\lambda - A)u\|^2 = \|(a - A)u\|^2 + |b|^2\|u\|^2 + 2\underbrace{\mathfrak{R}\langle (a - A)u, ibu\rangle}_{=0} \geqslant |b|^2\|u\|^2.$$

This implies that $\lambda - A$ is invertible with bounded inverse by the second lemma below.

3) We prove that $\sigma(A)$ is closed which is equivalent to showing that $\rho(A)$ is open.

Take $\lambda \in \rho(A)$, then we show that $\lambda' \in \rho(A)$ for $|\lambda - \lambda'|$ sufficiently small.

$$\lambda' - A = \lambda' - \lambda + \lambda - A = \big((\lambda' - \lambda)(\lambda - A)^{-1} + 1\big)(\lambda - A).$$

Since $(\lambda - A)^{-1}$ is bounded $(\lambda' - A)^{-1}$ is as well if $((\lambda' - \lambda)(\lambda - A)^{-1} + 1)^{-1}$ is. This is the case as $B = (\lambda' - \lambda)(\lambda - A)^{-1}$ satisfies

$$\|B\| = |\lambda' - \lambda|\|(\lambda - A)^{-1}\| < 1$$

if $|\lambda' - \lambda|$ is small enough. Thus $(1 + B)^{-1}$ is bounded.

4) Now we prove that $\|A\| = \max|\sigma(A)|$. We know already that $\sup|\sigma(A)| \leqslant \|A\|$. The other inequality is non-trivial. By third lemma below we have to prove that

$$\sup|\sigma(A)| \geqslant \sup_{\|u\|=1} |\langle u, Au\rangle|.$$

Denote $E := \sup|\sigma(A)|$. We shall prove that $E \geqslant \langle u, Au\rangle$ for all unit vectors u. By the definition of E, $E + t \in \rho(A)$ for all $t > 0$. Thus $(A - E - t)^{-1}$ is bounded. Define $f(t) = \langle u, (A - E - t)^{-1}u\rangle$ for $t > 0$. Then we have by the boundedness of the operators

$$f'(t) = \left\langle u, (A - E - t)^{-2}u\right\rangle = \|(A - E - t)^{-1}u\|^2 \geqslant 0.$$

Thus we know that $f(t)$ is an increasing function. Moreover,

$$\lim_{t\to\infty} f(t) = \lim_{t\to\infty} \left\langle u, (A - E - t)^{-1}u\right\rangle = 0.$$

This is left as an exercise. Thus $f(t) \leqslant 0$ for $t > 0$, i.e. for all $t > 0$

$$\left\langle u, (A - E - t)^{-1}u\right\rangle \leqslant 0$$

and thus replacing u by $(A - E - t)u$

$$\langle u, (A - E - t)u\rangle \leqslant 0$$

which implies that

$$\langle u, Au\rangle \leqslant E + t$$

for all unit vectors u and $t > 0$. Taking the limit $t \to 0$ yields the result.

Thus $\sup|\sigma(A)| \geqslant \sup_{\|u\|=1} \langle u, Au\rangle$. By the same argument,

$$\sup|\sigma(A)| \geqslant \sup_{\|u\|=1} (-\langle u, Au\rangle) = -\inf_{\|u\|=1} \langle u, Au\rangle$$

hence

$$\sup|\sigma(A)| \geqslant \sup_{\|u\|=1} |\langle u, Au\rangle| = \|A\|$$

q.e.d.

Lemma 4.13. *If B is a bounded operator and $\|B\| < 1$. Then $(1 - B)^{-1}$ is a bounded operator and $\|(1 - B)^{-1}\| \leqslant (1 - \|B\|)^{-1}$.* □

Proof. Note we can define

$$(1 - B)^{-1} := \sum_{k=0}^{\infty} B^k := \lim_{n\to\infty} \sum_{k=0}^{n} B^k =: \lim_{n\to\infty} A_n$$

Since $\|B\| \leqslant 1$ the right-hand side is well defined as for $n < m$

$$\|A_n - A_m\| = \left\| \sum_{k=n+1}^{m} B^k \right\| \leqslant \sum_{k=n+1}^{m} \|B^k\| \leqslant \sum_{k=n+1}^{m} \|B\|^k \xrightarrow{n,m\to\infty} 0.$$

Thus $(1 - B)^{-1} := \lim_{n\to\infty} A_n$ is well-defined and it is a bounded operator. Moreover,

$$\left\|(1 - B)^{-1}\right\| \leqslant \sum_{k=0}^{\infty} \|B\|^k = (1 - \|B\|)^{-1}.$$

The fact that $(1 - B)^{-1}$ is indeed the inverse follows as usual via

$$(1 - B)(1 - B)^{-1} = (1 - B) \sum_{k=0}^{\infty} B^k = 1 + \sum_{k=1}^{\infty} B^k - \sum_{k=1}^{\infty} B^k = 0$$

q.e.d.

Remark 4.14. Here we used the fact that the set $B(\mathscr{H})$ of bounded operators on $\mathscr{H}$ with the operator norm is a Banach space. □

Lemma 4.15. *If B is a bounded operator and $\|Bu\| \geqslant b\|u\|$ and $\|B^*u\| \geqslant b\|u\|$ for all $u \in \mathscr{H}$ then B^{-1} is a bounded operator.* □

Lemma 4.16. *If $A = A^*$ is a bounded operator, then*

$$\|A\| = \sup_{\|u\|=1} |\langle u, Au\rangle|.$$

$\square$

Theorem 4.17 (Continuous Functional Calculus for Bounded Operators)**.** *Let $A = A^*$ be a bounded operator. Then there exists a unique continuous linear map*

$$\mathscr{L} : \begin{aligned} \mathscr{C}(\sigma(A)) &\longrightarrow B(\mathscr{H}) \\ f &\longmapsto f(A) \end{aligned}$$

such that the following properties hold

1) If f is a polynomial $f(t) = \sum_j a_j t^j$, then

$$f(A) = \sum_j a_j A^j.$$

2) $\|f(A)\| = \|f\|_{L^\infty}$.

Moreover, we also have $f(A)g(A) = (fg)(A)$ for all $f, g \in \mathscr{C}(\sigma(A))$.
This means that $\mathscr{L}$ is an isometry of C^*-algebra $\mathscr{C}(\sigma(A))$. $\square$

Proof. If f is a a polynomial, $f(A)$ is well-defined. We need to prove that $\|f(A)\| = \|f\|_{L^\infty}$ for all polynomials f. To do this, we show that $\sigma(f(A)) = f(\sigma(A))$. We know that $\|f(A)\| = \sup|\sigma(f(A))|$. For every $\lambda \in \mathbb{C}$ we can write

$$f(t) - \lambda = C \prod_j (t - t_j)$$

for $t_j \in \mathbb{C}$, then

$$f(A) - \lambda = C \prod_j (A - t_j).$$

and

$$\begin{aligned}
\lambda \notin \sigma(f(A)) &\iff (f(A)-\lambda)^{-1} \text{ is bounded} \\
&\iff (A-t_j)^{-1} \text{ is bounded for all } j \\
&\iff t_j \notin \sigma(A) \text{ for all } j \\
&\iff (t-t_j)^{-1} \text{ is bounded for all } j \text{ on } \sigma(A) \\
&\iff (f(t)-\lambda)^{-1} \text{ is bounded on } \sigma(A) \\
&\iff \lambda \notin f(\sigma(A))
\end{aligned}$$

Furthermore, we thus have

$$\|f(A)\| = \sup|\sigma(f(A)| = \sup|f(\sigma(A))| = \|f\|_\infty.$$

By the Weierstrass theorem, we know that for any $\sigma(A) \subset \mathbb{R}$ compact, the polynomials on $\sigma(A)$ are dense in $\mathscr{C}(\sigma(A))$, i.e. for all $f \in \mathscr{C}(\sigma(A))$ there exists a sequence of polynomials $(f_n)_n$ such that $\|f_n - f\|_{L^\infty} \to 0$.
Then $\|f_n(A) - f_m(A)\| = \|f_n - f_m\|_{L^\infty} \to \infty$ as $n, m \to \infty$. Hence there exists a unique $f(A) = \lim_{n\to\infty} f_n(A)$ and $\|f(A)\| = \|f\|_{L^\infty}$.
Moreover $f(A)g(A) = (fg)(A)$ for all polynomials and thus the same holds for all continuous functions by the same density argument. *q.e.d.*

We now want to extend the functional calculus to a larger class of function f.

Theorem 4.18 (Spectral Measure)**.** *Let $A = A^*$ be a bounded operator on $\mathscr{H}$. Then for all $u \in \mathscr{H}$ there exists a unique Borel measure μ_u on $\sigma(A)$ such that*

$$\langle u, f(A)u\rangle = \int_{\sigma(A)} f(x)\mathrm{d}\mu_u(x)$$

for all $f \in \mathscr{C}(\sigma(A))$. Consequently $\|f(A)u\| = \|f\|_{L^2(\sigma(A),\mathrm{d}\mu_u)}$ for all $f \in \mathscr{C}(\sigma(A))$ and we can extend $f \mapsto f(A)$ for any $f \in L^2(\sigma(A), \mathrm{d}\mu_u)$.

□

Proof. Define the mapping

$$\mathscr{L} : \begin{aligned} \mathscr{C}(\sigma(A)) &\longrightarrow \mathbb{C} \\ f &\longmapsto \mathscr{L}(f) = \langle u, f(A)u\rangle \end{aligned}.$$

Then $\mathscr{L}$ is linear, continuous, ***positive***, i.e. $\mathscr{L}(f) \geqslant 0$ for all $f \geqslant 0$. Here the positivity follows as $f \geqslant 0$ implies that $f = \overline{g}g$ for some $g \in \mathscr{C}(\sigma(A))$.
Then

$$\mathscr{L}(f) = \langle u, f(A)u\rangle = \langle u, \overline{g}(A)g(A)u\rangle = \langle u, g(A)^* g(A)u\rangle = \|g(A)u\|^2 \geqslant 0.$$

as the continuous functional calculus is a C^* algebra homomorphism. Then the result follows from the following theorem.

Theorem 4.19 (Riesz-Markov Thorem)**.** *Let Ω be a Borel set in $\mathbb{R}^d$ and let $\mathscr{L} : \mathscr{C}_c(\Omega) \to \mathbb{C}$ be a linear and positive functional. Then there exists a unique Borel regular measure μ in Ω such that*

$$\mathscr{L}(\rho) = \int_\Omega f(x)\mathrm{d}\mu(x)$$

for all $f \in \mathscr{C}_c(\Omega)$ □

Remark 4.20 (Recall)**.** A Borel measure μ on Ω is regular if

1) $\mu(K) < \infty$ for all compact $K \subset \Omega$.

2)

$$\mu(E) = \inf\{\mu(U \cap \Omega) \,\big|\, U \text{ open, } E \subset U\} = \sup\{\mu(K \cap \Omega) \,\big|\, U \text{ open, } K \subset E\}$$

□

Sketch of Proof. For simplicity assume that $\Omega = \mathbb{R}^d$. Then the measure μ is defined as follows:
For all U open let

$$\mu(U) = \sup\{\mathscr{L}(f) \,\big|\, f \text{ continuous, } 0 \leqslant f \leqslant 1, \operatorname{supp} f \subset U\}$$

Then if K is compact define

$$\mu(K) = \inf\{\mathscr{L}(f) \,\big|\, f \text{ continuous, } 0 \leqslant f \leqslant 1,\ f \equiv 1 \text{ on } K\}.$$

Then μ can be extended to a Borel regular measure on $\mathbb{R}^d$. We can prove

$$\mathscr{L}(f) = \int f(x)\mathrm{d}\mu(x)$$

for all continuous f by approximation. *q.e.d.*

Continuation of Proof of Theorem 4.18. By the Riesz-Markov theorem, there exists a unique regular Borel measure μ_u on $\sigma(A)$ such that

$$\langle u, f(A)u\rangle = \mathscr{L}(f) = \int\limits_{\sigma(A)} f(x)\mathrm{d}\mu_u(x)$$

for all $f \in \mathscr{C}(\sigma(A))$. Moreover,

$$\|f(A)u\|^2 = \langle u, f(A)^* f(A)u\rangle = \big\langle u, \big| f \big|^2(A)u\big\rangle = \int\limits_{\sigma(A)} |f|^2(x)\mathrm{d}\mu_u(x) = \|f\|^2_{L^2(\sigma(A),\mathrm{d}\mu_u)}.$$

Thus $\|f(A)u\| = \|f\|_{L^2(\sigma(A),\mathrm{d}\mu_u)}$ for all $f \in \mathscr{C}(\sigma(A))$. This allows us to extend the map $f \mapsto f(A)u$, for any $f \in L^2(\sigma(A), \mathrm{d}\mu_u)$, i.e. if $f \in L^2(\sigma(A), \mathrm{d}\mu_u)$, then take a sequence $(f_n)_n$ of continuous functions converging to f in $L^2(\sigma(A), \mathrm{d}\mu_u)$ and define

$$f(A)u = \lim_{n\to\infty} f_n(A)u.$$

q.e.d.

Remark 4.21. Here we did not define $f(A)$ but only $f(A)u$ which is simpler. □

Theorem 4.22 (Spectral Theorem for Bounded Self-Adjoint Operators)**.** *Let $A = A^*$ be a bounded operator on $\mathscr{H}$. Then there exists a Borel measurable set $\Omega \subset \mathbb{R}^d$, and a Borel measure μ such that there exists a unitary mapping*

$$U : \begin{aligned} \mathscr{H} &\longrightarrow L^2(\Omega, \mathrm{d}\mu) \\ A &\longmapsto M_a \end{aligned}$$

i.e. $UAU^* = M_a$ with M_a being the multiplication operator on $L^2(\Omega, \mathrm{d}\mu)$ with a function *a, i.e.*

$$(M_a f)(x) = a(x)f(x)$$

for all $f \in L^2(\Omega, \mathrm{d}\mu)$. *Moreover,* a *is a bounded, real-valued function on* Ω. *We can take* $\Omega = \sigma(A) \times \mathbb{N} \subset \mathbb{R}^2$ *and* $a(\lambda, n) = \lambda$. □

Remark 4.23. An easy way to remember this theorem is to note

$$A \longleftrightarrow M_a,$$

i.e. A up to a unitary transformation is equivalent to a multiplication operator.

□

Example 4.24. The Fourier transform

$$f \longmapsto \hat{f}(k) = \int_{\mathbb{R}^d} e^{-2\pi i k \cdot x} f(x) \mathrm{d}x$$

defined on $L^2(\mathbb{R}^d)$ is a unitary operator by Placherl's Theorem 1.33.

Proof.

Step 1 Recall that for all $u \in \mathscr{H}$, there exists a unique μ_u on $\sigma(A)$ such that

$$\langle u, f(A)u \rangle = \int_{\sigma(A)} f(x) \mathrm{d}\mu_u(x)$$

for all $f \in L^2(\sigma(A), \mathrm{d}\mu_u)$ by the theorem on the Spectral measure.

In particular, there exists a unitary mapping

$$U_u^* : \begin{aligned} L^2(\sigma(A), \mathrm{d}\mu_u) &\longrightarrow \mathscr{H}_u \\ f &\longmapsto f(A) \end{aligned}$$

where

$$\mathscr{H}_u = \left\{ f(A)u \,\middle|\, f \in L^2(\sigma(A), \mathrm{d}\mu_u) \right\} \subset \mathscr{H}$$

which is a closed subspace, i.e. itself a Hilbert space, of the Hilbert space $\mathscr{H}$. It is left as an exercise to show that

$$\mathscr{H}_u = \overline{\operatorname{span}\left\{A^k u \,\middle|\, k \in \mathbb{N}_0\right\}} \subset \mathscr{H}.$$

If $\mathscr{H}_u = \mathscr{H}$ we are done. In this case $\Omega = \sigma(A)$ and $a(\lambda) = \lambda$ and we call u a ***cyclic vector***.

In general, if there is no cyclic vector, then we need the lemma below.

Noting that $A : \mathscr{H}_u \to \mathscr{H}_u$ (why?) we can write

$$A = \bigoplus_{n=1}^{\infty} A_{u_n}.$$

Define the unitary operator

$$U : \bigoplus_{n\in\mathbb{N}} \mathscr{H}_{u_n} = \mathscr{H} \longrightarrow L^2(\sigma(A) \times \mathbb{N}) = \bigoplus_{n\in\mathbb{N}} L^2(\sigma(A), \mathrm{d}\mu_{u_n})$$

via

$$U := \bigoplus_{n\in\mathbb{N}} U_{u_n}$$

Then we see that

$$UAU^* = \bigoplus_{n\in\mathbb{N}} \Big(U_{u_n} A\big|_{\mathscr{H}_{u_n}} U^*_{u_n} \Big) = \bigoplus_{n} M_{a(\lambda,n)}$$

where $a(\lambda, n) = \lambda$. This is because

$$U_{u_n} A\big|_{\mathscr{H}_{u_n}} U^*_{u_n} : \begin{aligned} L^2(\sigma(A), \mathrm{d}\mu_{u_n}) &\longrightarrow L^2(\sigma(A), \mathrm{d}\mu_{u_n}) \\ f &\longmapsto U_{u_n}(Af(A)) = xf(x) \end{aligned}$$

q.e.d.

Lemma 4.25. *For any bounded self-adjoint operator A on $\mathscr{H}$, there exists an at most countable orthonormal family $(u_n)_{n\in\mathbb{N}}$ such that*

$$\mathscr{H} = \oplus_{n=1}^{\infty} \mathscr{H}_{u_n}.$$

□

Axiom 4.26 (Zorn's Lemma)**.** *Let P be a partially ordered set, with order $\prec$, i.e. it satisfies*

1) $\forall a \in P : a \prec a$

2) $\forall a, b \in P : a \prec b \wedge b \prec a \implies a = b$

3) $\forall a, b, c \in P : a \prec b \wedge b \prec c \implies a \prec c$

Note that there may be elements that are not comparable, i.e. $a \not\prec b$ *and* $b \not\prec a$*.*
If for all totally ordered subsets $I \subset P$ *(any pair* (a, b) *in* I *is comparable) there exists a maximal element* a_I*, i.e.* $a \prec a_I$ *for all* $a \in I$*. Then there exists a maximal element in* P*, i.e.*

$$\exists p \in P \, \forall a \in P : p \prec a \implies p = a.$$

□

Proof. Let $P = \left\{ (u_n)_n \,\middle|\, (u_n)_n \text{ is an ONF of } \mathscr{H} \right\}$ and

$$(u_n)_n \prec (v_n)_n :\iff \bigoplus \mathscr{H}_{u_n} \subset \bigoplus \mathscr{H}_{v_n}$$

Then Zorn's Lemma tells us that there exists a maximal $(u_n)_n$. We claim that $\mathscr{H} = \bigoplus_{n\in\mathbb{N}} \mathscr{H}_{u_n}$.
Assume that $\mathscr{H} \supsetneq \bigoplus_{n\in\mathbb{N}} \mathscr{H}_{u_n}$. Then there exists a $u \in H$, $u \neq 0$ and $u \perp \mathscr{H}_{u_n}$ for all $n \in \mathbb{N}$. Because $A : \mathscr{H}_{u_n} \to \mathscr{H}_{u_n}$ it follows that $A : (\bigoplus \mathscr{H}_{u_n})^\perp \to (\bigoplus \mathscr{H}_{u_n})^\perp$. Then we can define $\mathscr{H}_u$ in the usual way. Then $(u_n)_n \prec (u_n)_n \cup \{u\}$ because

$$\bigoplus \mathscr{H}_{u_n} \subsetneq \bigoplus \mathscr{H}_{u_n} \oplus \mathscr{H}_u$$

which is a contradiction to the maximality of $(u_n)_n$. *q.e.d.*

Corollary 4.27 (Functional Calculus)**.** *Let $A = A^*$ be a bounded operator on $\mathscr{H}$. Then* *there exists a unique linear map*

$$\begin{aligned} B(\sigma(A), \mathbb{C}) &\longrightarrow B(\mathscr{H}) \\ f &\longmapsto f(A) \end{aligned}$$

from the set of measurable, bounded functions $\sigma(A) \to \mathbb{C}$ to the bounded operators on $\mathscr{H}$, such that

1) *If $f(x) = \sum t_j z^j$ then $f(A) = \sum t_j A^j$.*

2) $\|f(A)\| = \|f\|_{L^2}$

3) $f(A)g(A) = (fg)(A)$

4) $f(A)^* = \overline{f}(A)$

5) *$f(\sigma(A)) = \sigma(f(A))$, in particular if $f \geqslant 0$ then $f(A) \geqslant 0$, i.e. $\langle u, f(A)u \rangle \geqslant 0$ for all $u \in \mathscr{H}$.*

6) *(Monotone Convergence) If $f_n \uparrow f$ pointwise, then $f_n(A) \to f(A)$ strongly, i.e. for all $u \in \mathscr{H}$, $f_n(A)u \to f(A)u$ strongly.*

□

Proof. By the spectral theorem, there exists a unitary transformation $U : \mathscr{H} \to L^2(\Omega, \mathrm{d}\mu)$, $UAU^* = M_a$ is a multiplication operator. Then we can define $f(A)$ by

$$Uf(A)U^* = M_{f(a)}$$

i.e.

$$(M_{f(a)}g)(x) = f(a(x))g(x)$$

for all $g \in L^2(\Omega, \mathrm{d}\mu)$. Monotone convergence now follows from the usual monotone convergence for functions. *q.e.d.*

Theorem 4.28 (Spectral Theorem for Normal Operators)**.** *Let A be a bounded normal operator on $\mathscr{H}$, i.e. $AA^* = A^*A$. Then there exists a unitary operator $U : \mathscr{H} \to L^2(\Omega, \mathrm{d}\mu)$, such that $UAU^* = M_a$ is a multiplication operator with a function a. Here a is a bounded function Ω, however we do not know if a is real-valued* □

Remark 4.29. The proof is more complicated, e.g. in general $f(A)^* \neq \overline{f}(A)$ for a normal operator.
To prove the spectral theorem for normal operators we define the two self-adjoint operators

$$X_1 = \frac{A + A^*}{2}, \qquad X_2 = i\frac{A - A^*}{2}$$

which commute $X_1 X_2 = X_2 X_1$. We can apply the spectral theorem to X_1, X_2 and since they commute we can simultaneously diagonalise them. We can recover $A = X_1 - iX_2$ □

4.1 Unbounded Self-Adjoint Operators

Definition 4.30. Let $A : D(A) \to \mathscr{H}$ be a linear, unbounded operator, where $D(A) \subset \mathscr{H}$, $\overline{D(A)} \to \mathscr{H}$. □

Definition 4.31 (Extension)**.** An operator B is called a ***extension*** of A, $A \subset B$, iff $D(A) \subset D(B)$ and $B\big|_{D(A)} = A$. □

Definition 4.32 (Adjoint Operator)**.** We want to define A^* such that $\langle A^* x, y\rangle = \langle x, Ay\rangle$ for all $y \in D(A)$ and all $x \in D(A^*)$. Here

$$\begin{aligned} D(A^*) &:= \left\{x \in \mathscr{H} \,\middle|\, \exists z \in \mathscr{H}\, \forall y \in D(A) : \langle z, y\rangle = \langle x, y\rangle\right\} = \\ &= \left\{x \in \mathscr{H} \,\middle|\, \sup_{y \in D(A)} |\langle x, Ay\rangle| < \infty\right\} \end{aligned}$$

and we define $A^* x := z$. □

Remark 4.33. In general, it might happen that $D(A^*)$ is very small and $\overline{D(A^*)} \neq \mathscr{H}$. □

Definition 4.34 (Symmetric Operator)**.** An operator A such that for all $x, y \in D(A)$

$$\langle Ax, y \rangle = \langle x, Ay \rangle$$

is called ***symmetric***. □

Remark 4.35. It is left as an exercise to show that A is symmetric iff $\langle x, Ax \rangle \in \mathbb{R}$ for all $x \in D(A)$ which in turn is equivalent to $A \subset A^*$. □

Definition 4.36 (Self-Adjoint Operator)**.** An operator A is called ***self-adjoint*** iff $A = A^*$ (in particular $D(A) = D(A^*)$). □

Remark 4.37. Find example of symmetric but not self-adjoint operators. □

Definition 4.38. Let $A : D(A) \to \mathscr{H}$ be a (densely defined) unbounded operator. The resolvent set

$$\rho(A) := \left\{ z \in \mathbb{C} \,\middle|\, (z - A)^{-1} \text{ is well-defined as a bounded operator} \right\}$$

and the spectrum is $\sigma(A) := \mathbb{C} \setminus \rho(A)$ □

Example 4.39 (Multiplication Operator)**.** Let (Ω, μ) be a measure space. Let $f : \Omega \to \mathbb{C}$ be a measurable function. Define

$$M_f : \begin{aligned} D(M_f) &\longrightarrow L^2(\Omega, \mathrm{d}\mu) \\ u &\longmapsto (M_f u)(x) = f(x)u(x) \end{aligned}$$

where $D(M_f) = \left\{ u \in L^2(\Omega, \mu) \,\middle|\, fu \in L^2(\Omega, \mu) \right\}$. Note that $D(M_f)$ is indeed dense in $L^2(\Omega, \mu)$. (Exercise!)

This operator has the following properties

1) $\|M_f\| = \sup_{\|u\|_{L^2} \leqslant 1} \|M_f u\|_{L^2} = \|f\|_{L^\infty}$. In particular, M_f is a bounded operator iff f is bounded.

2) $(M_f)^* = M_{\bar{f}}$. To see this note that

$$\langle M_{\bar{f}}u, v\rangle = \int_\Omega \overline{\bar{f}u}v\mathrm{d}\mu = \int_\Omega \bar{u}fv\mathrm{d}\mu = \langle u, M_f v\rangle$$

and $D(M_{\bar{f}}) = D(M_f)$ as $fu \in L^2$ iff $\overline{f}u \in L^2$ iff $|f||u| \in L^2$.

3) M_f is self-adjoint iff $(M_f)^* = M_f$ iff $f = \overline{f}$ iff f is real-valued.

4)

$$\begin{aligned}\sigma(M_f) = \operatorname{ess\,ran}(f) &= \left\{z \in \mathbb{C} \,\middle|\, \forall \varepsilon > 0 : \mu(f^{-1}(B_{\mathbb{C}}(z,\varepsilon))) > 0\right\} = \\ &= \left\{z \in \mathbb{C} \,\middle|\, \forall \varepsilon > 0 : \mu\big(\left\{x \in \Omega \,\middle|\, |f(x) - z| < \varepsilon\right\}\big) > 0\right\}\end{aligned}$$

To see this note that $z - M_f = M_{z-f}$ and thus $(z - M_f)^{-1} = M_{(z-f)^{-1}}$. This is a bounded operator iff $(z - f)$ is bounded, i.e. $\|(z - f)^{-1}\|_{L^\infty} < \infty$.

Example 4.40. If $f : \mathbb{R}^d \to \mathbb{R}$, $f(x) = |x|^2$. Then M_f is a self-adjoint multiplication operator on $L^2(\mathbb{R}^d)$ and

$$\sigma(M_f) = \operatorname{ess\,ran}\big(x \mapsto |x|^2\big) = [0, \infty)$$

Theorem 4.41 (Basic Properties of the Spectrum)**.** *Let $A : D(A) \to \mathscr{H}$ be a (densely defined) unbounded operator on a Hilbert space $\mathscr{H}$.*

1) $\sigma(A)$ is a closed set in $\mathbb{C}$.

2) If A is self-adjoint ($A = A^*$) then $\sigma(A) \subset \mathbb{R}$.

3) If A is symmetric and $\sigma(A) \subset \mathbb{R}$ then A is self-adjoint.

□

Proof. 1) We proof that $\rho(A)$ is open. Take $z_0 \in \rho(A)$, then we prove that $z \in \rho(A)$ if $|z - z_0|$ is small enough. We have

$$\begin{aligned}(z - A)^{-1} = (z - z_0 + z_0 - A)^{-1} &= \Big(\big((z - z_0)(z_0 - A)^{-1} + \mathbb{I}\big)(z_0 - A)\Big)^{-1} = \\ &= (z_0 - A)^{-1}\big(\mathbb{I} + (z - z_0)(z_0 - A)^{-1}\big)^{-1}\end{aligned}$$

where we used that $(z_0 - A)^{-1}$ is a well-defined, bounded operator. Then if $|z - z_0|$ is small enough $\|(z - z_0)(z_0 - A)^{-1}\| < 1$ and thus $(\mathbb{I} + (z - z_0)(z_0 - A)^{-1})^{-1}$ is bounded by Lemma 4.13.

2) Assume that $A = A^*$. We prove that $\sigma(A) \subset \mathbb{R}$. Take $z \in \mathbb{C} \setminus \mathbb{R}$, then we prove that $(z - A)^{-1}$ is bounded. Consider $z = \pm i$. We see that

$$\|(A + i)x\|^2 = \langle (A + i)x, (A + ix) \rangle = \|Ax\|^2 + \|x\|^2.$$

This implies that $A \pm i$ is injective and, together with the self-adjointness of A, that $\operatorname{ran}(A \pm i) = \mathscr{H}$.

- $\operatorname{ran}(A + i)$ is dense in $\mathscr{H}$, because if $y \perp \operatorname{ran}(A + i)$ then $y \in \ker(A + i)^* = \ker(A - i) = \{0\}$.
- $\operatorname{ran}(A + i)$ is closed. Take $(A + i)x_n \to a$, we need to prove that $a \in \operatorname{ran}(A + i)$. Because $(A + i)x_n$ is Cauchy sequence it follows by the above inequality that

$$\|(A + i)x_n - (A + i)x_m\|^2 \geqslant \|Ax_n - Ax_m\|^2 + \|x_n - x_m\|^2$$

  and thus $(Ax_n)_n$ and $(x_n)_n$ are both Cauchy sequences. Thus $Ax_n \to y$ and $x_n \to x$ in $\mathscr{H}$.

  We need to prove that $x \in D(A)$ and $Ax = y$. We know that A is self-adjoint, $A = A^*$, thus it is sufficient to prove that $x \in D(A^*)$. We need to show that

$$\sup_{\substack{\varphi \in D(A) \\ \|\varphi\| \leqslant 1}} |\langle x, A\varphi \rangle| < \infty$$

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

$$\langle x, A\varphi \rangle = \lim_{n \to \infty} \langle x_n, A\varphi \rangle = \lim_{n \to \infty} \langle Ax_n, \varphi \rangle = \langle y, \varphi \rangle .$$

  Thus by definition, $x \in D(A^*) = D(A)$ and $Ax = y$, as $D(A)$ is dense.

  Thus

$$a = \lim_{n \to \infty} (A + i)x_n = (A + i)x$$

  with $x \in D(A)$, i.e. $a \in \operatorname{ran}(A + i)$. Thus $\operatorname{ran}(A + i)$ is closed.

The same analysis also holds true for $A - i$.

This means that $A \pm i$ is surjective and thus $(A \pm i)^{-1}$ is well-defined. Moreover, $\|(A \pm i)x\| \geqslant \|x\|$ thus $\|(A \pm i)^{-1}\| \leqslant 1$.

This proves that $z = \pm i \in \rho(A)$. In general, if $z \in \mathbb{C} \setminus \mathbb{R}$, then $z = \Re z + i\Im z$, $\Im z \neq 0$. Then

$$z - A = \Re z + \Im z - A = \left(i + \frac{\Re z - A}{\Im z}\right)\Im z$$

Since $\frac{\Re z - A}{\Im z}$ is still a self-adjoint operator and we may apply the previous result thus $(z - A)^{-1}$ is bounded.

This concludes

$$A = A^* \implies \sigma(A) \subset \mathbb{R}.$$

3) Assume that $\sigma(A) \subset \mathbb{R}$ and that A is symmetric.

Then $\pm i \in \rho(A)$. (The same prove as above holds since symmetric operators are closed.) Thus $(A \pm i)^{-1}$ is bounded.

We prove that $D(A^*) = D(A)$. Take $x \in D(A^*)$, then there exists $y \in D(A)$ such that

$$(A + i)y = (A^* + i)x$$

this implies that for all $z \in D(A)$

$$\langle y, (A - i)z\rangle = \langle (A + i)y, z\rangle = \langle (A^* + i)x, z\rangle = \langle x, (A - i)z\rangle$$

as A is symmetric. Thus $y = x$ because $\operatorname{ran}(A - i) = \mathscr{H}$ and hence $x \in D(A)$.

q.e.d.

Theorem 4.42 (Spectral Theorem for Unbounded Self-Adjoint Operators)**.** *Let $A : D(A) \to \mathscr{H}$ be a self-adjoint operator on a Hilbert space. Then there exists a measure space (Ω, μ) such that Ω is a Borel subset of $\mathbb{R}^d$, μ is a regular Borel measure and there exists a unitary operator $U : \mathscr{H} \to L^2(\Omega, \mu)$ such that*

$$UAU^* = M_a$$

for some measurable function $a : \Omega \to \mathbb{R}$.

Moreover $UD(A) = D(M_a) = \{u \in L^2 \,|\, au \in L^2\}$.
We can take $\Omega = \sigma(A) \times \mathbb{N} \subset \mathbb{R}^2$ *and* $a(\lambda, n) = \lambda$. $\square$

Proof. We know that $S = (A+i)^{-1}$ is a bounded operator as $i \in \rho(A)$. Further $S^* = (A-i)^{-1}$ and $S^*S = SS^*$. Thus S is a normal operator.
Applying the spectral theorem for the bounded normal operator S we find a measure space (Ω, μ) and a unitary operator

$$U : \mathscr{H} \longrightarrow L^2(\Omega, \mu)$$

such that $USU^* = M_f$ for some bounded function $f : \Omega \to \mathbb{C}$.
Now we want to find a function $a : \Omega \to \mathbb{R}$ such that $UAU^* = M_a$. Using $S = (A+i)^{-1}$ it follows that $A = S^{-1} - i$ thus we might guess that $a = f^{-1} - i$.
We now have to prove that this choice makes sense. Here $f \neq 0$ a.e. because from $USU^* = M_f$ we know that $\sigma(S) = \sigma(M_f) = \operatorname{ess\,ran}(f)$, however we know that $0 \in \rho(S)$ and thus $0 \notin \operatorname{ess\,ran}(f)$. To see this suppose that $f \equiv 0$ on $B \subset \Omega$ with $\mu(B) > 0$. Then $u = \mathbf{1}_B$ is a non-zero function with $M_f u = 0$, which means that 0 is an eigenvalue of M_f. Since $USU^* = M_f$ this means that 0 is also an eigenvalue of S. Thus there exists a $\varphi \neq 0$ such that $S\varphi = 0$, however we then have

$$0 = (A+i)S\varphi = (A+i)(A+i)^{-1}\varphi = \varphi$$

which is a contradiction.
Note that f^{-1} might have singularities and hence a might not be bounded.
Thus we can define $a = f^{-1} - i$ and we have

$$UAU^* = U(S^{-1} - i)U^* = US^{-1}U - i = (USU^*)^{-1} - i = M_f^{-1} - i = M_{f^{-1}} - i = M_a$$

Here a is a real-valued function because $UAU^* = M_a$ is self-adjoint. It is easy to check that $UD(A) = D(M_a)$.

q.e.d.

Theorem 4.43 (Functional Calculus of Self-Adjoint Operators)**.** *Let* $A : D(A) \to \mathscr{H}$ *be a self-adjoint operator on a Hilbert space* $\mathscr{H}$.

Then there exists a unique linear map

$$\Phi : \begin{aligned} B(\sigma(A), \mathbb{C}) &\longrightarrow B(\mathscr{H}) \\ f &\longmapsto f(A) \end{aligned}$$

such that

1) *If* $f = 1$ *(i.e.* $f(x) = 1$ *for all* $x \in \sigma(A)$*) then* $f(A) = \mathbb{I}$ *(the identity on* $\mathscr{H}$*).*

2) $\|f(A)\| = \|f\|_{L^\infty}$

3) $f(A)^* = \overline{f}(A)$

4) $f(A)g(A) = (fg)(A)$

5) $f(\sigma(A)) = \sigma(f(A))$

6) *Monotone Convergence: Let* $f_n \uparrow f$ *pointwise, then* $f_n(A) \to f(A)$ *strongly, i.e. for all* $u \in \mathscr{H}$, $f_n(A)u \to f(A)u$.

   Dominated Convergence: Let $f_n \to f$ *pointwise, and* $\sup_n \|f_n\|_{L^\infty} < \infty$ *then* $f_n(A) \to f(A)$ *strongly.*

7) *If* $AB = BA$ *is well-defined, then* $f(A)B = Bf(A)$ *for all bounded functions* f*.*

□

Proof. By the spectral theorem we have $UAU^* = M_a$. Define $f(A)$ by $Uf(A)U^* = M_{f(a)}$, i.e. $(M_{f(a)}u)(x) = f(a(x))u(x)$. *q.e.d.*

Remark 4.44. We used the seventh property to prove the Spectral theorem for normal operators. □

Example 4.45. Let $A = (-\Delta)$ on $L^2(\mathbb{R}^d)$. We that Fourier transform $\mathcal{F}$ is a unitary operator and

$$\widetilde{Af}(k) = |2\pi k|^2 \hat{f}(k),$$

i.e.

$$\mathcal{F}(-\Delta)\mathcal{F}^* = M_{|2\pi k|^2}$$

Consequently $\sigma(-\Delta) = [0, \infty)$ and

$$D(-\Delta) = \left\{ u \in L^2(\mathbb{R}^d) \,\middle|\, |2\pi k|^2 \hat{u}(k) \in L^2 \right\} = H^2(\mathbb{R}^d)$$

$-\Delta$ is only self-adjoint on $D(-\Delta)$.

Algebras of Observables

Classical Mechanics

An experiment is represented by a function $A(\boldsymbol{r}, \boldsymbol{p})$ on phase space Γ. Further it is physically reasonable to assume that A is a bounded function, as any experiment has only a finite range of possible results.
We can give this observable the supremum norm

$$\|A\|_\infty := \sup_{(\boldsymbol{r},\boldsymbol{p})\in\Gamma} |A(\boldsymbol{r}, \boldsymbol{p})| < \infty$$

A ***state*** is given by a certain reproducible procedure of preparing the system. Then

$$\underline{\omega} : \langle A \rangle_\omega = \frac{1}{N}\sum_{n=1}^{N} a_i^{(\omega)} \in \mathbb{R}$$

is called the result of the measurement A for the state ω.
To a high precision we have $\langle A^m \rangle_\omega = \langle A \rangle_\omega^m$.
The properties of ω are

- normalised: $\omega(\mathbf{1}) = 1$
- it is a linear functional: $\mathscr{A} \to \mathbb{C}(\mathbb{R})$ where $\mathscr{A}$ denotes the algebra of observables
- positivity: for $A(x, p) \geqslant 0$, $\omega(A) \geqslant 0$.

$$\omega(A) = \int_\Gamma \rho(x, p) A(x, p) \mathrm{d}x\mathrm{d}p$$

6

C^* Algebra

The experiments A are elements of a (C^*) algebra $\mathscr{A}$.
A state is a linear, positive functional on $\mathscr{A}$, i.e. for $A, B \in \mathscr{A}$ and $\lambda \in \mathbb{C}$

$$\omega(\lambda A) = \lambda\omega(A), \qquad \omega(A+B) = \omega(A) + \omega(B)$$

Further we assume that

- Normalisation: $\omega(\mathbf{1}) = 1$
- Positivity: A is positive, i.e. if $A = B^*B$ then $\omega(A) \geqslant 0$.

Two observables are called equal

$$A = B :\Longleftrightarrow \forall\omega : \omega(A) = \omega(B).$$

Note that these definitions apply that if $A + B = C$

$$\omega(C) = \omega(A) + \omega(B).$$

However, it is very much unclear what it means to take the sum of experiments.
We define a norm on $\mathscr{A}$ by taking

$$\|A\| = \sup_\omega |\omega(A)|.$$

Definition 4.46 (Algebra)**.** An algebra $\mathscr{A}$ is

1. $\mathscr{A}$ is a complex vector space
2. $\mathscr{A}$ has an associative multiplication operation.
3. the multiplication is distributive with respect to the addition in $\mathscr{A}$ and the multiplication by scalars
4. $\mathscr{A}$ contains a unit for the multiplication operation

$\square$

Definition 4.47 (*-Algebra)**.** $\mathscr{A}$ is an algebra equipped with a complex conjugation or adjoint operation $^* : \mathscr{A} \to \mathscr{A}$ satisfying

$$(PQ)^* = Q^* P^*, \qquad (P+Q)^* = P^* + Q^*$$
$$(\alpha Q)^* = \overline{\alpha} Q^*, \qquad (Q^*)^* = Q$$

□

Definition 4.48 (C_- - Algebra)**.** A C_--algebra is a C^*-algebra equipped with a norm which further satisfies

- $\|PQ\| \leqslant \|P\| \|Q\|$
- $\|Q^*\| = \|Q\|$
- $\|QQ^*\| = \|Q\| \|Q^*\|$
- $\|\mathbf{1}\| = 1$

□

Definition 4.49 (Classes of Elements on a C^*-Algebra)**.**

1. Self-Adjoint or Hermitean: $Q^* = Q$
2. Unitary: $Q^* Q = QQ^* = \mathbf{1}$
3. Normality: $QQ^* = Q^* Q$
4. Projector: $Q^2 = Q = Q^*$
5. Positive: there exists $C \in \mathscr{A} : Q = C^* C$

□

Definition 4.50 (Resolvent Set and Spectrum)**.** The resolvent set of $A \in \mathscr{A}$ is

$$\rho(A) = \left\{ z \in \mathbb{C} \,\middle|\, (A - z)^{-1} \in \mathscr{A} \right\}$$

The spectrum is the compliment of the resolvent. $\square$

Remark 4.51. Using the same argument as in the case of operators on Hilbert spaces we may conclude that the resolvent set is open. $\square$

Proposition 4.52 (Spectral Properties).

- *Hermitean:* $\sigma(A) \subset \mathbb{R}$
- *Unitary:* $\sigma(U) \subset S^1$
- *Projector:* $\sigma(P) = \{0, 1\}$
- *Positive:* $\sigma(Q) \subset [0, \infty)$

$\square$

Remark 4.53. A state is a positive linear functional, i.e. $\omega(A^*A) \geqslant 0$. $\square$

Example 4.54.

1) Classical: A state is a function ρ on phase space satisfying $\rho(x,p) \geqslant 0$, $\int \rho = 1$ and the action being given by

$$\int_\Gamma \rho(x,p)A(x,p)\mathrm{d}x\mathrm{d}p.$$

2) Quantum 1: For the bounded operators $B(\mathscr{H})$ of a Hilbert space $\mathscr{H}$ the observables are unit vectors $\psi \in \mathscr{H}$ with the action being given by

$$\langle \psi, A\psi \rangle \,.$$

3) Quantum 2: We can alternatively form the density operator $\rho_\psi = |\psi\rangle \langle\psi|$, where ρ is a positive operator of trace 1. The state action is given by

$$\operatorname{Tr} \rho A.$$

Proposition 4.55. *For a positive linear functional ω on $\mathscr{A}$ we have the following "Cauchy-Schwartz" inequality*

$$|\omega(A^*B)|^2 \leqslant \omega(A^*A)\omega(B^*B)$$

In particular this implies that ω is bounded and thus continuou. □

States form a ***convex space***, i.e. let ω_1, ω_2 be two states then the for all $\lambda \in [0,1]$, $\omega = \lambda\omega_1 + (1-\lambda)\omega_2$ is again a state.

Definition 4.56 (Pure and Mixed States)**.** A state is called ***pure*** if cannot be represented as a non-trivial convex combination of two states.
Otherwise a state is called mixed. □

Proposition 4.57. *Any state ω can be written as a convex combination of pure states $(\alpha_i)_{i\in\mathbb{N}}$ such that*

$$\omega = \sum_i \lambda_i \alpha_i, \qquad \sum_i \lambda_i = 1, \qquad \lambda_i \geqslant 0.$$

□

Definition 4.58 (Abelian Algebra)**.** An algebra is Abelian if all elements commute. □

Definition 4.59 (Algebraic *-Homomorphism)**.** A map $\pi : \mathscr{A} \to \mathscr{B}$ between *-algebras is called a *-homomorphism if

- $\pi(AB) = \pi(A)\pi(B)$
- $\pi(\alpha A + \beta B) = \alpha\pi(A) + \beta\pi(B)$
- $\pi(A^*) = \pi(A)^*$

□

Definition 4.60. A character χ is a *-homomorphism of $\mathcal{A} \to \mathbb{C}$ such that

(1) If exists $(\chi(A) - z)^{-1}$ if $z \in \sigma(A)$ then $\chi(A) \in \sigma(A)$.

(2) χ is positive, i.e. $\chi(A^*A) = \chi(A^*)\chi(A) = \chi(A)^*\chi(A) \geqslant 0$

(3) Any χ is a state: $\chi(A\mathbf{1}) = \chi(A)\chi(\mathbf{1})$, hence $\chi(\mathbf{1}) = 1$

(4) Cauchy-Schwartz $|\chi(A^*B)|^2 \leqslant \chi(A^*A)\chi(B^*B)$.

(5) Characters are pure states.

(6) There exist a character such that $\chi(A) = \|A\|$

□

Definition 4.61. The weak *-topology V, V^* define

$$B_{v,\varepsilon}(W^*) = \left\{U^* \in V^* \,\middle|\, |W^(v) - U^*(v)| < \varepsilon\right\}$$

for $W^* \in V^*$, $v \in V$. □

Definition 4.62. $X(A)$ is set of all characters, the set of all continuous functions $f : X(A) \to \mathbb{C} \sim A$ for any $A \in \mathcal{A}$???? □

Theorem 4.63 (Gel'fand Isomorphism)**.** *An Abelian C^* algebra is isomorphic to the weak *-continuous function $\mathscr{C}(X)$ on the character set $X = X(\mathcal{A})$. Norm on $\mathscr{C}(X)$ is given by the supremum norm*

$$\|f\| = \sup_{\chi \in X} |f(\chi)|.$$

Furthermore it is an isometry w.r.t. to this norm, i.e. $\|A\| = \|f_A\|$. □

Proof. (1) We define $A \mapsto f_A$, via the natural inclusion into the double dual, i.e. $f_A(\chi) = \chi(A)$. This is a *-homomorphism, as χ is one, e.g.

$$f_{AB}(\chi) = \chi(AB) = \chi(A)\chi(B) = f_A(\chi)f_B(\chi).$$

This inclusion map is naturally injective, as continuous linear functionals separate points.

(2) The Gel'fand map preserves the norm as

$$\|A\| = \sup_{\chi \in X} |\chi(A)| = \|f\|$$

To see the first equality note that for all states we have per definitionem $|\chi(A)| \leqslant \|A\|$ and there exists a pure state such that $|\omega(A)| = \|A\|$.

(3) The main problem is to prove surjectivity: For any $f \in \mathscr{C}(X)$ there exist A_f such that $f_{A_f} = f$ for any polynomial.

This obviouslyholds for polynomials. Thus by the "Weierstrass" theorem: any continuous function on a compact set on X can be arbitrarily well-approximated by polynomials. Compact is taken here w.r.t. *-topology.

Holes: Existence of ω such that $\omega(A) = \|A\|$, GNS construction, compactness and the Stone-Weierstrass theorem.

q.e.d.

Let $\mathcal{A}_A$ be the algebra generated by $\mathbf{1}, A, A^*$, i.e. all polynomial expressions of the form $\sum a_{mn} A^n (A^*)^m$ and the closure under the norm of the algebra.
$\mathcal{A}_A$ is commutative hence it follows that is isomorphic to $\mathscr{C}(X_{\mathcal{A}})$.

Definition 4.64 (Representation on $\mathcal{A}$ on $B(\mathscr{H})$)**.** A representation π of the C^*-algebra $\mathcal{A}$ is a *-homomorphism of $\mathcal{A}$ into $\mathcal{B}(\mathscr{H})$.
If π is injective, then the representation is called faithful. Two representation are called ***equivalent***, if there exists an isomorphism $U : \mathscr{H}_1 \to \mathscr{H}_2$ if for all $A \in \mathcal{A}$

$$\pi_2(A) = U \pi_1(A) U^{-1}$$

□

Definition 4.65 (Invariant Subspace)**.** Let $V \in \mathscr{H}$ be a ***subspace*** of $\mathscr{H}$. V is called an invariant subspace of $\pi(\mathcal{A})$ iff

$$\forall A \in \mathcal{A} : v \in V \implies \pi(A) v \in V$$

□

Definition 4.66. A vector $c \in \mathscr{H}$ is called ***cyclic*** for a representation π if

$$\mathcal{C} := \left\{ \pi(A)c \,\middle|\, A \in \mathcal{A} \right\}$$

is dense in $\mathscr{H}$, i.e. $\overline{\mathcal{C}} = \mathscr{H}$. □

Definition 4.67 (Irreducible Representation)**.** A representation is called ***irreducible*** on of the two equivalent properties holds

(1) The only closed invariant subspaces $V \subset \mathscr{H}$ are $\{0\}$ and $\mathscr{H}$.

(2) Any vector $\varphi \in \mathscr{H}$ is cyclic.

□

Definition 4.68 (GNS - Construction (Gel'fand, Naimark, Segal))**.** A C^*-algebra $\mathcal{A}$ induces a Hilbert space using a state ω.
We define a scalar product $A, B \in \mathscr{A}$ via $\langle A, B \rangle := \omega(A^* B)$. This hermitean, however, it is not necessarily strictly positive.
To remedy this define

$$\mathcal{N}_\omega = \left\{ A \in \,\middle|\, \omega(A^* A) = 0 \right\}.$$

and then the induced scalar product on $\mathcal{A}/\mathcal{N}_\omega$ is strictly positive. The completion of $\mathcal{A}/\mathcal{N}_\omega$ is a Hilbert space. □

Remark 4.69. Irreducible representations of a commutative algebra are one-dimensional.

□

Definition 4.70 (GNS - Representation)**.** Let $\overline{B} \in \mathscr{H}_{\mathrm{GNS}}$ with $B \in \mathcal{A}$, then define the representation $\pi : \mathcal{A} \to B(\mathscr{H}_{\text{GNS}})$ via

$$\pi(A)\overline{B} = \overline{AB}.$$

□

Remark 4.71.

- The GNS representation for a pure state is irreducible.
- For any given representation of $\mathcal{A}$ on $\mathscr{H}$, an element $\psi \in \mathscr{H}$ defines a pure state via

$$\omega_\psi(A) = \langle \psi, A\psi \rangle$$

The corresponding subspace $\left\{\pi(A)\psi \,\middle|\, A \in \mathcal{A}\right\}$, is invariant and isomorphic to the GNS Hilbert space.

□

Chapter 5

Self-Adjoint Extensions

Remark 5.1 (Question)**.** Given a symmetric operator A, can we find a self-adjoint extension B of A., i.e. $D(B) \supset D(A)$, $B\big|_{D(A)} = a$ and $B = B^*$. Thus $A \subset B = B^* \subset A^*$.
It is left as an exercise to show that if $A : D(A) \to \mathscr{H}$ and $B : D(B) \to \mathscr{H}$ are symmetric operators and $A \subset B$ then $B^* \subset A^*$, i.e.

$$A \subset B \subset B^* \subset A^*$$

□

Method 1 (Closure) Given $A : D(A) \to \mathscr{H}$ symmetric. Define its closure $\overline{A} : D(\overline{A}) \to \mathscr{H}$ as follows:

Let $\|x\|_A := \|Ax\| + \|x\|$ for all $x \in D(A)$

$$\begin{aligned} D(\overline{A}) &:= \overline{D(A)}^{\|\cdot\|_A} = \\ &= \left\{ x \in \mathscr{H} \,\middle|\, \exists (x_n)_n \subset D(A), (x_n)_n \text{ Cauchy w.r.t. } \|\cdot\|_A : x = \lim_{n\to\infty} x_n \text{ in } \mathscr{H} \right\} = \\ &= \left\{ x \in \mathscr{H} \,\middle|\, \exists (x_n)_n \subset D(A) : \|x_n - x_m\|_A \xrightarrow{n,m\to\infty} 0 : x = \lim_{n\to\infty} x_n \text{ in } \mathscr{H} \right\} \end{aligned}$$

This is well-defined because A is a symmetric operator. More precisely, if $(x_n)_n$ is a Cauchy sequence in $\|\cdot\|_A$, then $(Ax_n)_n$ and $(x_n)_n$ are Cauchy sequences in $\mathscr{H}$. Thus we have in $\mathscr{H}$

$$Ax_n \xrightarrow{n\to\infty} y, \qquad x_n \xrightarrow{n\to\infty} x$$

Here the limit $y = \lim Ax_n$ is independent of the choice of $(x_n)_n$. Indeed if $(x'_n)_n$ is another sequence in $D(A)$ such that

$$Ax'_n \xrightarrow{n\to\infty} y', \qquad x'_n \xrightarrow{n\to\infty} x$$

Then $y = y'$ because for all $\varphi \in D(a)$

$$\langle y, \varphi\rangle = \lim_{n\to\infty} \langle Ax_n, \varphi\rangle = \lim_{n\to\infty} \langle x_n, A\varphi\rangle = \langle x, A\varphi\rangle = \lim_{n\to\infty} \langle x'_n, A\varphi\rangle = \lim_{n\to\infty} \langle Ax'_n, \varphi\rangle = \langle y', \varphi\rangle$$

and thus $y = y'$ as $D(A)$ is dense in $\mathscr{H}$.

Definition 5.2. We define the closure of symmetric operator $A : D(A) \to \mathscr{H}$ to be the operator defined on $D(\overline{A})$ via $\overline{A}x := \lim_{n\to\infty} Ax_n$, where $(x_n)_n \subset D(A)$ is a Cauchy sequence w.r.t. $\|\cdot\|_A$ and $x_n \to x$ in $\mathscr{H}$.
By the above this well-defined for all $x \in D(\overline{A})$. □

Remark 5.3. Often $\overline{A}$ is already a self-adjoint operator, in which case we are done. For example let $A = -\Delta$ on $D(A) = \mathscr{C}_c^\infty(\mathbb{R}^d) \subset \mathscr{H} = L^2(\mathbb{R}^d)$. Then since $\|\cdot\|_\Delta = \|-\Delta(\cdot)\| + \|\cdot\|$ is equivalent to $\|\cdot\|_{H^2}$ we find that

$$D(\overline{A}) = \overline{\mathscr{C}_c^\infty(\mathbb{R}^d)}^{\|\cdot\|_A} = \overline{\mathscr{C}_c^\infty(\mathbb{R}^d)}^{\|\cdot\|_{H^2}} = H^2(\mathbb{R}^d)$$

and as we have already proven $-\Delta u$ for $u \in H^2(\mathbb{R}^d)$ is just the extension of $-\Delta$ on $\mathscr{C}_c^\infty(\mathbb{R}^d)$. Since $-\Delta$ on $H^2(\mathbb{R}^d)$ is self-adjoint $\overline{A}$ is as well. □

Example 5.4. Let $A = -\Delta - \frac{1}{|x|}$ on $\mathscr{C}_c^\infty(\mathbb{R}^{\not\Vdash})$ be the Hydrogen atom Hamiltonian. Then $D(\overline{A}) = H^2(\mathbb{R}^3)$ and $\overline{A}u = \left(-\Delta - \frac{1}{|x|}\right)u$ for all $u \in H^2(\mathbb{R}^3)$.
Here the proof is not trivial! For all $u \in H^2(\mathbb{R}^d)$, $-\Delta u \in L^2$ per definitionem and $-\frac{u(x)}{|x|} \in L^2$ by the Hardy-Littlewood-Sobolev inequality Theorem 1.30.
But the inverse is more difficult: Does $\left(-\Delta - \frac{1}{|x|}\right)u \in L^2$ for $u \in L^2$ imply that $u \in H^2(\mathbb{R}^3)$?
In particular does $-\Delta u - \frac{u(x)}{|x|} \in L^2$ imply that $-\Delta u$ and $\frac{u(x)}{|x|} \in L^2$?

Example 5.5 (Counter Example to Closure Being Self-Adjoint)**.** Let $A = -i\frac{d}{dx}$ on $D(A) = \mathscr{C}_c^\infty(0,1) \subset \mathscr{H} = L^2(0,1)$.
Then A is symmetric (which can be checked easily via integration by parts). But

$$D(\overline{A}) = \overline{\mathscr{C}_c^\infty(0,1)}^{\|\cdot\|_A} = \overline{\mathscr{C}_c^\infty(0,1)}^{\|\cdot\|_{H^1}} = H_0^1(0,1) := \left\{u \in H^1(0,1) \,\middle|\, u(0) = u(1) = 0\right\}.$$

However,

$$D\left(\overline{A}^*\right) = \left\{u \in L^2 \,\middle|\, \sup_{\substack{v \in D(\overline{A}) \\ \|v\|_{L^2} \leqslant 1}} |\left\langle u, \overline{A}v\right\rangle_{L^2}| < \infty\right\} = H^1(0,1)$$

where checking the last equality is left as an exercise. Hence $\overline{A}$ is not self-adjoint.

Definition 5.6. If $A = \overline{A}$, i.e. $D(A)$ is closed w.r.t. $\|\cdot\|_A = \|A\cdot\| + \|\cdot\|$, then we call A a closed operator. □

Proposition 5.7. *Assume that $A : D(A) \to \mathscr{H}$ is symmetric, $A \subset B$ and B is closed and symmetric. Then $\overline{A} \subset B \subset A^*$.*
This means that $\overline{A}$ is the smallest closed extension of A and A^* is the largest closed extension of A. In particular A^* is closed. □

Proof. Exercise! *q.e.d.*

Definition 5.8. Let $A : D(A) \to \mathscr{H}$ be a symmetric operator. If $\overline{A}$ is self-adjoint then we call A ***essentially self-adjoint***. □

Theorem 5.9. *Let $A : D(A) \to \mathscr{H}$ by symmetric. Then the following are equivalent*

(1) *A is self-adjoint.*

(2) $\sigma(A) \subset \mathbb{R}$

(3) $\operatorname{ran}(A \pm i) = \mathscr{H}$

□

Proof. The first two items are just a reformulation of Theorem 4.41 and third follows from their proof. *q.e.d.*

In fact we have the even stronger result

Proposition 5.10. *Let $A : D(A) \to \mathscr{H}$ be a symmetric operator. If $\sigma(A) \neq \mathbb{C}$, then A is closed.* □

Proof. Exercise! *q.e.d.*

Theorem 5.11. *Let $A : D(A) \to \mathscr{H}$ be symmetric. Then the following are equivalent.*

(1) A is essentially self-adjoint.

(2) $\operatorname{ran}(A \pm i)$ is dense in $\mathscr{H}$.

□

Proof. Easy once one has proven that $\operatorname{ran}\left(\overline{A} \pm i\right) = \overline{\operatorname{ran}(A \pm i)}$ which is left as exercise. *q.e.d.*

Method 2 (Kato-Rellich Method) Assume that $A : D(A) \to \mathscr{H}$ is self-adjoint. When is $A + B : D(A) \to \mathscr{H}$ is self-adjoint, if B is a small "perturbation" of A?

Theorem 5.12 (Kato-Rellich)**.** *Let $A : D(A) \to \mathscr{H}$ be self-adjoint, $B : D(A) \to \mathscr{H}$ symmetric. If for some $\varepsilon < 1$ and some $C_\varepsilon v$*

$$\|Bx\| \leqslant \varepsilon\|Ax\| + C_\varepsilon\|x\|$$

holds for all $x \in D(A)$, we say that ε is an A-bound for B, then $A + B$ is self-adjoint on $D(A + B) = D(A)$, i.e. "small perturbations" do not destroy self-adjointness. □

Lemma 5.13. *Let A and B be as above. Then for all $\mu > 0$, $B(A + i\mu)^{-1}$ is a bounded operator and*

$$\limsup_{\mu \to \infty} \|B(A \pm i\mu)^{-1}\| \leqslant \varepsilon$$

where ε is the A-bound of B. □

Proof. Because A is self-adjoint, $i\mu \in \rho(A)$ for all $\mu > 0$ thus $(A \pm i\mu)^{-1}$ is a bounded operator with

$$(A \pm i\mu)^{-1} : \mathscr{H} \longrightarrow D(A)$$

thus $B(A \pm i\mu)^{-1}$ is well-defined on $\mathscr{H}$. We have

$$\begin{aligned}\left\|B(A \pm i\mu)^{-1}\right\| &= \sup_{\substack{x \in \mathscr{H} \\ x \neq 0}} \frac{\|B(A \pm i\mu)^{-1}x\|}{\|x\|} = \sup_{\substack{y \in D(A) \\ y \neq 0}} \frac{\|By\|}{\|(A \pm i\mu)y\|} \leqslant \sup_{\substack{y \in D(A) \\ y \neq 0}} \frac{\varepsilon\|Ay\| + C_\varepsilon\|y\|}{\|(A \pm i\mu)y\|} = \\ &= \sup_{\substack{y \in D(A) \\ y \neq 0}} \frac{\varepsilon\|Ay\| + C_\varepsilon\|y\|}{\sqrt{\|Ay\|^2 + \mu^2\|y\|^2}} \leqslant \sup_{\substack{y \in D(A) \\ y \neq 0}} \frac{\varepsilon\|Ay\| + C_\varepsilon\|y\|}{\max\{\|Ay\|, \mu\|y\|\}} \leqslant \varepsilon + \frac{C_\varepsilon}{\mu}\end{aligned}$$

where the penultimate inequality follows from $\sqrt{a^2 + b^2} \geqslant \max\{|a|, |b|\}$. *q.e.d.*

Proof of Theorem 5.12. To show that $A + B$ is self-adjoint in on $D(A)$, we need to prove that $\operatorname{ran}(A + B \pm i\mu) = \mathscr{H}$ for some $\mu > 0$.
We have $A + B + i\mu = (1 + B(A + i\mu)^{-1})(A + i\mu)$. Here $(A + i\mu)^{-1}$ is well-defined because A is self-adjoint. Then

$$(A + B + i\mu)(D(A)) = \big(1 + B(A + i\mu)^{-1}\big)(A + i\mu)(D(A)) = \big(1 + B(A + i\mu)^{-1}\big)(\mathscr{H})$$

Then this is equal to $\mathscr{H}$ if $1 + B(A + i\mu)^{-1}$ has an inverse. This holds true when $\|B(A + i\mu)^{-1}\| < 1$ by Lemma 4.13. Then we can apply the lemma which in particular states that

$$\|B(A + i\mu)^{-1}\| \leqslant \varepsilon + \frac{C_\varepsilon}{\mu}.$$

Since $\varepsilon < 1$ for μ large enough this is indeed smaller than 1. *q.e.d.*

Theorem 5.14 (Kato-Rellich for Schrödinger Operators)**.** *Consider the operator $A = -\Delta + V$ on $D(A) = H^2(\mathbb{R}^d)$, where V is some real-valued potential function. This is self-adjoint if $V \in L^p(\mathbb{R}^d) + L^q(\mathbb{R}^d)$ for $2 \leqslant p, q \leqslant \infty$, for $d = 1, 2, 3$.* □

Remark 5.15. If $f \in L^p(\mathbb{R}^d)$ for some $1 \leqslant r \leqslant p \leqslant \infty$, then we can write $f = f_1 + f_2$ with $f_1 \in L^r(\mathbb{R}^d)$ and $f_2 \in L^\infty(\mathbb{R}^d)$.
Moreover, we can take f_1 such that $\|f_1\|_{L^r} \leqslant \delta$ for any $\delta > 0$.

This statement can be proven using dominated convergence and its proof is left as an exercise. □

Proof. Because V is real valued, $A = -\Delta + V$ is symmetric and we only need to verify that

$$\|Vu\|_{L^2} \leqslant \varepsilon\| - \Delta u\|_{L^2} + C_\varepsilon\|u\|_{L^2}$$

for some $\varepsilon < 1$. In particular this also shows that $M_V : D(A) \to \mathscr{H}$ is well-defined.
This is equivalent to

$$\|Vu\|_{L^2} \leqslant \varepsilon\|u\|_{H^2} + C_\varepsilon\|u\|_{L^2}$$

and we shall prove that this holds for all $\varepsilon > 0$.
By assumption we can write $V = V_1 + V_2 \in L^2 + L^\infty$ with $\|V_1\|_{L^2} \leqslant \delta$.
By the Sobolev inequality Theorem 3.23 we have for $d = 1, 2, 3$, $L^\infty(\mathbb{R}^d) \subset H^2(\mathbb{R}^d)$ and thus

$$\|Vu\|_{L^2} \leqslant \|V_1u\|_{L^2} + \|V_2u\|_{L^2} \leqslant \|V_1\|_{L^2}\|u\|_{L^\infty} + \|V_2\|_{L^\infty}\|u\|_{L^2} \leqslant \delta C_d\|u\|_{H^2(\mathbb{R}^d)} + C_\delta\|u\|_{L^2}$$

Choosing $C_d\delta = \varepsilon$ yields the result. *q.e.d.*

Example 5.16. $A = -\Delta - \frac{1}{|x|}$ is self-adjoint on $D(A) = H^2(\mathbb{R}^d)$, on $L^2(\mathbb{R}^3)$. This is the case by Kato-Rellich as

$$V(x) = -\frac{1}{|x|} = -\frac{1}{|x|}\mathbf{1}_{\{|x|\leqslant 1\}} - \frac{1}{|x|}\mathbf{1}_{\{|x|>1\}} \in L^p(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$$

for any $p < 3$.
In particular, since for all $u \in L^2(\mathbb{R})^3$ such that $Au = \left(-\Delta u - \frac{1}{|x|}\right)u \in L^2$ then $u \in H^2(\mathbb{R}^3)$ and $-\Delta u, -\frac{u(x)}{|x|} \in L^2$
In fact, $A = -\Delta - \frac{1}{|x|^s}$ is self-adjoint on $D(A) = H^2(\mathbb{R}^3)$ for all $s < \frac{3}{2}$ by the same proof.
But $A = -\Delta - \frac{1}{|x|^s}$ with $s \geqslant \frac{3}{2}$ cannot be extended to a self-adjoint operator on $H^2(\mathbb{R}^3)$.
For this the Kato-Rellich theorem is not enough.

5.1 Quadratic Forms

Let $A : D(A) \to \mathscr{H}$ be self-adjoint operator. Assume that $A \geqslant 1$, i.e. that $\langle u, Au\rangle \geqslant \|u\|^2$ for all $u \in D(A)$.

Then $D(A)$ is a Hilbert space with $\|x\|_A = \|Ax\|$, $\langle x, y\rangle_A = \langle Ax, Ay\rangle$.

Definition 5.17 (Quadratic From Domain)**.** Let $Q(A) = \overline{D(A)}^{\|\cdot\|_{Q(A)}}$, where $\|x\|^2_{Q(A)} = \langle x, Ax\rangle$ for all $x \in D(A)$.
Equivalently

$$Q(A) = \left\{ x \in \mathscr{H} \,\middle|\, x = \lim_{n\to\infty} x_n \text{ in } \mathscr{H} \text{ and } (x_n)_n \subset D(A) \text{ is a } \|\cdot\|_{Q(A)}\text{-Cauchy sequence.} \right\}$$

□

Remark 5.18. Note that this also implies that $x_n \xrightarrow{n\to\infty} x$ in $\big(Q(A), \|\cdot\|_{Q(A)}\big)$. Thus $Q(A)$ is a Hilbert space with norm $\|\cdot\|_{Q(A)}$.
Conversely, $Q(A)$ contains the information of $(A, D(A))$ in the sense that $x \in D(A)$ iff $x \in Q(A)$ and

$$\sup_{\substack{y\in Q(A)\\ \|y\|\leqslant 1}} \left|\langle x, y\rangle_{Q(A)}\right| < \infty.$$

- Indeed, if $x \in D(A)$ then for all $y \in D(A)$ then $\langle x, y\rangle_{Q(A)} = \langle x, Ay\rangle = \langle Ax, y\rangle$. By denseness it follows that $\langle x, y\rangle_{Q(A)} = \langle Ax, y\rangle$ for all $y \in Q(a)$.

  Thus $\sup_{\substack{y\in Q(A)\\ \|y\|\leqslant 1}} \left|\langle x, y\rangle_{Q(A)}\right| \leqslant \|Ax\| < \infty$.

- If $x \in Q(A)$ and $\sup_{\substack{y\in Q(A)\\ \|y\|\leqslant 1}} \left|\langle x, y\rangle_{Q(A)}\right| < \infty$. Then

$$y \longmapsto \langle x, y\rangle_Q$$

  is a continuous, linear functional on $(Q(A), \|\cdot\|_Q)$ (trivially from the Schwartz inequality), but also a continuous linear functional on $(Q(A), \|\cdot\|)$ and by denseness also on the whole Hilbert space $\mathscr{H}$. Thus by the Riesz representation theorem there exists a unique $z \in \mathscr{H}$ such that $\langle x, y\rangle_Q = \langle z, y\rangle$ for all $y \in Q(A)$ and in particular also $\langle x, Ay\rangle = \langle z, y\rangle$ for all $y \in D(A)$. Thus $x \in D(A^*) = D(A)$ as $A^* = A$.

□

Example 5.19. Take $A = 1-\Delta$ on $L^2(\mathbb{R}^d)$. $D(A) = H^2(\mathbb{R}^d)$ and $Q(A) = \overline{H^2(\mathbb{R}^d)}^{\|\cdot\|_{Q(A)}}$ where $\|u\|_{Q(A)} = \sqrt{\langle u, (1-\Delta)u\rangle_{L^2}} = \|u\|_{H^1(\mathbb{R}^d)}$, i.e. $Q(A) = H^1(\mathbb{R}^d)$.

Example 5.20. Take $A = M_a$ on $L^2(\Omega, \mu)$ for $a \geqslant 1$, then

$$D(A) = \left\{u \in L^2 \,\middle|\, au \in L^2\right\}$$
$$Q(A) = \left\{u \in L^2 \,\middle|\, \sqrt{a}u \in L^2\right\}$$

because

$$\|u\|_{Q(A)} = \sqrt{\langle u, Au\rangle_{L^2}} = \sqrt{\langle u, au\rangle_{L^2}} = \|\sqrt{a}u\|_{L^2}.$$

Remark 5.21. If A is self-adjoint and $A \geqslant 1$ then $Q(A) = D\left(\sqrt{A}\right)$. Here $\sqrt{A}$ is defined via Spectral theorem and functional calculus. It satisfies

$$\sqrt{A} \geqslant 0, \qquad \left(\sqrt{A}\right)^2 = A.$$

□

Remark 5.22 (Friedrich Self-Adjoint Extension)**.** Take a symmetric $A : D(A) \to \mathscr{H}$ with $A \geqslant 1$. Then proceeding as follows

$$(A, D(A)) \longrightarrow \left(\langle\cdot,\cdot\rangle_{Q(A)}, Q(A)\right) \xrightarrow{\text{closing}} \left(\langle\cdot,\cdot\rangle_{Q(\widetilde{A})}, Q(\widetilde{A})\right) \longrightarrow \left(\widetilde{A}, D(\widetilde{A})\right)$$

we get a self-adjoint extension $\widetilde{A}$ of A. In general only $\overline{A} \subset \widetilde{A}$ holds. □

Theorem 5.23 (Friedrich's Extension)**.** *Take $A : D(A) \to \mathscr{H}$, $A \geqslant 1$. Define $\|u\|_Q = \sqrt{\langle u, Au\rangle}$ for $u \in D(A)$ and $Q(A) = \overline{D(A)}^{\|\cdot\|_{Q(A)}}$ as above.*

Define $A_F : D(A_F) \to \mathscr{H}$ as

$$D(A_F) = \left\{ x \in Q(A) \,\middle|\, \sup_{\substack{y \in Q \\ \|y\| \leqslant 1}} \left| \langle x, y \rangle_Q \right| < \infty \right\} =$$
$$= \left\{ x \in Q(A) \,\middle|\, \exists z \in \mathscr{H} \; \forall y \in Q(A) : \langle x, y \rangle_Q = \langle z, y \rangle \right\}$$

and $A_F x = z$ for all $x \in D(A_F)$.

Then A_F is a self-adjoint operator and $Q(A_F) = Q$, $A_F\big|_{D(A)} = A$. □

Proof. 1) $D(A) \subset D(A_F)$ because if $x \in D(A)$, then for all $y \in D(A)$

$$\langle x, y \rangle_Q = \langle Ax, y \rangle$$

and thus by denseness $\sup_{\substack{y \in Q(A) \\ \|y\| \leqslant 1}} \left| \langle x, y \rangle_Q \right| < \infty$ and therefore $x \in D(A_F)$.

In particular, $D(A_F)$ is dense in $(\mathscr{H}, \| \cdot \|_{\mathscr{H}})$ and it is also dense in $(Q(A), \| \cdot \|_Q)$.

2) We prove that A_F is a symmetric operator. Take $x, y \in D(A_F) \subset Q(A)$. Then

$$\langle A_F x, y \rangle = \langle x, y \rangle_Q = \overline{\langle y, x \rangle_Q} = \overline{\langle A_F y, x \rangle} = \langle x, A_F y \rangle .$$

3) We prove that $D(A_F) = D(A_F^*)$. Assume that $x \in D(A_F^*)$ then

$$\sup_{\substack{y \in D(A_F) \\ \|y\| \leqslant 1}} |\langle x, A_F y \rangle| < \infty$$

Then by the lemma below $x \in Q$ and thus $\langle x, A_F y \rangle = \langle x, y \rangle_Q$ and therefore

$$\sup_{\substack{y \in D(A_F) \\ \|y\| \leqslant 1}} \left| \langle x, y \rangle_Q \right| < \infty$$

holds. Since $D(A_F)$ is dense in $(Q(A), \| \cdot \|_Q)$ we have

$$\sup_{\substack{y \in Q(A) \\ \|y\| \leqslant 1}} \left| \langle x, y \rangle_Q \right| < \infty \quad \therefore \quad x \in D(A_F).$$

Thus $D(A_F)$ is self-adjoint, $A_F\big|_{D(A)} = A$, $\|x\|_{Q(A_F)} = \|x\|_{Q(A)}$ and therefore $Q(A_F) = Q(A)$. *q.e.d.*

Lemma 5.24. *If $x \in \mathscr{H}$, and $\sup_{\substack{y\in D(A)\\ \|y\|\leqslant 1}} |\langle x, Ay\rangle| < \infty$, then $x \in Q$.* □

Proof. Because $D(A)$ is dense in $\mathscr{H}$, there exists a sequence $(x_n)_n \subset D(A)$ such that $x_n \xrightarrow{n\to\infty} x$ in $\mathscr{H}$. Then for all $y \in D(A)$

$$\langle x, Ay\rangle = \lim_{n\to\infty} \langle x_n, Ay\rangle = \lim_{n\to\infty} \langle x_n, y\rangle_Q$$

Then for all $n \in \mathbb{N}$, $y \mapsto \langle x_n, y\rangle_Q$ is a linear, continuous functional $(Q, \|\cdot\|_Q) \to \mathbb{C}$ and $\|\mathscr{L}_n\| = \|x_n\|_Q$.
The assumption that

$$\sup_{\substack{y\in D(A)\\ \|y\|\leqslant 1}} \left|\lim_{n\to\infty} \langle x_n, Ay\rangle\right| < \infty$$

implies by the uniform boundedness principle that $\sup_{n\in\mathbb{N}} \|x_n\|_Q < \infty$.
Descending to a subsequence we may assume that $x_n \rightharpoonup z$ in Q by the Banach-Alaoglu Theorem 1.20 and therefore also $x_n \rightharpoonup z$ in $\mathscr{H}$ and since $x_n \to x$ strongly in $\mathscr{H}$ it follows that $x = z \in Q$. *q.e.d.*

Remark 5.25. If A is a bounded from below, i.e. $A \geqslant -C$ for some constant C, then we can define the Friedrichs extension of A by

$$A_F = (A + C + 1)_F - C - 1.$$

□

Example 5.26. Let $A = -\Delta - \frac{1}{|x|^s}$ in $L^2(\mathbb{R}^3)$. If $s < \frac{3}{2}$, then A is self-adjoint on $D(A) = H^2(\mathbb{R}^3)$ by Kato-Rellich. If $\frac{3}{2} \leqslant s < 2$, then

$$\langle u, Au\rangle = \int |\nabla u|^2 - \int \frac{|u(x)|^2}{|x|^s} \mathrm{d}s$$

is well-defined on $H^1(\mathbb{R}^d)$. Then we can define a self-adjoint operator $A_F : D(A_F) \to \mathscr{H} = L^2(\mathbb{R}^3)$ by the Friedrichs extension.
Note that $D(A_F) \neq H^2(\mathbb{R}^3)$ but $Q(A_F) = H^1(\mathbb{R}^3)$.

Remark 5.27. If $A : D(A) \to \mathscr{H}$, $A \geqslant -C$ then there exist self-adjoint extensions $A_{\min}, A_{\max}$ such that if B is a self-adjoint extension of A, then

$$A_{\min} \leqslant B \leqslant A_{\max}$$

in the sense that

$$\langle u, A_{\min} u \rangle \leqslant \langle u, Bu \rangle \leqslant \langle u, A_{\max} u \rangle .$$

In fact, $A_{\max} = A_F$ and $A_{\min}$ is the so-called Krein extension. $\square$

Chapter 6

Quantum Dynamics

Given $A : D(A) \to \mathscr{H}$. We want to solve

$$\begin{cases} i\frac{d}{dt}x(t) = Ax(t), & \text{for } t \in \mathbb{R} \\ x(0) = x_0 \end{cases}$$

If A is a bounded, self-adjoint operator, then this equation has a unique solution

$$x(t) = e^{-itA}x_0$$

for all $x_0 \in \mathscr{H}$. Here

$$e^{-itA} = \sum_{n=0}^{\infty} \frac{(-itA)^n}{n!}$$

is well-defined, bounded operator, as A is. Since A is self-adjoint e^{-itA} is a unitary operator on $\mathscr{H}$, i.e. $\left\|e^{-itA}x_0\right\| = \|x_0\|$.

Theorem 6.1 (Stone's Theorem)**.** *Let $A : D(A) \to \mathscr{H}$ be a self-adjoint operator. Then the equation*

$$\begin{cases} i\frac{d}{dt}x(t) = Ax(t), & \textit{for } t \in \mathbb{R} \\ x(0) = x_0 \end{cases}$$

has a unique solution for all $x_0 \in D(A)$. In fact

$$x(t) = e^{-itA}x_0$$

where e^{-itA} is defined via the Spectral theorem. Here the derivative means that for all t

$$\lim_{s\to 0} \frac{x(t+s)-x(t)}{s} = Ax(t)$$

strongly in $\mathscr{H}$. $\square$

Proof. 1) Assume that $A = M_a$ on $\mathscr{H} = L^2(\Omega, \mu)$ and $D(A) = \left\{x \,\middle|\, ax \in L^2\right\}$. Then

$$x(t)(\xi) = e^{-ita(\xi)} x_0(\xi) \in L^2.$$

Moreover, $x_0 \in D(A)$ implies that $ax_0 \in L^2$, thus also $ax(t) \in L^2$ and therefore $x(t) \in D(A)$.

The key-point here is that $\left|e^{-ita(\xi)}\right| = 1$.

2) Generally, for $A : D(A) \to \mathscr{H}$ self-adjoint, we have by the Spectral theorem a unitary operator $U : \mathscr{H} \to L^2(\Omega, \mu)$ such that $UAU^* = M_a$. Then you define

$$e^{-itA} = U^* M_{e^{-ita}} U.$$

and then $x(t) = e^{-itA}x_0$ is well-defined.

3) The differential equation holds as

$$i\frac{d}{dt} e^{-ita(\xi)} = a(\xi) e^{-ita(\xi)}$$

4) Concerning the conservation of the norm note that

$$\begin{aligned}\frac{d}{dt}\|x(t)\|^2 = \frac{d}{dt}\langle x(t), x(t)\rangle = \left\langle \frac{d}{dt}x(t), x(t)\right\rangle + \left\langle x(t), \frac{d}{dt}x(t)\right\rangle = \\ = \langle -iAx(t), x(t)\rangle + \langle x(t), -iAx(t)\rangle = 0\end{aligned}$$

Thus $\|x(t)\| = \|x_0\|$ for all $t \in \mathbb{R}$.

5) Concerning uniqueness assume that $x(t)$ and $y(t)$ are two solutions of differential equation, then $z(t) = x(t) - y(t)$ solves

$$\begin{cases} i\frac{d}{dt}z(t) = Az(t), & \text{for } t \in \mathbb{R} \\ z(0) = 0 \end{cases}$$

then by conservation of norm $\|z(t)\| = \|z(0)\| = 0$, i.e. $x(t) = y(t)$ for all $t \in \mathbb{R}$.

q.e.d.

Theorem 6.2 (Stone's Theorem, Weak Solution)**.** *Let $A : D(A) \to \mathscr{H}$ be self-adjoint. Then the equation*

$$\begin{cases} i\dfrac{d}{dt}x(t) = Ax(t) \\ \quad x(0) = x_0 \in \mathscr{H} \end{cases}$$

has a unique weak solution $x(t) \in \mathscr{H}$, i.e. for all $\varphi \in D(A)$

$$\begin{cases} \frac{d}{dt}\langle ix(t), \varphi\rangle = \langle x(t), A\varphi\rangle \\ x(t) \xrightarrow{t\to 0} x_0 \text{ strongly in } \mathscr{H} \end{cases}$$

Moreover, the unique weak solution is $x(t) = e^{-itA}x_0$. □

Proof. 1) Take $x(t) = e^{-itA}x_0 \in \mathscr{H}$. Then $x(t) \xrightarrow{t\to 0} x_0$ strongly as follows from the Spectral theorem and dominated convergence.

Take $\varphi \in D(A)$. We prove that

$$\frac{d}{dt}\langle ix(t), \varphi\rangle = \langle x(t), A\varphi\rangle$$

By the Spectral theorem, we can assume that $A = M_a$ on $L^2(\Omega, \mu)$.

Then the above equation becomes

$$\frac{d}{dt}\int \overline{ie^{-ita(\xi)}x_0(\xi)}\varphi(\xi)\mathrm{d}\xi = \int \overline{ie^{-ita(\xi)}x_0(\xi)}a(\xi)\varphi(\xi)\mathrm{d}\xi$$

which is equivalent to

$$\lim_{s\to t}\int (-i)\frac{e^{ita(\xi)} - e^{isa(\xi)}}{t-s}\overline{x_0(\xi)}\varphi(\xi)\mathrm{d}\xi = \int \overline{ie^{-ita(\xi)}x_0(\xi)}a(\xi)\varphi(\xi)\mathrm{d}\xi$$

This is correct by dominated convergence as for all $\xi \in \Omega$

$$\lim_{s\to t}\frac{e^{ita(\xi)} - e^{isa(\xi)}}{t-s} = ia(\xi)e^{ita(\xi)}$$

and we have the majorant

$$\left|\frac{e^{ita(\xi)}-e^{isa(\xi)}}{t-s}\right| = \left|\frac{e^{i(t-s)a(\xi)}-1}{t-s}\right| = \frac{\sqrt{(\cos((t-s)\xi)a(\xi)-1)^2+\sin((t-s)a(\xi))^2}}{|t-s|} \leqslant$$
$$\leqslant 2|a(\xi)|$$

Here $\varphi \in D(A)$ implies that $a(\xi)\varphi(\xi) \in L^2$ and thus that $\overline{x_0(\xi)}a(\xi)\varphi(\xi) \in L^1$. We conclude that $x(t) = e^{-itA}x_0$ is a weak solution.

2) Assume that $x(t)$ is a weak solution. We need to prove that $x(t) = e^{-itA}x_0$. The difficulty is that

$$\frac{d}{dt}\langle x(t), x(t)\rangle = 2\,\Re\left\langle \frac{d}{dt}x(t), x(t)\right\rangle = -2\,\Re\langle iAx(t), x(t)\rangle$$

does not make sense as we only know that $x(t) \in \mathscr{H}$.

Indeed, take any $\varphi \in D(A)$, then

$$\begin{aligned}\frac{d}{dt}\left\langle x(t), e^{-itA}\varphi\right\rangle &= \left\langle \frac{d}{dt}x(t), e^{-itA}\varphi\right\rangle + \left\langle x(t), \frac{d}{dt}e^{-itA}\varphi\right\rangle = \\ &= \left\langle x(t), iAe^{-itA}\varphi\right\rangle + \left\langle x(t), (-i)Ae^{-itA}\varphi\right\rangle = 0\end{aligned}$$

where we have to justify the first equality. Indeed,

$$\begin{aligned}\frac{d}{dt}\left\langle x(t), e^{-itA}\varphi\right\rangle &= \lim_{s\to t}\frac{\left\langle x(t), e^{-itA}\varphi\right\rangle - \left\langle x(s), e^{-isA}\varphi\right\rangle}{t-s} = \\ &= \lim_{s\to t}\left\langle \frac{x(t)-x(s)}{t-s}, e^{-itA}\varphi\right\rangle + \lim_{s\to t}\left\langle x(t), \frac{e^{-itA}\varphi - e^{-isA}\varphi}{t-s}\right\rangle = \\ &= \left\langle x(t), iAe^{-itA}\varphi\right\rangle + \left\langle x(t), (-i)e^{-itA}\varphi\right\rangle = 0\end{aligned}$$

We may conclude that, if $x(t)$ is a weak solution, then for all $\varphi \in D(A)$ and all $t \in \mathbb{R}$

$$\left\langle x(t), e^{-itA}\varphi\right\rangle = \langle x_0, \varphi\rangle$$

Consequently, since $e^{-itA}x_0$ is another weak solution then

$$\left\langle e^{-itA}x_0, e^{-itA}\varphi\right\rangle = \langle x_0, \varphi\rangle$$

thus for all $\varphi \in D(A)$ and all $t \in \mathbb{R}$

$$\left\langle x(t) - e^{-itA}x_0, e^{-itA}\varphi \right\rangle = 0$$

choosing $\varphi = e^{itA}\varphi_0$ for some $\varphi_0 \in D(A)$ yields that for all $\varphi_0 \in D(A)$

$$\left\langle x(t) - e^{-itA}x_0, \varphi_0 \right\rangle = 0$$

hence by the denseness of $D(A)$ in $\mathscr{H}$

$$x(t) = e^{-itA}x_0$$

for all $t \in \mathbb{R}$.

q.e.d.

Remark 6.3. If $x(t)$ is a weak solution, then $\|x(t)\| = \|x_0\|$ for all $t \in \mathbb{R}$. □

Definition 6.4. A family of unitary operators $\left\{U(t) \,\middle|\, t \in \mathbb{R}\right\}$ on Hilbert space $\mathscr{H}$ is called a strongly continuous one-parameter unitary group if

- $U(t+s) = U(t)U(s) = U(s)U(t)$
- $\lim_{s\to t} U(s)x = U(t)x$ strongly in $\mathscr{H}$ for all $x \in \mathscr{H}$.

□

Theorem 6.5 (Stone's Theorem, Strongly Continuous One-Parameter Unitary Group)**.**

1) *If $A : D(A) \to \mathscr{H}$ is self-adjoint, then $U(t) = e^{-itA}$ for $t \in \mathbb{R}$ forms a strongly continuous one-parameter unitary group.*

2) *If $\left\{U(t) \,\middle|\, t \in \mathbb{R}\right\}$ is a strongly continuous one-parameter unitary group, then there exists a unique self-adjoint operator $A : D(A) \to \mathscr{H}$ such that $U(t) = e^{-itA}$.*

Moreover,

$$D(A) = \left\{ x \in \mathscr{H} \,\middle|\, \lim_{t\to 0} \frac{U(t)x - x}{t} \text{ exists strongly in } \mathscr{H} \right\}$$

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

$$Ax := i \lim_{t\to 0} \frac{(U(t)-1)x}{t}.$$

A is called the infinitesimal generator of $\{U(t) \,|\, t \in \mathbb{R}\}$.

$\square$

Proof. 1) Trivial by the above!

2) Define the operator $A : D(A) \to \mathscr{H}$ via

$$\begin{aligned} D(A) &= \left\{ x \in \mathscr{H} \,\middle|\, \lim_{t\to 0} \frac{U(t)x - x}{t} \text{ exists weakly in } \mathscr{H} \right\} = \\ &= \left\{ x \in \mathscr{H} \,\middle|\, \exists z \in \mathscr{H}\, \forall \varphi \in \mathscr{H} : \lim_{t\to\infty} \left\langle \frac{(U(t)-1)x}{t}, \varphi \right\rangle = \langle z, \varphi\rangle \right\} \end{aligned}$$

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

$$Ax := i \operatorname*{w-lim}_{t\to 0} \frac{(U(t)-1)x}{t}.$$

Step 1 We prove hat $D(A)$ is dense in $\mathscr{H}$. For all $x \in \mathscr{H}$ and $f \in \mathscr{C}_c^\infty(\mathbb{R})$, define

$$x_f = \int_{\mathbb{R}} f(t)U(t)x\mathrm{d}t$$

where $t \mapsto U(t)x$ is continuous. We prove that $x_f \in D(A)$. Indeed,

$$\begin{aligned} \frac{U(t)-1}{t} x_f &= \int_{\mathbb{R}} \frac{U(t)-1}{t} f(s)U(s)x\mathrm{d}s = \int_{\mathbb{R}} f(x)\frac{U(t+s)-U(s)}{t} x\mathrm{d}s = \\ &= \int_{\mathbb{R}} \frac{f(s-t)-f(s)}{t} U(t)x\mathrm{d}s \end{aligned}$$

Now interchange the limit $t \to 0$ by using the dominated convergence theorem for Bochner integrals as for all $t \in \mathbb{R}$ there is some $\xi \in (s-t,t)$ such that

$$\left| \frac{f(s-t)-f(s)}{t} \right| = |f'(\xi)| \leqslant \|f'\|_{L^\infty} < \infty$$

where the last estimate follows from the compact support of f and thus f'. Thus

$$\lim_{t\to\infty} \frac{U(t)-1}{t} x_f = \lim_{t\to 0} \int_{\mathbb{R}} \frac{f(s-t)-f(t)}{t} U(s)x\mathrm{d}s = -\int_{\mathbb{R}} f'(s)U(s)x\mathrm{d}s = -x_{f'}$$

Thus for all $x \in \mathscr{H}$ and all $f \in \mathscr{C}_c^\infty(\mathbb{R})$

$$\lim_{t\to\infty} \frac{U(t)-1}{t} x_f = -x_{f'}$$

strongly in $\mathscr{H}$. This means that $x_f \in D(A)$ for all $x \in \mathscr{H}$ and all $f \in \mathscr{C}_c^\infty(\mathbb{R})$.

Now we need to prove that for all $x \in \mathscr{H}$ there exists a sequence $(f_n)_n \subset \mathscr{C}_c^\infty(\mathbb{R})$ such that $x_{f_n} \xrightarrow{n\to\infty} x$ strongly in $\mathscr{H}$.

Take any $f \in \mathscr{C}_c^\infty$ with $\int f = 1$ and define $f_n(t) = nf(nt)$. Then

$$x_{f_n} = \int_{\mathbb{R}} f_n(s)U(s)x\mathrm{d}s = \int_{\mathbb{R}} nf(ns)U(s)x\mathrm{d}s = \int_{\mathbb{R}} f(t)\underbrace{U\left(\frac{t}{n}\right)x}_{\xrightarrow{n\to\infty} x}\,\mathrm{d}t \xrightarrow{n\to\infty} \int_{\mathbb{R}} f(t)x = x$$

strongly in $\mathscr{H}$. Thus $D(A)$ is dense in $\mathscr{H}$. We may again interchange the limit $n \to \infty$ and the integral by the dominated convergence theorem for Bochner integrals as

$$\left\| f(t)U\left(\frac{t}{n}\right)x \right\| = |f(t)| \left\| U\left(\frac{t}{n}\right)x \right\| = |f(t)|\|x\|$$

which is an integrable majorant.

Step 2 We need to prove that A is symmetric. For $x, y \in D(A)$ we have by the assumed weak convergence

$$\begin{aligned}\langle x, Ay\rangle &= \lim_{t\to 0}\left\langle x, i\frac{U(t)-1}{t}y\right\rangle = \lim_{t\to 0}\left\langle -i\frac{U(t)^*-1}{t}x, y\right\rangle = \lim_{t\to 0}\left\langle i\frac{U(-t)-1}{-t}x, y\right\rangle = \\ &= \langle Ax, y\rangle\end{aligned}$$

where we used that for a unitary operator $U(t)^* = U(t)^{-1} = U(-t)$ as

$$U(t)U(-t) = U(-t)U(t) = U(0) = \mathbb{I}.$$

Step 3 We need to prove that A is self-adjoint, i.e. $D(A^*) = D(A)$. Take $x \in D(A^*)$, i.e.

$$\sup_{\substack{y\in D(A)\\ ||y||\leqslant 1}} |\langle x, Ay\rangle| < \infty \quad \therefore \quad \sup_{\substack{y\in D(A)\\ ||y||\leqslant 1}} \left|\lim_{t\to 0}\left\langle x, i\frac{U(t)-1}{t}y\right\rangle\right| < \infty$$

Since

$$\lim_{t\to 0}\left\langle x, i\frac{U(t)-1}{t}y\right\rangle = \lim_{t\to 0}\left\langle i\frac{U(-t)-1}{-t}x, y\right\rangle = \lim_{t\to 0}\left\langle i\frac{U(t)-1}{t}x, y\right\rangle$$

it follows that

$$\sup_{\substack{y\in D(A)\\ ||y||\leqslant 1}} \left|\lim_{t\to 0}\left\langle i\frac{U(t)-1}{t}x, y\right\rangle\right| < \infty$$

If we define for all $y \in D(A)$

$$\mathscr{L}_t(y) := \left\langle i\frac{U(t)-1}{t}x, y\right\rangle$$

then $\mathscr{L}_t$ can be extended to be a bounded functional on $\mathscr{H}$ and since $\lim_{t\to 0}\mathscr{L}_t(y)$ is finite it follows that for every $y \in \mathscr{H}$

$$\sup_{t\in\mathbb{R}} |\mathscr{L}_t(y)|$$

is bounded. Note that $\|\mathscr{L}_t\| \leqslant \frac{2}{t}\|x\|$ which is bounded for $|t| \to \infty$.

Thus by the uniform bounded principle, $\sup_t \|\mathscr{L}_t\| \leqslant C < \infty$, i.e. for all t

$$\left\|\frac{U(t)-1}{t}x\right\| \leqslant C$$

Take any sequence $t_n \xrightarrow{n\to\infty} 0$, then the sequence

$$\left(\frac{U(t_n)-1}{t_n}x\right)_n$$

is bounded in $\mathscr{H}$ and thus by the Banach-Alaoglu Theorem 1.20 we can assume by descending to a subsequence that

$$\frac{U(t_n)-1}{t_n}x \xrightarrow[]{n\to\infty} z \in \mathscr{H}$$

weakly. Here the limit z is independent of the choice of $(t_n)_n$ as for all $\varphi \in D(A)$

$$\langle z, \varphi \rangle = \lim_{n\to\infty} \left\langle \frac{U(t_n)-1}{t_n} x, \varphi \right\rangle = \lim_{n\to\infty}, \left\langle \frac{U(-t_n)-1}{t_n} x\varphi \right\rangle = \langle x, -iA\varphi \rangle$$

Then because the limit z is unique we can conclude that

$$\frac{U(t)-1}{t} x \xrightarrow{t\to 0} z$$

Thus for all $x \in D(A^*)$ there limit w-$\lim_{t\to} \frac{U(t)-1}{t} x$ exists and thus $x \in D(A)$.

Therefore $A = A^*$.

Step 4 We show that $U(t) = e^{-itA}$. We can easily check that $U(t)A = AU(t)$ on $D(A)$. We know that for all $x \in D(A)$ that $i\frac{U(t)-1}{t} x \rightharpoonup Ax$, thus $x(t) = U(t)x$ is a weak solution to

$$\begin{cases} i\frac{d}{dt} x(t) = Ax(t) \\ x(0) = x \end{cases}$$

i.e. for all $\varphi \in D(A)$

$$\frac{d}{dt} \langle ix(t), \varphi \rangle = \langle x(t), A\varphi \rangle .$$

Thus $x(t) = U(t)x$ and $e^{-itA}x$ are two weak solutions thus $U(t)x = e^{-itA}x$ for all $x \in \mathscr{H}$ by the uniqueness of weak solutions. Hence $U(t) = e^{-itA}$

Step 5

$$\begin{aligned} D(A) = \left\{ x \in \mathscr{H} \,\middle|\, \underset{t\to 0}{\text{w-lim}} \frac{U(t)-1}{t} x \text{ exists} \right\} = \\ = \left\{ x \in \mathscr{H} \,\middle|\, \lim_{t\to 0} \frac{U(t)-1}{t} x \text{ exists} \right\} \end{aligned}$$

q.e.d.

Remark 6.6. In Mathematical Quantum Mechanics we are generally interested in the following three questions

- Is A self-adjoint?
- $\sigma(A)$ spectral properties

- What is the behaviour of e^{-itA} as $t \to \infty$. Scattering Theory.

$\square$

Chapter 7

Bound States

Remark 7.1. Consider the spectrum of the Hydrogen atom Schrödinger operator $A = -\Delta + V(x)$, $V(x) = -\frac{1}{|x|}$. This potential goes to 0 at infinity and its spectrum consists of two parts: $\{\lambda \in \sigma(A) \mid \lambda < 0\}$ which is discrete, i.e. its is made up of disjoint points, and $\{\lambda \in \sigma(A) \mid \lambda \geqslant 0\}$ which is continuous. □

Definition 7.2. Let $A : D(A) \to \mathscr{H}$ be a self-adjoint operator.
The discrete spectrum is defined to be

$$\sigma_{\text{disc}}(A) := \{\lambda \in \sigma(A) \mid \lambda \text{ is an eigenvalue with finite multiplicity}\}.$$

The essential spectrum is its compliment

$$\sigma_{\text{ess}}(A) := \sigma(A) \setminus \sigma_{\text{disc}}(A).$$

$\lambda \in \sigma_{\text{ess}}(A)$ iff λ is not an eigenvalue or it has infinite multiplicity.

□

Remark 7.3. Recall that λ is an eigenvalue of A iff there exists a non-zero vector in $D(A)$ such that

$$Av = \lambda v.$$

□

Theorem 7.4 (Weyl Sequences)**.** *Let $A : D(A) \to \mathscr{H}$ be a self-adjoint operator and $\lambda \in \mathbb{C}$. Then*

1) *$\lambda \in \sigma(A)$ iff there exists a of unit-vectors sequence $(u_n)_n \subset D(A)$ such that*

$$\|(A-\lambda)u_n\| \xrightarrow{n\to\infty} 0$$

The sequence $(u_n)_n$ is called a ***singular sequence****, or Weyl sequence for λ.*

2) *$\lambda \in \sigma_{disc}(A)$ iff $\lambda \in \sigma(A)$ and any Weyl sequence $(u_n)_n$ for λ is pre-compact, i.e. it contains a subsequence $(u_{n_k})_k$ converging strongly in $\mathscr{H}$.*

3) *$\lambda \in \sigma_{ess}(A)$ iff there exists a Weyl sequence $(u_n)_n$ converging weakly to 0 in $\mathscr{H}$ or equivalently iff there exists an orthonormal Weyl sequence $(u_n)_n$ for λ.*

$\square$

Proof. By the spectral theorem we may assume w.l.o.g. that $A = M_a$ on $L^2(\Omega,\mu)$ and $\sigma(A) = \operatorname{ess\,ran}(a)$.

1) Let $\lambda \in \sigma(A)$. We have to find a Weyl sequence $(u_n)_n$, i.e. a sequence of function satisfying $\|u_n\|_{L^2} = 1$, $\|au_n\|_{L^2} < \infty$ and $\|(a-\lambda)u_n\| \xrightarrow{n\to\infty} 0$, i.e.

$$\lim_{n\to\infty} \int_\Omega |a(\xi)-\lambda|^2 |u_n(\xi)|^2 \mathrm{d}\mu(\xi) = 0.$$

By assumption we have $\lambda \in \sigma(A) = \operatorname{ess\,ran}(a)$, i.e. for all $\varepsilon > 0$

$$\mu\big(\big\{\xi \,\big|\, |a(\xi)-\lambda| < \varepsilon\big\}\big) > 0.$$

We choose

$$u_n = \frac{\mathbf{1}_{\left\{|a(\xi)-\lambda|<\frac{1}{n}\right\}}}{\mu\big(\big\{|a(\xi)-\lambda| < \frac{1}{n}\big\}\big)}$$

for which $\|u_n\|_{L^2} = 1$ holds. Then

$$\int_\Omega |a(\xi)-\lambda|^2 |u_n(\xi)|^2 \mathrm{d}\mu(\xi) \leqslant \int_\Omega \frac{1}{n^2} |u_n(\xi)|^2 \mathrm{d}\mu(\xi) = \frac{\|u_n\|_{L^2}^2}{n^2} = \frac{1}{n^2} \xrightarrow{n\to\infty} 0$$

Conversely, assume that there exists a Weyl sequence $(u_n)_n$ for λ. We have to prove that $\lambda \in \sigma(A) = \operatorname{ess\,ran}(a)$. Assume that $\lambda \notin \operatorname{ess\,ran}(a)$ then there exists a $\varepsilon > 0$ such that

$$\mu(\{|a - \lambda| < \varepsilon\}) = 0.$$

Then $|a(\xi) - \lambda| \geqslant \varepsilon$ for almost every $\xi \in \Omega$. It follows that

$$0 \xleftarrow{\infty \leftarrow n} \int_\Omega |a(\xi) - \lambda|^2 |u_n(\xi)|^2 \mathrm{d}\mu(\xi) \geqslant \varepsilon^2 \int_\Omega |u_n(\xi)|^2 \mathrm{d}\mu(\xi) \geqslant \varepsilon^2$$

where the leftmost convergence from the fact that $(u_n)_n$ is a Weyl sequence. This is a contradiction. ↯

2) Assume that $\lambda \in \sigma_{\text{disc}}(A)$ and let $(u_n)_n$ be a Weyl sequence for λ. We have to prove that $(u_n)_n$ is pre-compact. By the lemma below it follows from $\lambda \in \sigma_{\text{disc}}(A)$ that there exists an $\varepsilon > 0$ such that

$$\mu\big(a^{-1}((\lambda - \varepsilon, \lambda + \varepsilon) \setminus \{\lambda\})\big) = 0$$

Then since $(u_n)_n$ is Weyl sequence

$$0 \xleftarrow{\infty \leftarrow n} \int_\Omega |a(\xi) - \lambda|^2 |u_n(\xi)|^2 \mathrm{d}\mu(\xi) = \int_{a^{-1}(\lambda)} \cdots + \int_{\Omega \setminus a^{-1}(\lambda)} \cdots \geqslant \int_{a^{-1}(\lambda)} \varepsilon^2 |u_n(\xi)|^2 \mathrm{d}\mu(\xi)$$

thus

$$\int_{a^{-1}(\lambda)} |u_n(\xi)|^2 \mathrm{d}\mu(\xi) \xrightarrow{n \to \infty} 0.$$

It therefore suffices to show that

$$\big(\mathbf{1}_{a^{-1}(\lambda)} u_n(\xi)\big)_n$$

is pre-compact in L^2. However, as $\lambda \in \sigma_{\text{disc}}(A)$ iff λ is an eigenvalue of M_a with finite multiplicity which in turn is equivalent to $\mathbf{1}_{a^{-1}(\lambda)} L^2$ being a non-empty, finite-dimensional subspace of $L^2(\Omega, \mu)$.

Thus since $(u_n)_n$ is bounded, $\big(\mathbf{1}_{a^{-1}(\lambda)} u_n(\xi)\big)_n$ is a bounded subset of a finite-dimensional Hilbert space and is thus pre-compact.

Note here that u is an eigenfunction of M_a with eigenvalue of λ, iff

$$\begin{aligned} M_a u = \lambda u &\iff a(\xi)u(\xi) = \lambda u(\xi) \text{ for a.e. } \xi \iff \\ &\iff a(\xi) = \lambda \text{ for a.e. } \xi \in \operatorname{supp}(u) \iff \\ &\iff u \text{ is supported on } a^{-1}(\lambda) \iff \\ &\iff u \in \mathbf{1}_{a^{-1}(\lambda)} L^2(\Omega, \mu) \text{ the eigenspace of } M_a \text{ with eigenvalue } \lambda. \end{aligned}$$

Conversely, assume that $\lambda \in \sigma(A)$ and that for every Weyl sequence $(u_n)_n$, there exists a subsequence converging strongly. We have to prove that $\lambda \in \sigma_{\text{disc}}(A)$.

We shall fist prove that λ is an isolated point in $\sigma(A) = \operatorname{ess\,ran}(a)$. Assume that λ is not an isolated point. The for all $\varepsilon > 0$

$$\mu\Big(a^{-1}((\lambda - \varepsilon, \lambda + \varepsilon) \setminus \{\lambda\})\Big) > 0.$$

Choose a positive, monotonously decreasing sequence $(\varepsilon_n)_n$ converging to 0 such that the following sequence of sets have positive measure

$$B_n := \Big(a^{-1}((\lambda - \varepsilon_n, \lambda - \varepsilon_{n+1}) \cup (\lambda + \varepsilon_{n+1}, \lambda + \varepsilon_n))\Big)$$

Define $u_n := \frac{\mathbf{1}_{B_n}}{\mu(B_n)}$, then $(u_n)_n$ is a Weyl sequence, as $\|u_n\|_{L^2} = 1$, and

$$\int\limits_{\Omega} |a(\xi) - \lambda|^2 |u_n(\xi)|^2 \mathrm{d}\mu(\xi) \leqslant \int\limits_{\Omega} \varepsilon_n^2 |u_n(\xi)| \mathrm{d}\mu(\xi) = \varepsilon_n^2 \xrightarrow{n\to\infty} 0.$$

But $(u_n)_n$ is an orthonormal family because $\operatorname{supp} u_n \cap \operatorname{supp} u_m = \emptyset$ if $n \neq m$. Thus $u_n \xrightharpoonup{n\to\infty} 0$ weakly. Thus u_n cannot have any strongly convergent subsequence since any possible limit would need to have norm 1 which is a contradiction to the above. ↯

If λ is an isolated point of $\operatorname{ess\,ran}(a)$ then $a^{-1}(\lambda)$ has to have positive measure (why?). Thus λ is an eigenvalue with eigenvector

$$u = \frac{\mathbf{1}_{a^{-1}(\lambda)}}{\mu(a^{-1}(\lambda))}.$$

Moreover, the eigenspace of λ has to finite-dimension, for otherwise we could choose an infinite sequence $(u_n)_n$ of orthonormal vectors within it. This would form a Weyl sequence weakly converging to zero contradicting its pre-compactness.

3) Let $\lambda \in \sigma_{\text{ess}}(A)$. We need to find a Weyl sequence $(u_n)_n$ that is an orthonormal family.

If λ possesses an infinite-dimensional eigenspace, then we can choose an orthonormal basis $(u_n)_n$ of that eigenspace which would also be a Weyl sequence.

If λ is not an isolated point in $\operatorname{ess\,ran}(a)$, then for all $\varepsilon > 0$

$$\mu\big(a^{-1}((\lambda-\varepsilon,\lambda+\varepsilon)\setminus\{\lambda\})\big) > 0$$

Then we can define a Weyl sequence $(u_n)_n$ as above, with $\operatorname{supp} u_n \cap \operatorname{supp} u_m = \emptyset$ for $n \neq m$ thus forming an orthonormal basis.

Conversely, if there exists a Weyl sequence $(u_n)_n$, such that $u_n \xrightarrow{n\to\infty} 0$ weakly. Then $\lambda \notin \sigma_{\text{disc}}(A)$ and thus $\lambda \in \sigma_{\text{ess}}(A)$.

q.e.d.

Lemma 7.5. *$\lambda \in \sigma_{disc}(A)$ implies that λ is an isolated point in the spectrum of A, i.e. there exists an $\varepsilon > 0$ such that*

$$\mu\big(a^{-1}((\lambda-\varepsilon,\lambda+\varepsilon)\setminus\{\lambda\})\big) = 0$$

□

7.1 Weyl Theory

Definition 7.6. Let $A : D(A) \to \mathscr{H}$ be a self-adjoint operator and $B : D(A) \to \mathscr{H}$. We say that B is A-relatively compact iff $B(A+i)^{-1}$ is a compact operator on $\mathscr{H}$, or equivalently for every bounded sequence $(u_n)_n$ in $(D(A), \|\cdot\|_A)$, there exists a subsequence $(u_{n_k})_k$ such that Bu_{n_k} converges strongly in $\mathscr{H}$ (why?). □

Theorem 7.7 (Weyl)**.** *Let $A : D(A) \to \mathscr{H}$ be a self-adjoint operator and $B : D(A) \to \mathscr{H}$ symmetric and A-relatively compact. Then*

1) B is A-relatively bounded with arbitrarily small bound ε, i.e. for all $\varepsilon > 0$, there *exists a constant C_ε such that for all $u \in D(A)$*

$$\|Bu\| \leqslant \varepsilon\|Au\| + C_\varepsilon\|u\|.$$

Consequently, $A+B$ is self-adjoint on $D(A)$ by the Kato-Rellich Theorem 5.12.

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

□

Proof. 1) We shall prove this by showing that for any $\varepsilon > 0$

$$\lim_{\mu\to\infty} \|B(A+i\mu)^{-1}\| < \varepsilon$$

or equivalently

$$\lim_{\mu\to\infty} \|B(A+i\mu)^{-1}\| = 0$$

For $\mu > 0$ write

$$B(A+i\mu)^{-1} = \underbrace{B(A+i)^{-1}}_{\text{compact}}\underbrace{(A+i)(A+i\mu)^{-1}}_{\text{bounded}}$$

The result now directly follows from the lemma below.

2) Let $\lambda \in \sigma(A)$ then there exists a Weyl sequence of unit vectors $(u_n)_n \subset D(A)$, such that $(A-\lambda)u_n \xrightarrow{n\to\infty} 0$ and $u_n \xrightarrow{n\to\infty} 0$. Then to prove that $(u_n)_n$ is a Weyl sequence for $A+B$ it suffices to show that $Bu_n \xrightarrow{n\to\infty} 0$ strongly in $\mathscr{H}$.

To see this note that

$$Bu_n = B(A+i)^{-1}(A-\lambda+\lambda+i)u_n = \underbrace{B(A+i)^{-1}}_{\text{compact}}\big(\underbrace{(A-\lambda)u_n}_{\xrightarrow{n\to\infty}0} + \underbrace{(\lambda+i)u_n}_{\xrightarrow{n\to\infty}0}\big) \xrightarrow{n\to\infty} 0$$

strongly.

The converse follows by replacing A with $A+B$ and B with $-B$ as B, and thus $-B$ are relatively $A+B$-compact. To see this note that

$$B(A+B+i)^{-1} = B\big(\big(1+B(A+i)^{-1}\big)(A+i)\big)^{-1} = \underbrace{B(A+i)^{-1}}_{\text{compact}}\big(1+B(A+i)^{-1}\big)^{-1}$$

The rightmost operator is bounded. To see this note that as $B(A+i)^{-1}$ is compact

$$B(A+i)^{-1} = \sum_n \lambda_n |v_n\rangle \langle v_n| \,.$$

Then $1 + B(A+i)^{-1}$ has a bounded inverse iff there is an open neighbourhood of -1 not disjoint from $(\lambda_n)_n$. This is the case since $-1 \in \rho(B(A+i)^{-1})$. Suppose that $-1 \in \sigma(B(A+i)^{-1})$ then it must be an eigenvalue and therefore there must exist some $u \in \mathscr{H}$ such that

$$B(A+i)^{-1}u = -u \iff Bv = -(A+i)v \iff (A+B)v = -iv$$

where $v \in D(A)$ such that $(A+i)v = u$, which exists since A is self-adjoint. Now the rightmost equality is a contradiction since $A+B$ is self-adjoint.

q.e.d.

Lemma 7.8. *(i) Let A be a self-adjoint operator. Then for all $u \in \mathscr{H}$*

$$\lim_{\mu\to\infty} \left\|(A+i)(A+i\mu)^{-1}u\right\| = 0.$$

(ii) Let B be a compact operator, and $(A_n)_n$ a sequence of bounded operator such that for all $u \in \mathscr{H}$, $\|A_n u\| \xrightarrow{n\to\infty} 0$, then $\|BA_n\| \xrightarrow{n\to\infty} 0$.

□

Proof. Exercise! *q.e.d.*

Example 7.9. Let $V : \mathbb{R}^d \to \mathbb{R}$ be a potential with $V \in L^2(\mathbb{R}^d) + L^p(\mathbb{R}^d)$, $2 \leqslant p < \infty$. Then V $(-\Delta)$-relatively compact (Exercise!), and thus

$$\sigma_{\mathrm{ess}}(-\Delta + V) = \sigma_{\mathrm{ess}}(-\Delta) = [0,\infty)$$

For example this holds for $V(x) = -\frac{1}{|x|}$ in $\mathbb{R}^3$.

7.2 Bound States

Definition 7.10. Let A be a self-adjoint operator. If u is an eigenfunction of A with eigenvalue λ outside the essential spectrum, then u is called a bound state. □

We shall now investigate two questions concerning bound states:

1) How many bound states are there?

2) What are the basic properties of bound states.

Theorem 7.11 (Min-Max Principle)**.** *Let $A : D(A) \to \mathscr{H}$ be a self-adjoint operator and bound from below. Define the n^{th} min-max value or singular value for $n \in \mathbb{N}$ to be*

$$\mu_n = \inf_{\substack{M \subset D(A) \\ \dim M = n}} \max_{\substack{u \in M \\ \|u\|=1}} \langle u, Au \rangle$$

1) μ_n is increasing, i.e. $\mu_1 \leqslant \mu_2 \leqslant \cdots$ with $\mu_n \xrightarrow{n\to\infty} \mu_\infty$ where $\mu_\infty = \inf \sigma_{ess}(A)$.

2) If $\mu_n < \mu_\infty$, then μ_n is the n^{th} lowest eigenvalue of A.

□

Proof. Look at

$$\mu_1 = \inf_{\substack{u \in D(A) \\ \|u\|=1}} \langle u, Au \rangle = \inf \sigma(A) \in \sigma(A)$$

There are two possibilities.

1) If $\mu_1 = \mu_\infty$, we need to prove that $\mu_\infty = \inf \sigma_{\text{ess}}(A)$. We know that

$$\mu_\infty = \mu_1 = \inf \sigma(A) \leqslant \inf \sigma_{\text{ess}}(A)$$

so it is enough to prove that $\mu_\infty \in \sigma_{\text{ess}}(A)$.

2) If $\mu_1 < \mu_\infty$, we need to prove that μ_1 is an eigenvalue.

Then we proceed by an induction argument: Split $H = W \oplus W^\perp$, $W = \text{span}\{u_1\}$, where $Au_1 = \mu_1 u_1$ then $A : W \to W$ and thus $A : W^\perp \to W^\perp$. Thus we consider $A\big|_{W^\perp}$ instead for which we have

$$\mu_n(A\big|_{W^\perp}) = \mu_{n+1}(A).$$

Let us check the details. By the spectral theorem, we may assume w.l.o.g. that $A = M_a$ on $L^2(\Omega, \nu)$. Consider

$$\mu_1 = \inf_{\|u\|=1} \langle u, Au\rangle = \inf \sigma(A).$$

- If μ_1 is an isolated point of $\sigma(A)$ or if $\nu(a^{-1}(\mu_1)) > 0$, then μ_1 is an eigenvalue of A (the proof of this is similar to that of Weyl theory) and we can proceed by the induction argument.

  If μ_1 has infinite multiplicity then trivially $\mu_n = \mu_1$ for all $n \in \mathbb{N}$.

- If μ_1 is not an isolated point of $\sigma(A)$, and $\nu(a^{-1}(\mu_1)) = 0$ (i.e. $\mu_1 \in \sigma_{\text{ess}}(A)$) then we have $\mu_1 = \mu_\infty$. Indeed, we will prove that $\mu_n = \mu_1$ for all $n \in \mathbb{N}$.

  Since $\mu_1 \in \sigma(A)$ we have for all $\varepsilon > 0$

$$\nu\big(a^{-1}(\mu_1 - \varepsilon, \mu_1 + \varepsilon)\big) > 0$$

  but for any positive, monotonous zero sequence $(\varepsilon_n)_n$

$$\lim_{n\to\infty} \nu\big(a^{-1}(\mu_1 - \varepsilon_n, \mu_1 + \varepsilon_n)\big) = \nu\big(a^{-1}(\mu_1)\big) = 0$$

  Furthermore, we can choose the sequence in such a way that

$$\nu\big(a^{-1}(\mu_1 - \varepsilon_n, \mu_1 + \varepsilon_n)\big) > \nu\big(a^{-1}(\mu_1 - \varepsilon_{n+1}, \mu_1 + \varepsilon_{n+1})\big)$$

  Then define $\varphi_n = \frac{\mathbf{1}_{\Omega_n}}{\sqrt{\nu(\Omega_n)}}$ where

$$\Omega_n = a^{-1}((\mu_1 - \varepsilon_n, \mu_1 + \varepsilon_n) \setminus (\mu_1 - \varepsilon_{n+1}, \mu_1 + \varepsilon_{n+1}))$$

  which is an orthonormal family in $L^2(\Omega)$. Define $M_{m,n} := \operatorname{span}\{\varphi_m, \varphi_{m+1}, \ldots, \varphi_{m+n-1}\big)$, $\dim M_{m,n} = n$. Then for all $u \in M_n$ with $\|u\| = 1$

$$\langle u, Au\rangle = \int_\Omega a(\xi)|u(\xi)| \mathrm{d}\nu(\xi) \leqslant \max_{k=m,\ldots,m+n-1} \langle \varphi_k, A\varphi_k\rangle \leqslant \mu_1 + \varepsilon_m$$

  Thus for all $m \in \mathbb{N}$

$$\mu_n(A) \leqslant \max_{\substack{u\in M_{m,n}\\ \|u\|=1}} \langle u, Au\rangle \leqslant \mu_1 + \varepsilon_m$$

taking m to infinity we thus find that

$$\mu_n(A) \leqslant \mu_1$$

which proves the claim that $\mu_1 = \mu_\infty$ and together with the case of an eigenfunction of infinite multiplicity, then if $\mu_1 \in \sigma_{\text{ess}}(a)$ then $\mu_\infty = \inf \sigma_{\text{ess}}(A)$ and $\mu_\infty = \inf \sigma_{\text{ess}}(A)$.

q.e.d.

Remark 7.12.1) (Max-Min Principle) We also have

$$\mu_n(A) = \sup_{\substack{M_{n-1} \subset D(A)8 \\ \dim M_{n-1} = n-1}} \inf_{\substack{u \perp M_{n-1} \\ \|u\|=1}} \langle u, Au \rangle \,.$$

In particular if $\mu, \ldots, \mu_{n-1}$ are eigenvalues with eigenfunctions $u_1, \ldots, u_{n-1}$ then

$$\mu_n(A) = \inf_{\substack{u \perp \{u_1, \ldots, u_{n-1}\} \\ \|u\|=1}} \langle u, Au \rangle$$

2) $\mu_n(A)$ is determined by the quadratic form of A, i.e.

$$\mu_n(A) = \inf_{\substack{M \subset Q(A) \\ \dim M = n}} \max_{\substack{u \in M \\ \|u\|=1}} Q(u)$$

where $Q(u) = \langle u, Au \rangle$ if $u \in D(A)$. If B is a symmetric operator bounded from below let B_F be its Friedrichs extension then

$$\mu_n(B) = \mu_n(B_F).$$

3) The mapping $A \mapsto \mu_n(A)$ is monotone

$$A \geqslant B \quad \Longrightarrow \quad \mu_n(A) \geqslant \mu_n(B).$$

and thus for $B \geqslant 0$

$$\mu_n(A + B) \geqslant \mu_n(A).$$

$\square$

Theorem 7.13. *Consider $A = -\Delta + V$ on $L^2(\mathbb{R}^3)$ with $V \in L^2 + L^p$, $\infty > p > 2$. Then A is self-adjoint on $D(A) = H^2$ and $\sigma_{ess}(A) = [0, \infty)$.*

1) *If $V(x) \leqslant -\frac{1}{|x|^a}$ for $|x|$ large enough and $0 < a < 2$, then A infinitely many negative eigenvalues.*

2) *If $V(x) \geqslant -\frac{1}{|x|^a}$ for $|x|$ large and $a > 2$, then A has finitely many negative eigenvalues.*

□

Sketch of Proof. 1) From the min-max principle, we need to show that $\mu_n(A) < 0 = \inf \sigma_{\text{ess}}(A) = \mu_\infty$ for all $n \geqslant 1$. We have to find an orthonormal family $(\varphi_n)_n$ with disjoint support such that $\langle \varphi_n, A\varphi_n \rangle < 0$ for all $n \geqslant 1$.

2) Again by the min-max principle we have to prove that fro some $\mu_n(A) \geqslant 0$ for n large enough. Note that

$$A = -\Delta + V = -\frac{\Delta}{2} + V\mathbf{1}_{|x|\leqslant R} + \underbrace{\left(-\frac{\Delta}{2}\right)}_{\geqslant \frac{1}{8|x|^2}} + \underbrace{V\mathbf{1}_{|x|\geqslant R}}_{\geqslant -\frac{1}{|x|}} \geqslant -\frac{\Delta}{2} + V\mathbf{1}_{|x|\leqslant R} =: B$$

for R large enough since $a > 2$. So $\mu_n(A) \geqslant \mu_n(B)$ and it suffice to prove that $\mu_n(B) \geqslant 0$ if n is large. This step allows us to assume that V has compact support. Assume that B infinitely many eigenvalues below 0, i.e. there exists an orthonormal family $(u_n)_n$ of eigenfunctions such that

$$-\frac{1}{2}\Delta u_n + V u_n = \mu_n u_n$$

We can check that u_n is bound in $H^2(\mathbb{R}^3)$ thus by the Sobolev embedding theorem $u_n \xrightarrow{n\to\infty} u$ strongly in L^∞_{loc}. On the other hand, $(u_n)_n$ is an orthonormal family and thus weakly converges to 0 in L^2. Hence $u_n \to 0$ in L^∞_{loc}.

$V u_n \to 0$ strongly in L^2 because $V \in L^2$ and V has compact support. Thus

$$-\Delta u_n = -V u_n + \mu_n u_n \xrightarrow{n\to\infty} 0$$

strongly in L^2. However, $(-\Delta - \mu_n)u_n = -Vu_n$ hence $\|u_n\| = 1$ and

$$u_n = -\underbrace{(-\Delta - \mu_n)^{-1}}\to (-\Delta)^{-1}\underbrace{Vu_n}_{\to 0}$$

which is a contradiction (why?).

Another way of seeing this is by proving that

$$\sqrt{|V|}u_n = -\operatorname{sgn}(V)\sqrt{|V|}(-\Delta - \mu_n)^{-1}\sqrt{|V|}\sqrt{|V|}u_n$$

where $\sqrt{|V|}(-\Delta - \mu_n)^{-1}\sqrt{|V|}$ is a compact operator.

q.e.d.

Theorem 7.14 (Schrödinger Operator with Trapping Potential)**.** *Consider $A = -\Delta + V$ on $L^2(\mathbb{R}^3)$, $V \in L^{3/2}_{loc}$, $V(x) \to \infty$ as $|x| \to \infty$. Then: A is bounded from below and can be extended to be a self-adjoint operator by Friedrichs extension. Moreover, A has a compact resolvent, i.e. $(A+z)^{-1}$ is compact for all $z \in \rho(A)$.*
Consequently, there exists an orthonormal basis $(u_n)_n$ and $\mu_n \uparrow \infty$ such that $Au_n = \mu_n u_n$. □

Proof. By the min-max principle we need to show that $\mu_n \uparrow \infty$. Assume by contradiction that $\mu_n \xrightarrow{n\to\infty} \mu_\infty < \infty$. Thus $\mu_\infty \in \sigma_{\text{ess}}(A)$. Consequently there exists a singular Weyl sequence $(\varphi_n)_n$ of orthonormal vectors, converging weakly to 0, such that

$$\|(A - \mu_\infty)\varphi_n\|_{L^2} \xrightarrow{n\to\infty} 0$$

Then we can show that φ_n is bounded in H^1 and thus by descending to a subsequence we have that $\varphi_n \to 0$ in $L^p_{\text{loc}}(\mathbb{R}^3)$ for $p < 6$.
Then

$$\langle \varphi_n, A\varphi_n\rangle = \int |\nabla\varphi_n|^2 + \int V|\varphi_n|^2 \geqslant \int V|\varphi_n|^2 = \int_{|x|\leqslant R} V|\varphi_n|^2 + \int_{|x|\geqslant R} V|\varphi_n|^2$$

and

$$\int_{|x|\geqslant R} V|\varphi_n|^2 \geqslant \underbrace{\inf_{|x|\geqslant R} V(x)}_{\xrightarrow{R\to\infty} 0} \underbrace{\int_{|x|\geqslant R} |\varphi_n|^2}_{\xrightarrow{n\to\infty} 1} \longrightarrow +\infty$$

as $n \to \infty$ and then $R \to \infty$.
Thus $\langle \varphi_n, A\varphi_n \rangle \xrightarrow{n\to\infty} 0$. But this contradicts $\langle \varphi_n, A\varphi_n \rangle \xrightarrow{n\to\infty} \mu_\infty < \infty$.

q.e.d.

Theorem 7.15 (Exponential Decay of Bound States). *Consider $A = -\Delta + V$ with $V \in L^2(\mathbb{R}^3) + L^p(\mathbb{R}^3)$ and $2 < p < \infty$. Assume that $V(x) \to \infty$ as $|x| \to \infty$. If u is an eigenfunction of A with eigenvalue $E < 0$, then*

$$\int_{\mathbb{R}^3} |u(x)|^2 e^{2\alpha|x|} \mathrm{d}x < \infty$$

for all $0 < \alpha < \sqrt{|E|}$. □

Lemma 7.16 (IMS Localisation). *If $\varphi : \mathbb{R}^d \to \mathbb{R}$ is smooth, then as quadratic forms in L^2*

$$\frac{\varphi^2(-\Delta) + (-\Delta)\varphi^2}{2} = \varphi(-\Delta)\varphi - |\nabla\varphi|^2.$$

Consequently, if $(\varphi_i)_i$ with

$$\sum_{i\in I} \varphi_i^2 = 1$$

then

$$-\Delta = \sum_{i\in I} \varphi_i(-\Delta)\varphi_i - \sum_i |\nabla\varphi_i|^2,$$

i.e.

$$\int |\nabla u|^2 = \sum_{i\in I} \int |\nabla(\varphi_i u)|^2 - \sum_i \int |\nabla\varphi_i|^2|u|^2$$

□

Proof. This follows from a simple integration by parts. *q.e.d.*

Proof of Theorem. Let $-\Delta u + Vu = Eu$. Then for a real-valued, smooth φ

$$\left\langle \varphi^2 u, (-\Delta + V - E)u \right\rangle = 0$$

Thus

$$\left\langle u, \frac{\varphi^2(-\Delta + V - E) + (-\Delta + V - E)\varphi^2}{2} u \right\rangle = 0$$

By IMS localisation

$$\int |\nabla(\varphi u)|^2 + \int V\varphi^2|u|^2 - E\int \varphi^2|u|^2 - \int |\nabla\varphi|^2|u|^2 = 0$$

Since $V(x) \to \infty$ as $|x| \to \infty$, if $\operatorname{supp}\varphi \subset \{|x| \geqslant R\}$ with R large, then

$$\left|\int V\varphi^2|u|^2\right| \leqslant \varepsilon \int \varphi^2|u|^2$$

for $\varepsilon > 0$ small. Thus

$$\int |\nabla(\varphi u)|^2 \geqslant (E-\varepsilon)\int \varphi^2|u|^2$$

To conclude we need to show φ appropriately

$$0 = \underbrace{\int |\nabla(\varphi u)|^2}_{\geqslant 0} + \underbrace{\int V\varphi^2|u|^2}_{\geqslant -\varepsilon\int\varphi^2|u|^2} - E\int \varphi^2|u|^2 - \int |\nabla\varphi|^2|u|^2$$

thus

$$(|E|-\varepsilon)\int \varphi^2|u|^2 \leqslant \int |\nabla\varphi|^2|u|^2$$

A good choice of φ is $\operatorname{supp}\varphi \subset \{|x| \geqslant R\}$ for R large and $|\nabla\varphi| \sim \varphi$. Thus we can choose $\varphi = e^f$ on $|x| \geqslant R$ for some function f such that $|\nabla f| \leqslant \kappa$ and $f \sim \kappa|x|$ where $\kappa < \sqrt{|E|-\varepsilon}$ This tells us that

$$\int e^{2f}u^2 < \infty.$$

q.e.d.

Theorem 7.17 (CLR - Cwikel-Lieb-Rozenblum)**.** *If $d \geqslant 3$, $V \in L^{\frac{d}{2}}(\mathbb{R}^d)$, then*

$$\big|\{\textit{negative eigenvalues of } -\Delta + V\}\big| \leqslant C\int_{\mathbb{R}^d} |V_-|^{\frac{d}{2}}$$

for a universal constant C that only depends on the dimension, and

$$V_- = \begin{cases} -V, & \text{if } V \leqslant 0 \\ 0, & \text{if } V \geqslant 0 \end{cases}$$

$\square$

Remark 7.18. 1) Semi-Classical Analysis: We have the approximate principle that

$$\text{one quantum bound state of } -\Delta+V \quad \leftrightsquigarrow \quad \text{one unit volume in phase space in } \mathbb{R}^d\times\mathbb{R}^d$$

in particular

$$\dim \mathbf{1}_{(-\Delta+V)<0} \leftrightsquigarrow \int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} \mathbf{1}_{\{|2\pi k|^2+V(x)<0\}} \mathrm{d}k\mathrm{d}x = C_{\mathrm{cl}} \int\limits_{\mathbb{R}^d} V_-^{\frac{d}{2}}$$

Note that $\{|2\pi k|^2 + V(x) < 0\}$ is the region in phase space where the particular has energy less than 0.

2) The assumption $d \geqslant 3$ is crucial! If $d = 1, 2$ and if $V \leqslant 0, V \not\equiv 0$, then $-\Delta + V$ has at least one negative eigenvalue (exercise!).

$\square$

Proof. Let

$$W = \overline{\operatorname{span}\{\text{eigenfunctions of } -\Delta+V \text{ with negative eigenvalue}\}} = \operatorname{ran} \mathbf{1}_{\{-\Delta+V<0\}}.$$

We have to prove that $\dim W \leqslant C \int V_-^{\frac{d}{2}}$. Assume that $\dim W \geqslant N$, then $\dim(\sqrt{-\Delta}W) \geqslant N$ (why?).

Then there exists an orthonormal family $\left(\sqrt{-\Delta}u_j\right)_j$ in $L^2(\mathbb{R}^d)$, i.e. $\left\langle\sqrt{-\Delta}u_j, \sqrt{-\Delta}u_k\right\rangle = \delta_{jk}$ and $u_j \in W$.

Then per assumption for all $j = 1, \ldots, N$

$$\langle u_j, (-\Delta+V)u_j\rangle \leqslant 0$$

since $u_j \in W$. Thus

$$1 + \int V|u_j|^2 \leqslant 0$$

and therefore taking the sum over j yields

$$N + \int V\rho \leqslant 0$$

where

$$\rho(x) = \sum_{j=1}^{N} |u_j(x)|^2.$$

It follows that

$$N \leqslant -\int V\rho \leqslant V_{-}\rho$$

On the other hand:

$$N = \sum_{j=1}^{N} \langle u_j, -\Delta u_j \rangle = \sum_{j=1}^{N} \int_{\mathbb{R}^d} |2\pi k|^2 \left|\widehat{u}_j(k)\right|^2 \mathrm{d}k = \sum_{j=1}^{N} \int_{\mathbb{R}^d} \int_{0}^{\infty} \mathbf{1}_{\{|2\pi k|^2 > e\}} \left|\widehat{u}_j(k)\right|^2 \mathrm{d}e\mathrm{d}k =$$

Define u_j^e via its Fourier transform

$$\widehat{u_j^e}(k) = \mathbf{1}_{|2\pi k|^2 > e} \widehat{u}_j(k)$$

then

$$N = \sum_{j=1}^{N} \int_{\mathbb{R}^d} \int_{0}^{\infty} \left|\widehat{u_j^e}(k)\right|^2 \mathrm{d}e\mathrm{d}k = \sum_{j=1}^{N} \int_{0}^{\infty} \int_{\mathbb{R}^d} \left|\widehat{u_j^e}(k)\right|^2 \mathrm{d}e\mathrm{d}k = \sum_{j=1}^{N} \int_{0}^{\infty} \int_{\mathbb{R}^d} \left|u_j^e(k)\right|^2 \mathrm{d}e\mathrm{d}k =$$
$$= \sum_{j=1}^{N} \int_{\mathbb{R}^d} \int_{0}^{\infty} \left|u_j^e(k)\right|^2 \mathrm{d}e\mathrm{d}k$$

where the exchange of integrations is allowed by Tonelli's theorem as the integrand is always positive.

By the triangle inequality

$$\sqrt{\sum_{j=1}^{N} |u_j^e(x)|^2} \geqslant \sqrt{\sum_{j=1}^{N} |u_j(x)|^2} - \sqrt{\sum_{j=1}^{N} |u_j(x) - u_j^e(x)|^2}$$

and thus

$$\sum_{j=1} |u_j^e(x)|^2 \geqslant \left[\sqrt{\rho} - \sqrt{\sum_{j=1}^{N} |u_j(x) - u_j^e(x)|^2}\right]_{+}^{2}$$

Note that

$$\sum_{j=1}^{N}|u_j(x)-u_j^e(x)|^2=\sum_{j=1}^{N}\left|\int e^{2\pi ik\cdot x}\widehat{u_j-u_j^e}(k)\mathrm{d}k\right|^2=\sum_{j=1}^{N}\left|\int e^{2\pi ik\cdot x}\mathbf{1}_{\{|2\pi k|^2\leqslant e\}}\hat{u}_j(k)\mathrm{d}k\right|^2=$$
$$=\sum_{j=1}^{N}\left|\int e^{2\pi ik\cdot x}\frac{\mathbf{1}_{\{|2\pi k|^2\leqslant e\}}}{|2\pi k|}|2\pi k|\hat{u}_j(k)\mathrm{d}k\right|^2\leqslant$$
$$\leqslant\sum_{j=1}^{N}\left|\int e^{2\pi ik\cdot x}\frac{\mathbf{1}_{\{|2\pi k|^2\leqslant e\}}}{|2\pi k|}\right|^2\mathrm{d}k=K_d e^{\frac{d}{2}-1}.$$

where the inequality follows from Bessel's inequality as the $|2\pi k|\hat{u}_j(k)$ form an orthonormal family in $L^2(\mathbb{R}^d)$.

Thus

$$\sum_{j=1}^{N}|u_j^e(x)|^2\geqslant\left[\sqrt{\rho(x)}-\sqrt{K_d e^{\frac{d}{2}-1}}\right]_+^2$$

and therefore

$$N\geqslant\int_{\mathbb{R}^d}\int_0^\infty\left[\sqrt{\rho(x)}-\sqrt{K_d e^{\frac{d}{2}-1}}\right]_+^2\mathrm{d}e\mathrm{d}x=\widetilde{K}_e\int_{\mathbb{R}^d}\rho(x)^{\frac{d}{d-2}}\mathrm{d}x.$$

To conclude we now use Hölder's inequality to see that

$$N\leqslant\int V_-\rho\leqslant\left(\int V_-^{\frac{d}{2}}\right)^{\frac{2}{d}}\left(\int\rho^{\frac{d}{d-2}}\right)^{\frac{d-2}{d}}\leqslant\left(\int V_-^{\frac{d}{2}}\right)^{\frac{2}{d}}\left(\frac{N}{\widetilde{K}_d}\right)^{\frac{d-2}{d}}$$

and therefore

$$N\leqslant C_d\int V_-^{\frac{d}{2}}$$

and thus also $\dim W\leqslant C_d\int V_-^{\frac{d}{2}}$ since either there exists some $N\in\mathbb{N}$ such that $\dim W=N$ or $\dim W=\infty$ and thus the above inequality holds for all $N\in\mathbb{N}$ and therefore also

$$C_d\int V_-^{\frac{d}{2}}=\infty.$$

q.e.d.

Symmetries

Definition 7.19 (Strongly Continuous One-Parameter Unitary Group)**.** A family of operators $\left\{U(t) \,\middle|\, t \in \mathbb{R}\right\}$ such that for all $t_1, t_2 \in \mathbb{R}$

$$U(t_1)U(t_2) = U(t_1 + t_2)$$

and for $(t_n)_n \subset \mathbb{R}$, $t_n \xrightarrow{n\to\infty} t \in \mathbb{R}$

$$U(t_n) \xrightarrow[s]{n\to\infty} U(t).$$

□

Theorem 7.20. *Let A be a self-adjoint operator and $U(t) = \exp(-itA)$. Then*

(1) $U(t)$ is a strongly continuous unitary group.

(2) The limit for all $\psi \in D(A)$

$$\lim_{t\to 0} \frac{1}{t}(U(t)\psi - \psi) = -iA\psi.$$

(3) $D(A)$ is left invariant under $U(t)$, i.e. $U(t)D(A) \subset D(A)$.

□

Theorem 7.21 (Stone)**.** *Let $U(t)$ be a strongly continuous one-parameter unitary group. Then there exists the operator A on*

$$D(A) = \left\{\psi \in \mathscr{H} \,\middle|\, \lim_{t\to 0} \frac{1}{t}(U(t)\psi - \psi) \text{ exists}\right\}$$

defined via

$$A\psi = \lim_{t\to 0} \frac{i}{t}(U(t)\psi - \psi).$$

is self-adjoint. In particular $U(t) = \exp(-itA)$. □

Definition 7.22 (Symmetry Transformation)**.** A map $T : \mathscr{H} \to \mathscr{H}$, $\widehat{T} : \mathscr{L}(\mathscr{H}, \mathscr{H}) \to \mathscr{L}(\mathscr{H}, \mathscr{H})$ (a map from a suitable class of linear operators of the Hilbert space to itself) such that for all $\psi \in \mathscr{H}$ and all suitable operators $A \in \mathscr{L}(\mathscr{H}, \mathscr{H})$

$$\left\langle T\psi, \widehat{T}(A)T\psi \right\rangle = \langle \psi, A\psi\rangle$$

If $A = \sum_a |a\rangle \langle a|$, then if $a' = Ta$ and $A' = \widehat{T}A$ we

$$A' = \sum_a T\, |a\rangle\, T^* \langle a| = \sum_a |a'\rangle \langle a'|$$

and the symmetry condition translates to

$$\langle T\psi, a'\rangle \langle a', T\psi\rangle = |\, \langle a', T\psi\rangle\, |^2 \overset{!}{=} |\, \langle a, \psi\rangle\, |$$

for all $\psi \in \mathscr{H}$. □

Theorem 7.23 (Wigner)**.** *Let T be a bounded linear operator on $\mathscr{H}$ such that for all $u, v \in \mathscr{H}$*

$$|\, \langle u', v'\rangle\, | = |\, \langle u, v\rangle\, |$$

then T has the form $Tu = \varphi(u)Vu$ where $\varphi : \mathscr{H} \to S^1 \subset \mathbb{C}$ is some phase factor and V is either unitary or anti-unitary, i.e.

$$\langle Vu, Vv\rangle = \langle v, u\rangle\, .$$

□

Proof. Let $(e_j)_j$ be an orthonormal basis of $\mathscr{H}$, and define $e'_j = Te_j$.
For $j \geqslant 2$ define $f_j = e_1 + e_j$, the per our assumption

$$|\, \left\langle e'_2, f'_j\right\rangle | = |\, \langle e_1, f_j\rangle\, | = 1, \qquad |\, \left\langle e'_j, f'_k\right\rangle | = |\, \langle e_j, f_k\rangle\, | = \delta_{jk}$$

thus $f'_j = x_j e'_1 + y_j e'_j$ with $|x_j| = |y_j| = 1$.
Redefine $\widetilde{T}$ such that

$$\widetilde{f}'_j = \widetilde{T} f_j = \frac{f'_j}{x_j}, \qquad \widetilde{e}'_j = \frac{y_j}{x_j} e'_j$$

then $\widetilde{f}'_j = \widetilde{e}'_1 + \widetilde{e}'_j$. We shall now drop the tilde and simply consider $\widetilde{T}$ as the transition form T to $\widetilde{T}$ is simply a multiplication with a unitary operator.
Now let $Tu = \sum_i a'_i e'_i$. Then

$$|a'_j| = |\left\langle e'_j, u' \right\rangle| = |\left\langle e_j, u \right\rangle| = |a_j|$$

and

$$|a_1 + a_j| = |\left\langle e_1 + e_j, u \right\rangle| = |\left\langle e'_1 + e'_j, u' \right\rangle| = |a'_1 + a'_j|$$

which implies

$$|a_1|^2 + 2\,\Re\,\overline{a_1} a_j + |a_j|^2 = |a'_1|^2 + 2\,\Re\,\overline{a'_1} a'_j + |a'_j|^2 \iff \Re\,\overline{a_1} a_j = \Re\,\overline{a'_1} a'_j$$

If ϑ and ϑ' are the phases of $\overline{a_1} a_j$ and $\overline{a'_1} a'_j$ respectively, then this implies that $\cos(\vartheta) = \cos(\vartheta')$ since the norms of $\overline{a_1} a_j$ and $\overline{a'_1} a'_j$ are equal by the above.
Therefore $\vartheta = \pm\vartheta'$. If $\vartheta = \vartheta'$ then we can redefine T such that $a'_1 = a_1$ and if $\vartheta = -\vartheta'$ such that $a'_1 = \overline{a_1}$. In the first case this means that the symmetry is T is unitary and in the second anti-unitary. *q.e.d.*

Remark 7.24. A symmetry continuous connected to the identity must always be unitary by connectedness. □

Definition 7.25. A density matrix ρ is a positive operator on the Hilbert space $\mathscr{H}$ of trace 1. This means that there exists an orthonormal basis $(u_i)_i$ of $\mathscr{H}$ such that

$$\rho = \sum_i p_i \left| u_i \right\rangle \left\langle u_i \right|, \qquad \sum_i p_i = 1$$

p_i can be interpreted as the probability that a particle described by ρ is in the state $|u_i\rangle$.

□

Remark 7.26. ρ is the most general form of a "state" (as introduced with C^*-algebras) together with normality. □

Definition 7.27. The (von Neumann) entropy of ρ is defined to be

$$S(\rho) = -\operatorname{Tr}(\rho \log(\rho)) = -\sum_i p_i \log p_i.$$

□

Remark 7.28. Entropy is a measure for the "fuzzyness" of our knowledge of the state of a particle described by ρ. If ρ is a pure state, i.e. $\rho = |u\rangle \langle u|$, then $S(\rho) = 0$. □

The time-evolution of ρ is given by

$$\rho(t) = U(t)\rho U(t)^\dagger.$$

7.3 Argument for Unitary Evolution

Suppose that we have some general time evolution $v(t)$, $u(t)$ for some initial states u, v. Then the density matrix

$$\rho = \frac{1}{2} |u\rangle \langle u| + \frac{1}{2} |v\rangle \langle v|$$

would generically evolve as

$$\rho(t)\frac{1}{2} |u(t)\rangle \langle u(t)| + \frac{1}{2} |v(t)\rangle \langle v(t)|$$

Then for $\psi(t) = c_u u(t) + c_v v(t)$ the density matrix would be

$$\rho_\psi = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \langle u(t), v(t)\rangle \\ \frac{1}{2} \langle v(t), u(t)\rangle & \frac{1}{2} \end{pmatrix}$$

Suppose that $\langle u, v\rangle = 0$ but for some $t > 0$ $\langle u(t), v(t)\rangle \neq 0$. Then

$$S(\rho(0)) = \log(2), \qquad S(\rho(t)) = w_+ \log(w_+) + w_- \log(w_-)$$

where $w_\pm = \frac{1}{2}(1 \pm |\langle u, v\rangle|)$. Then since $S(\rho(0))$ is maximal entropy would decrease.
This gives one argument for why time evolution must behave as a symmetry and thus be unitary.

7.4 Trace Out of Density Matrix

Suppose that $\mathscr{H} = \mathscr{H}_S \otimes \mathscr{H}_0$ and suppose that only make an observation on $\mathscr{H}_S$, i.e. our observable decomposes as $A = A_S \otimes \mathbb{I}$. Then for a state

$$\psi_\rho = \sum_i \sqrt{p_i} \varphi_{iS} \otimes x_{i0}.$$

we have

$$\langle \psi_\rho, A\psi_\rho\rangle = \sum_{ij} \sqrt{p_i p_j} \langle \varphi_i, A\varphi_j\rangle \underbrace{\langle x_i, \mathbb{I}x_j\rangle}_{=\delta_{ij}} = \sum_i p_i \langle \varphi_i, A\varphi_i\rangle = \mathrm{Tr}(\rho A)$$

where $\rho = \sum_i p_i |\varphi_i\rangle \langle \varphi_i|$.

Chapter 8

Scattering Theory

Let us start with $u(t) = e^{-itA}u_0$, where $A = -\Delta + V$ on $L^2(\mathbb{R}^d)$. We are interested in the asymptotic behaviour of $u(t)$ as $t \to \pm\infty$.

- If u_0 is a bound state, then $u(t)$ remains localised as $t \to \pm\infty$.
- If u_0 is orthogonal to all bound states, then $u(t)$ escapes to infinity as $t \to \pm\infty$.

Theorem 8.1. *Let A be a self-adjoint operator on $L^2(\mathbb{R}^d)$ and $u(t) = e^{-itA}u_0$ with $u_0 \in \overline{\operatorname{span}\{\textit{eigenfunctions of } A\}}$.*
Then for all $\varepsilon > 0$ there exists a $R = R_\varepsilon$ such that

$$\inf_{t\in\mathbb{R}} \int\limits_{|x|\leqslant R} |u(t,x)|^2 \mathrm{d}x \geqslant \int\limits_{\mathbb{R}^d} |u_0(x)|^2 \mathrm{d}x - \varepsilon.$$

Note that

$$\int\limits_{\mathbb{R}^d} |u(t,x)|^2 \mathrm{d}x = \int\limits_{\mathbb{R}^d} |u_0(x)|^2$$

thus

$$\sup_{t\in\mathbb{R}} \int\limits_{|x|>R} |u(t,x)|^2 \mathrm{d}x \leqslant \varepsilon.$$

□

Proof. Exercise! *q.e.d.*

Next we show that if u_0 is orthogonal to all eigenfunctions of A, then $u(t) = e^{-itA}u_0$ escapes to infinity in the sense that for all $R > 0$

$$\lim_{t\to\pm\infty} \int\limits_{|x|\leqslant R} |u(t,x)|^2 \mathrm{d}x = 0$$

which is a particular case of the so-called RAGE theorem.

Our goal in studying scattering theory is as follows: if $A = -\Delta + V$, $V \to 0$ as $|x| \to \infty$ then for u_0 orthogonal to the bounds states there exist some $v_0^\pm \in L^2(\mathbb{R}^d)$ such that

$$\lim_{t\to\pm\infty} \left\| e^{-itA}u_0 - e^{it\Delta}v_0^\pm \right\|_{L^2} = 0.$$

Theorem 8.2 (RAGE for the free Schrödinger Operator)**.** *For all $f \in L^2(\mathbb{R}^d)$, then for all $R > 0$*

$$\int\limits_{|x|\leqslant R} \left|\left(e^{it\Delta}f\right)(x)\right|^2 \mathrm{d}x \xrightarrow{t\to\pm\infty} 0$$

□

Lemma 8.3. *If $f \in L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$, then*

$$\left(e^{it\Delta}f\right)(x) = \frac{1}{(4\pi i t)^{\frac{d}{2}}} \int\limits_{\mathbb{R}^d} e^{i\frac{|x-y|^2}{4t}} f(y)\mathrm{d}y$$

for a.e. $x \in \mathbb{R}^d$. □

Remark 8.4. Recall the heat kernel

$$\left(e^{t\Delta}f\right)(x) = \frac{1}{(4\pi t)^{\frac{d}{2}}} \int\limits_{\mathbb{R}^d} e^{-\frac{|x-y|^2}{4t}} f(y)\mathrm{d}y$$

□

Proof. For all $\varepsilon > 0$ and

$$\left(\widehat{e^{(it+\varepsilon)\Delta}f}\right)(k) = e^{-(it+\varepsilon)|2\pi k|^2}\hat{f}(k) =: \widehat{G}_\varepsilon(k)\hat{f}(k) = \widehat{G_\varepsilon * f}(k)$$

where

$$G(x) = \frac{1}{(4\pi(it+\varepsilon))^{\frac{d}{2}}} e^{-\frac{|x|^2}{4(it+\varepsilon)}}$$

by the formula for the Fourier transform of a Gaussian. Thus

$$\big(e^{(it+\varepsilon)\Delta} f\big)(x) = \frac{1}{(4\pi(it+\varepsilon))^{\frac{d}{2}}} \int\limits_{\mathbb{R}^d} e^{-\frac{|x-y|^2}{4(it+\varepsilon)}} f(y)\mathrm{d}y$$

for all $\varepsilon > 0$. The left-hand side converges to $e^{it\Delta} f$ as $\varepsilon \downarrow 0$ since $e^{-(it+\varepsilon)x}$ is bounded for all $\varepsilon \geqslant 0$ and converges pointwise and thus $e^{(it+\varepsilon)\Delta}$ converges strongly by functional calculus. The right-hand side on the other hand also converges pointwise and is dominated by $|f(y)| \in L^1$ and therefore by dominated convergence

$$\big(e^{it\Delta} f\big)(x) = \frac{1}{(4\pi it)^{\frac{d}{2}}} \int\limits_{\mathbb{R}^d} e^{-\frac{|x-y|^2}{4it}} f(y)\mathrm{d}y.$$

q.e.d.

Consequently if $f \in L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$, then

$$\big|e^{it\Delta} f(x)\big| = \left| \frac{1}{(4\pi it)^{\frac{d}{2}}} \int\limits_{\mathbb{R}^d} e^{i\frac{|x-y|^2}{4t}} f(y)\mathrm{d}y \right| \leqslant \frac{1}{(4\pi|t|)^{\frac{d}{2}}} \|f\|_{L^1}$$

for a.e. x and thus

$$\|e^{it\Delta} f\|_\infty \leqslant \frac{\|f\|_1}{(4\pi|t|)^{\frac{d}{2}}} \xrightarrow{t\to\pm\infty} 0$$

and for all $R > 0$

$$\int\limits_{\|x\|\leqslant R} \big|e^{it\Delta} f(x)\big|^2 \mathrm{d}x \leqslant \big\|e^{it\Delta} f\big\|_\infty^2 |B_R(0)| \xrightarrow{t\to\pm\infty} 0$$

Proof of Theorem 8.2. If $f \in L^1 \cap L^2$ we are done by the above. Now take any $f \in L^2(\mathbb{R}^d)$. We claim that for all $\varepsilon > 0$ there exist $f_1 \in L^1 \cap L^2$ and $f_2 \in L^2$ such that $f = f_1 + f_2$ and $\|f_2\|_{L^2} < \varepsilon$.

Indeed, if we take $f_1 = f\mathbf{1}_{\{|f|>\lambda\}}$ then

$$\int |f_1| = \int |f|\mathbf{1}_{\{|f|>\lambda\}} \leqslant \int \frac{|f|^2}{\lambda} = \frac{\|f\|^2}{\lambda} < \infty$$

and $f_2 = f\mathbf{1}_{\{|f|\leqslant\lambda\}}$ where

$$\|f_2\| = \int |f|^2\mathbf{1}_{\{|f|\leqslant\lambda\}} \xrightarrow{\lambda\to 0} 0$$

by dominated convergence. We can also take $f_1 = f\mathbf{1}_{\{|x|\leqslant L\}}$ which is $L^1 \cap L^2$ as $\{|x| \leqslant L\}$ has finite measure and for a set of finite measure $L^p \subset L^q$ for $p > q$. Then $f_2 = f\mathbf{1}_{\{|x|>L\}}$ which also converges to 0 as $L \to \infty$.

Thus

$$\int\limits_{|x|\leqslant R} \left|e^{it\Delta}f(x)\right|^2 \mathrm{d}x = \int\limits_{|x|\leqslant R} \left|e^{it\Delta}f_1(x) + e^{it\Delta}f_2(x)\right|^2 \mathrm{d}x \leqslant 2\int\limits_{|x|\leqslant R} \left|e^{it\Delta}f_1(x)\right|^2 \mathrm{d}x + 2\int\limits_{|x|\leqslant R} \left|e^{it\Delta}f_2(x)\right|^2 \mathrm{d}x \leqslant$$

$$\leqslant 2\int\limits_{|x|\leqslant R} \left|e^{it\Delta}f_1(x)\right|^2 \mathrm{d}x + 2\varepsilon^2$$

and therefore

$$\limsup_{t\to\pm\infty} \int\limits_{|x|\leqslant R} \left|e^{it\Delta}f(x)\right|^2 \mathrm{d}x \leqslant 2\varepsilon^2 \xrightarrow{\varepsilon\downarrow 0} 0.$$

q.e.d.

8.1 General RAGE

Let A be a self-adjoint operator on $\mathscr{H}$.

Theorem 8.5. *For $u_0 \in D(A)$ orthogonal to all eigenfunctions of A*

$$e^{itA}u_0 \xrightarrow[\text{ergodic}]{t\to\pm\infty} 0$$

weakly in $\mathscr{H}$. Equivalently, for all compact operators K, $Ke^{itA}u_0 \xrightarrow[\text{ergodic}]{t\to\pm\infty} 0$ strongly in $\mathscr{H}$, i.e.

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \left\|Ke^{itA}u_0\right\|_{\mathscr{H}}^2 = 0.$$

□

Remark 8.6 (Spectral Decomposition)**.**

$$\mathscr{H} = \mathscr{H}_{\mathrm{pp}} \oplus \mathscr{H}_{\mathrm{ac}} \oplus \mathscr{H}_{\mathrm{sc}}$$

which is the quantum version of the Lebesgue decomposition of a measure

$$\mu = \mu_{\text{pp}} + \mu_{\text{ac}} + \mu_{\text{sc}}$$

where $\mu - \mu_{\text{pp}}$ does not have any support on single points, $d\mu_{\text{ac}} = g\mathrm{d}x$ for some $g \in L^1(\mathbb{R}^d)$ and μ_{sc} is singular to the Lebesgue measure.
Which however, only consider the simpler decomposition

$$\mathscr{H}_p = \overline{\text{span}\{\text{eigenfunctions of } A\}}$$

point spectrum and $\mathscr{H}_c = \mathscr{H}_p^{\perp}$. □

Theorem 8.7 (Ruelle)**.** *Let A be a self-adjoint operator on $\mathscr{H}$. Then for all $u_0 \in \mathscr{H}$ and all K compact operators*

$$\frac{1}{T}\int_0^T \|Ke^{-itA}u_0\|^2 \mathrm{d}t \xrightarrow{T\to\pm\infty} 0$$

□

Remark 8.8. If K is a compact operator on a Hilbert space, then we can write K as

$$K = \sum_{n=1}^{\infty} \lambda_n \left|u_n\right\rangle \left\langle v_n\right|$$

where $(u_n)_n$, $(v_n)_n$ are orthonormal bases. By definition K is trace-class if

$$\operatorname{Tr}|K| = \sum_n |\lambda_n| < \infty.$$

where $|K| = \sqrt{K^*K}$. In this case

$$\operatorname{Tr} K = \sum_{n=1}^{\infty} \langle \varphi_n, K\varphi_n \rangle$$

for any orthonormal basis $(\varphi_n)_n$ (Exercise!).

By definition, K is Hilbert-Schmidt if

$$\|K\|_{\mathrm{HS}}^2 = \sum_{n=1}^{\infty} |\lambda_n|^2 < \infty.$$

In this case

$$\|K\|_{\mathrm{HS}}^2 = \sum_{n=1}^{\infty} \|K\varphi_n\|^2$$

for any orthonormal basis $(\varphi_n)_n$.

In fact we have

$$B(\mathscr{H}) \supset \text{compact operators} \supset \text{Hilbert-Schmidt operators } \sigma^2 \supset \text{Trace-Class operators } \sigma^1$$

or equivalently

$$\|K\| \leqslant \|K\|_{\mathrm{HS}} \leqslant \mathrm{Tr}\,|K| = \mathrm{Tr}\,\sqrt{K^*K}$$

If K is compact and $K = \sum \lambda_n |u_n\rangle \langle v_n|$ then

$$\|K\| = \sup_n |\lambda_n|, \quad \|K\|_{\mathrm{HS}} = \sqrt{\sum |\lambda_n|^2}, \quad \mathrm{Tr}\,|K| = \sum |\lambda_n|$$

In particular, if K is Hilbert-Schmidt then K^*K is trace class. In fact, σ^2 is a Hilbert space with inner product

$$\langle K_1, K_2 \rangle_{\mathrm{HS}} = \mathrm{Tr}(K_1^* K_2)$$

if K_1, K_2 are Hilbert-Schmidt.

In fact one can relate that any Hilbert-Schmidt operator K to an L^2 integral kernel. Recall that the kernel $K(x,y)$ of an operator K on $L^2(\Omega)$ is defined via

$$(Kf)(x) = \int_\Omega K(x,y) f(y) \mathrm{d}y$$

for all $f \in L^2(\Omega)$ and a.e. $x \in \Omega$.

Then an operator K is Hilbert-Schmidt on $L^2(\Omega)$ iff $K(x,y) \in L^2(\Omega \times \Omega)$ and $\|K\|_{HS} = \|K(\cdot,\cdot)\|_{L^2(\Omega\times\Omega)}$.

This proven by using $K = \sum_n \lambda_n |u_n\rangle \langle v_n|$ and accordingly defining

$$K(x,y) = \sum_n \lambda_n u_n(x) \overline{v_n(y)}.$$

□

Proof.

Step 1 Consider the sequence of operators

$$M_T = \frac{1}{T}\int_0^T |e^{-itA}u_0\rangle\langle e^{-itA}u_0|\,\mathrm{d}t$$

Then $M_T \geqslant 0$ and

$$\operatorname{Tr} M_T = \frac{1}{T}\int_0^T \operatorname{Tr}\big(|e^{-itA}u_0\rangle\langle e^{-itA}u_0|\big)\mathrm{d}t = \frac{1}{T}\int_0^T 1\mathrm{d}t = 1$$

Thus $(M_T)_T$ is a bounded set of trace-class operators. Thus $(M_T)_T$ is bounded in the Hilbert-Schmidt norm, and σ^2 is a Hilbert space. By the Banach-Alaoglu Theorem 1.20, there exists a sequence $T_n \xrightarrow{n\to\infty}$ and $M_\infty \in \sigma^2$ such that

$$M_{T_n} \xrightarrow{n\to\infty} M_\infty$$

weakly in the Hilbert-Schmidt space, i.e. for all Hilbert-Schmidt operators D

$$\lim_{n\to\infty} \operatorname{Tr}[M_{T_n}D] = \operatorname{Tr}[M_\infty D]$$

Step 2 We prove that $M_\infty = 0$. We first show that

$$e^{-itA}M_\infty e^{itA} = M_\infty$$

for all $t \in \mathbb{R}$. We have for all $T \in [0, \infty)$

$$\begin{aligned}
e^{-itA} M_T e^{itA} &= e^{-itA} \left(\frac{1}{T} \int_0^T |e^{-isA} u_0\rangle \langle e^{-isA} u_0| \,\mathrm{d}s \right) e^{itA} = \\
&= \frac{1}{T} \int_0^T |e^{-i(t+s)A} u_0\rangle \langle e^{-i(t+s)A} u_0| \,\mathrm{d}s = \\
&= \frac{1}{T} \int_t^{T+t} |e^{-isA} u_0\rangle \langle e^{-isA} u_0| \,\mathrm{d}s = \\
&= \frac{1}{T} \left(\int_0^T - \int_0^t + \int_T^{T+t} \right) |e^{-isA} u_0\rangle \langle e^{-i(s)A} u_0| \,\mathrm{d}s = \\
&= M_T + \frac{1}{T} \left(- \int_0^t + \int_T^{T+t} \right) |e^{-isA} u_0\rangle \langle e^{-isA} u_0| \,\mathrm{d}s =
\end{aligned}$$

However,

$$\operatorname{Tr} \left| e^{-itA} M_T e^{itA} - M_T \right| \leqslant \frac{1}{T} \left(\int_0^t + \int_T^{T+t} \right) \underbrace{\operatorname{Tr} |e^{-isA} u_0\rangle \langle e^{-isA} u_0|}_{=1} \,\mathrm{d}s = \frac{1}{T} 2t \xrightarrow{T \to \infty} 0$$

On the other hand, $M_T \rightharpoonup M_\infty$, thus $e^{-itA} M_T e^{itA} - M_T \rightharpoonup e^{-itA} M_\infty e^{itA} - M_\infty$ weakly in the Hilbert-Schmidt space. Thus $e^{-itA} M_\infty e^{itA} M_\infty$.

Taking the t-derivative we find

$$0 = \frac{d}{dt} \big(e^{-itA} M_\infty e^{itA} \big) = -ie^{-itA} (A M_\infty - M_\infty A) e^{itA}$$

hence $A M_\infty = M_\infty A$, i.e. M_∞ commutes with A.

Because M_T, and $M_T \rightharpoonup M_\infty$ weakly in Hilbert-Schmidt space it follows that $M_\infty \geqslant 0$, and that M_∞ is Hilbert-Schmidt operator.

Thus we can write $M_\infty = \sum_n \lambda_n |u_n\rangle \langle u_n|$. In particular if λ is an eigenvalue of M_∞ and $\lambda \neq 0$, then the eigenspace W_λ of λ has finite dimension.

Since A commutes with M_∞ it follows that $A : W_\lambda \to W_\lambda$ and A is a self-adjoint operator on W_λ there exists an orthonormal basis of eigenfunctions of A in W_λ.

In summary there exists an orthonormal basis $(\varphi_n)_n$ of $\mathscr{H}$ such that φ_n are both eigenfunctions of M_∞ and A and

$$M_\infty = \sum_{n=1}^{\infty} \lambda_n \left|\varphi_n\right\rangle \left\langle\varphi_n\right|$$

To conclude that $M_\infty = 0$, we need to use $u_0 \in \mathscr{H}_c$, i.e. u_0 is orthogonal to all eigenfunctions of A. From weak-convergence $M_T \rightharpoonup M_\infty$ in the Hilbert-Schmidt topology we know that

$$\lambda_n = \langle\varphi_n, M_\infty \varphi_n\rangle = \lim_{T\to\infty} \langle\varphi_n, M_T\varphi_n\rangle = \lim_{T\to\infty} \left\langle \varphi_n, \frac{1}{T}\int_0^T \left|e^{-itA}\right\rangle \left\langle e^{-itA}\right| \mathrm{d}t\varphi_n \right\rangle =$$

$$= \lim_{T\to\infty} \frac{1}{T}\int_0^T \left|\left\langle\varphi_n, e^{-itA}\varphi_n\right\rangle\right|^2 \mathrm{d}t = 0$$

Here

$$\left\langle\varphi_n, e^{-itA}u_0\right\rangle = \left\langle e^{itA}\varphi_n, u_0\right\rangle = \left\langle e^{it\xi_n}\varphi_n, u_0\right\rangle = 0$$

where $A\varphi_n = \xi_n\varphi_n$.

Thus $M_\infty = 0$, i.e.

$$\frac{1}{T}\int_0^T \left|e^{-itA}u_0\right\rangle \left\langle e^{-itA}u_0\right| \mathrm{d}t \xrightarrow{T\to\infty} 0$$

in the Hilbert-Schmidt topology. Strictly speaking, we have only proven this for some sequence $T_n \xrightarrow{n\to\infty} 0$. However, since the limit is independent of the sequence the convergence $T \to \infty$ follows.

Step 3 Now take K to be any compact operator, then

$$\frac{1}{T}\int_0^T \|Ke^{-itA}u_0\|^2 \mathrm{d}t = \mathrm{Tr}[M_T K^* K]$$

since

$$\|Ke^{-itA}u_0\|^2 = \mathrm{Tr}\big[K\left|e^{-itAu_0}\right\rangle \left\langle e^{-itA}u_0\right| K^*\big] = \mathrm{Tr}\big[\left|e^{-itAu_0}\right\rangle \left\langle e^{-itA}u_0\right| K^*K\big].$$

By the spectral theorem $K^*K \geqslant 0$ and compact, and thus we can write

$$K^*K = \sum_{n=1}^{\infty} \ell_n \left|v_n\right\rangle \left\langle v_n\right|$$

with $\ell_n \xrightarrow{n\to\infty} 0$.

Now

$$\begin{aligned}\operatorname{Tr}[M_T K^* K] &= \sum_{n=1}^{\infty} \ell_n \langle v_n, M_T v_n\rangle = \sum_{\ell_n \leqslant \varepsilon} \ell_n \langle v_n, M_T v_n\rangle + \sum_{\ell_n > \varepsilon} \ell_n \langle v_n, M_T v_n\rangle \leqslant \\ &\leqslant \varepsilon \underbrace{\sum_{n=1}^{\infty} \langle v_n, M_T v_n\rangle}_{=\operatorname{Tr} M_T = \|u_0\|^2} + \underbrace{\sum_{\ell_n > \varepsilon} \ell_n \langle v_n, M_T v_n\rangle}_{\text{finite sum}}\end{aligned}$$

Thus for all $\varepsilon > 0$

$$\limsup_{T\to\infty} \operatorname{Tr}[M_T K^* K] \leqslant \varepsilon \|u_0\|^2 + 0,$$

therefore

$$\operatorname{Tr}[M_T K^* K] \xrightarrow{T\to\infty} 0$$

q.e.d.

Corollary 8.9. *Let A be self-adjoint and K relatively A-compact and bounded, then*

$$\frac{1}{T}\int_0^T \left\|K e^{-itA} u_0\right\|^2 \mathrm{d}t \xrightarrow{T\to\infty} 0$$

for $u_0 \in \mathscr{H}_c$ and $u_0 \in D(A)$. 0 □

Proof. If $u_0 \in \mathscr{H}_c$ and $u_0 \in D(A)$, then

$$\frac{1}{T}\int_0^T \left\|K e^{-itA} u_0\right\|^2 \mathrm{d}t = \frac{1}{T}\int_0^T \big\| \underbrace{K(A+i)^{-1}}_{\text{compact}} e^{-itA}(A+i)u_0\big\|^2 \mathrm{d}t \xrightarrow{T\to\infty} 0$$

where we use that $A : \mathscr{H}_c \cap D(A) \to \mathscr{H}_c$ hence $(A+i)u_0 \in \mathscr{H}_c$ and Ruelle's theorem.

If $u_0 \in \mathscr{H}_c$ and $u_0 \in D(A)$ then by Jensen's inequality

$$\frac{1}{T}\int\limits_0^T \|Ke^{-itA}u_0\|\mathrm{d}t \leqslant \sqrt{\frac{1}{T}\int\limits_0^T \|Ke^{-itA}u_0\|^2\mathrm{d}t} \xrightarrow{T\to\infty} 0$$

If $u_0 \in \mathscr{H}_c$ (not necessarily in $D(A)$), then there exists a sequence $(u_n)_n \subset \mathscr{H}_c \cap D(A)$ such that $u_n \xrightarrow{n\to\infty} u_0$ in $\mathscr{H}$.

Then

$$\frac{1}{T}\int\limits_0^T \|Ke^{-itA}u_0\|\mathrm{d}t \leqslant \frac{1}{T}\int\limits_0^T \|Ke^{-itA}u_n\|\mathrm{d}t + \frac{1}{T}\int\limits_0^T \|Ke^{-itA}(u_n-u_0)\|\mathrm{d}t$$

The first term converges to 0 as $T\to\infty$ by the above and the second term can be estimated by

$$\frac{1}{T}\int\limits_0^T \|Ke^{-itA}(u_n-u_0)\|\mathrm{d}t \leqslant \|K\|\|u_n-u_0\|\frac{1}{T}\int\limits_0^T \mathrm{d}t = \|K\|\|u_n-u_0\|$$

and thus be made arbitrarily small by taking $n\to\infty$. Now noting that

$$\|Ke^{-itA}u_0\|^2 \leqslant \|Ke^{-itA}u_0\|\|K\|\|u_0\|$$

the convergence of the square follows as well. *q.e.d.*

Theorem 8.10 (RAGE). *Let A be self-adjoint $(K_n)_n$ a sequence of A-relatively compact bounder operator such that $K_n \xrightarrow{n\to\infty} 1$ strongly, i.e. for all $u \in \mathscr{H}$.*

$$\|K_n u - u\| \xrightarrow{n\to 0} 0$$

Then

$$\mathscr{H}_p = \left\{ u_0 \in \mathscr{H} \;\middle|\; \lim_{n\to\infty}\sup_{t\in\mathbb{R}}\left\|(1-K_n)e^{-itA}u_0\right\| = 0 \right\}$$
$$\mathscr{H}_c = \left\{ u_0 \in \mathscr{H} \;\middle|\; \forall n\in\mathbb{N}: \lim_{T\to\infty}\frac{1}{T}\int\limits_0^T \left\|K_n e^{-itA}u_0\right\| = 0 \right\}$$

$\square$

Proof. If $u_0 \in \mathscr{H}_c$, then

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \left\| K_n e^{-itA} u_0 \right\| = 0$$

by the corollary and by the assumption $K_n u \xrightarrow{n\to\infty} u$ strongly for all $u \in \mathscr{H}$, i.e. $\|K_n\| \leqslant C$ for all $n \in \mathbb{N}$ by the uniform boundedness principle.
If $u_0 \in \mathscr{H}_p$

$$(1 - K_n) e^{-itA} u_0 \xrightarrow{t\to\pm\infty} 0$$

strongly (Exercise!). Combining $\mathscr{H} = \mathscr{H} \oplus \mathscr{H}_p$ implies the conclusion. *q.e.d.*

Theorem 8.11. *Assume that $A = -\Delta + V$ is a self-adjoint operator on $L^2(\mathbb{R}^d)$, as V is $(-\Delta)$-compact. Then*

$$\mathscr{H}_c = \left\{ u \in L^2(\mathbb{R}^d) \,\middle|\, \forall \mathbb{R}^+ : \frac{1}{T} \int_0^T \int_{|x|\leqslant R} \left| \left(e^{-itA} u\right)(x) \right| \mathrm{d}x \mathrm{d}t \xrightarrow{T\to\infty} 0 \right\}$$

$$\mathscr{H}_p = \left\{ u \in L^2(\mathbb{R}^d) \,\middle|\, \lim_{R\to\infty} \inf_{t\in\mathbb{R}} \int_{|x|\leqslant R} \left| \left(e^{-itA} u\right)(x) \right| \mathrm{d}x = \|u\|_{L^2}^2 \right\}$$

□

Proof. The first part follows from Exercise 11.4.
The second part uses that $\mathbf{1}_{\{|x|\leqslant R\}}$ is relatively compact w.r.t. A which is equivalent to $\mathbf{1}_{\{|x|\leqslant R\}}(A+i)^{-1}$ being compact which follows from $\mathbf{1}_{\{|x|\leqslant R\}}(-\Delta+i)^{-1}(-\Delta+i)(A+i)^{-1}$ being the product of a compact and a bounded operator. *q.e.d.*

Remark 8.12. If we know that $u \in H_c(A)$, then $\int_{|x|\leqslant R} \left| \left(e^{-itA} u\right)(x) \right|^2 \to 0$ in the time average. Can we prove that pointwise convergence, i.e.

$$\lim_{t\to\pm\infty} \int_{|x|\leqslant R} \left| \left(e^{-itA} u\right)(x) \right|^2 \longrightarrow 0$$

This can proven for $A = -\Delta$ using

$$\left\|e^{it(-\Delta)}u\right\|_{L^\infty} \leqslant C\frac{\|u\|_{L^1}}{t^{3/2}}$$

To prove this for a general potential we hope that we can approximate $e^{-itA}u$ via free dynamics $e^{it\Delta}v$. □

8.2 Wave Operator

Let $A = -\Delta + V$, $A_0 = -\Delta$ on $L^2(\mathbb{R})$. We aim at finding $u_0 \in D(A)$ for each $v_0 \in D(A-0)$ such that

$$\lim_{t\to\infty} \|e^{-itA}u_0 - e^{-itA_0}v_0\|_{L^2} = 0 \iff u_0 = \lim_{t\to\pm\infty} e^{itA}e^{-itA_0}v_0$$

Definition 8.13 (Wave Operator)**.** If it exists we define the wave operator to be

$$\Omega_\pm := \operatorname*{s-lim}_{t\to\pm\infty} e^{-itA}e^{itA_0}$$

If the wave operator exists, then it is a unitary operator $L^2(\mathbb{R}^3) \to \operatorname{ran}\Omega_\pm$. In fact $\operatorname{ran}\Omega_\pm \subset \mathscr{H}_c$. □

Definition 8.14. We say that A is asymptotically complete iff $\operatorname{ran}\Omega_+ = \operatorname{ran}\Omega_- = \mathscr{H}_c$ which is equivalent to the existence of

$$\operatorname*{s-lim}_{t\to\pm\infty} e^{itA_0}e^{-itA}$$

□

Remark 8.15. When does $\Omega_\pm$ exist? The main in the following shall be that if $V(x) \xrightarrow{|x|\to\infty} 0$ "fast enough", i.e. if it is a so-called short range potential, then the wave operators exist. □

Theorem 8.16. *If $V \in L^2(\mathbb{R}^3) + L^p(\mathbb{R}^3)$, for $2 \leqslant p < 3$, then $\Omega_\pm$ exist.* □

Remark 8.17. If $|V(x)| \leqslant \frac{1}{|x|^{1+\varepsilon}}$, for $\varepsilon > 0$ and $|x|$ large, then $V\mathbf{1}_{|x|\geqslant R} \in L^{3-\delta}(\mathbb{R}^3)$, where $\delta = \delta_\varepsilon > 0$. Then the wave operators exist.
But if $|V(x)| \geqslant \frac{1}{|x|}$ for $|x|$ large, then the wave operators do not exist. We need to modify the approximation $\lim_{t\to\pm\infty} e^{-itA}e^{itS}$ where $S \neq -\Delta$. □

Theorem 8.18 (Cook's Method)**.** *If A and B are two self-adjoint operators on $\mathscr{H}$ with the same domain and if for $\varphi \in \mathscr{H}$*

$$\int_T^\infty \left\|(A-B)e^{itB}\varphi\right\| \mathrm{d}t < \infty$$

for some $T > \infty$, then

$$\Omega_+\varphi := \lim_{t\to+\infty} e^{-itA}e^{itB}\varphi$$

exists (as a limit in the norm topology.) □

Proof. We need to check that $t \mapsto e^{-itA}e^{itB}\varphi$ is a Cauchy sequence/net then existence follows from the completeness of $\mathscr{H}$. This is equivalent to

$$\left\|e^{-itA}e^{itB}\varphi - e^{-isA}e^{isB}\varphi\right\| \xrightarrow{t,s\to+\infty} 0.$$

In order to estimate this norm let us take the derivative

$$\frac{d}{dt}\left(e^{-itA}e^{itB}\varphi\right) = e^{itA}(-iA+iB)e^{itB}$$

where we used that $[f(C), C] = 0$ for any self-adjoint operator C and bounded function f.

Then

$$
\begin{aligned}
\left\|e^{-it_2A}e^{it_2B}\varphi - e^{-it_1A}e^{it_1B}\varphi\right\| &= \left\|\int_{t_1}^{t_2}(-i)e^{-itA}(A-B)e^{itB}\varphi \mathrm{d}t\right\| \leqslant \\
&\leqslant \int_{t_1}^{t_2}\left\|e^{-itA}(A-B)e^{itB}\varphi\right\|\mathrm{d}t = \\
&= \int_{t_1}^{t_2}\left\|(A-B)e^{itB}\varphi\right\|\mathrm{d}t = \\
&= \int_{T}^{t_2}\left\|(A-B)e^{itB}\varphi\right\|\mathrm{d}t - \int_{T}^{t_1}\left\|(A-B)e^{itB}\varphi\right\|\mathrm{d}t \xrightarrow{t_1,t_2\to\infty} 0
\end{aligned}
$$

since

$$
\int_{T}^{+\infty}\left\|(A-B)e^{itB}\varphi\right\|\mathrm{d}t < \infty
$$

q.e.d.

Proof of Theorem 8.16. From Cook's theorem, we need to check that

$$
\int_{T}^{\infty}\left\|Ve^{it(-\Delta)}\varphi\right\| < \infty
$$

if φ is "nice enough", i.e. $\varphi \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$. We shall argue later that this is indeed enough.

Assume that $V \in L^2(\mathbb{R}^3)$. Then

$$
\left\|Ve^{it(-\Delta)}\varphi\right\|_{L^2} \leqslant \|V\|_{L^2}\left\|e^{it(-\Delta)}\varphi\right\|_{L^\infty} \leqslant C\|V\|_{L^2}\frac{\|\varphi\|_{L^1}}{t^{3/2}}
$$

hence

$$
\int_{T}^{\infty}\left\|Ve^{it(-\Delta)}\varphi\right\| \leqslant C\frac{\|V\|_{L^2}\|\varphi\|_{L^1}}{\sqrt{T}} < \infty
$$

Assume that $V \in L^p(\mathbb{R}^3)$ with $2 \leqslant p < 3$. Then by Hölder's inequality

$$
\left\|Ve^{it(-\Delta)}\varphi\right\|_{L^2} \leqslant \|V\|_{L^p}\left\|e^{it(-\Delta)}\varphi\right\|_{L^q}
$$

with $\frac{1}{p}+\frac{1}{q}=\frac{1}{2}$. Here $\left\|e^{it(-\Delta)}\varphi\right\|_{L^q}$ can be controlled by $\left\|e^{it(-\Delta)}\varphi\right\|_{L^\infty}$ and $\left\|e^{it(-\Delta)}\varphi\right\|_{L^2}=\|\varphi\|_{L^2}$ for $q\in[2,\infty]$ by interpolation (Exercise 13.5)
Thus we have already proven that if $V\in L^2+L^p$ for $2\leqslant p<3$, then

$$\Omega_+\varphi:=\lim_{t\to\infty}e^{-it(-\Delta+V)}e^{it(-\Delta)}\varphi$$

exists strongly in L^2 for all $\varphi\in L^1\cap L^2$.
First note that Ω_+ is an isometric operator on its domain which is dense hence it can be uniquely extend to all of L^2. More precisely let $\varphi\in L^2$ and $(\varphi_n)_n\subset L^1\cap L^2$ converging to φ. Define $M_t:=e^{-itA}e^{it(-\Delta)}$ then

$$\begin{aligned}\|M_{t_2}\varphi-M_{t_1}\varphi\|&\leqslant\|M_{t_2}\varphi_n-M_{t_1}\varphi_n\|+\|M_{t_2}(\varphi-\varphi_n)-M_{t_1}(\varphi-\varphi_n)\|\leqslant\\&\leqslant\|M_{t_2}\varphi_n-M_{t_1}\varphi_n\|+\underbrace{(\|M_{t_2}\|+\|M_{t_1}\|)}_{=2}\|\varphi-\varphi_n\|=\\&=\|M_{t_2}\varphi_n-M_{t_1}\varphi_n\|+2\|\varphi-\varphi_n\|\xrightarrow{t_1,t_2\to+\infty}2\|\varphi-\varphi_n\|\xrightarrow{n\to\infty}0\end{aligned}$$

q.e.d.

Remark 8.19 (Completeness)**.** If V is nice enough, then

$$\Omega_+:=\operatorname*{s-lim}_{t\to\infty}e^{-it(-\Delta)V}e^{it(-\Delta)}$$

is well-defined on $L^2(\mathbb{R}^3)$. However, by the RAGE theorem we only know that $\operatorname{ran}(\Omega_+)\subset H_c(-\Delta+V)$. When does $\operatorname{ran}(\Omega_+)=H_c(-\Delta+V)$ hold.
If this is correct, then we say that Ω_+ is ***complete***. As a consequence, we can approximate every $u\in\mathscr{H}_c(-\Delta+V)$

$$\left\|e^{it(-\Delta+V)}u-e^{it(-\Delta)}\varphi\right\|_{L^2}\xrightarrow{t\to+\infty}0$$

as a consequence

$$\int\limits_{|x|\leqslant R}\left|\left(e^{it(-\Delta+V)}u\right)(x)\right|\mathrm{d}x\xrightarrow{t\to+\infty}0$$

$\square$

Remark 8.20. Kato prove that Ω_+ is complete iff

$$(\Omega_+)^{-1}u := \lim_{t\to\infty} e^{it(-\Delta)}e^{-itA}u$$

exists for all $u \in \mathscr{H}_c(A)$. $\square$

Theorem 8.21. *If V is short-range $V \in L^1 \cap L^\infty$ and $\|V\|_1 + \|V\|_\infty$ is small enough, then*

$$\left\|Ve^{it(-\Delta+V)}\varphi\right\|_{L^2} \leqslant \frac{C}{1+t^{3/2}}$$

for all $t \in \mathbb{R}$ where $\varphi \in L^1 \cap L^\infty$. C is independent of t but depends on φ. Consequently

$$\int_{-\infty}^{\infty} \left\|Ve^{it(-\Delta+V)}\varphi\right\|_{L^2}\mathrm{d}t < \infty$$

and hence

$$(\Omega_+)^{-1} := \operatorname*{s-lim}_{t\to\infty} e^{-it(-\Delta)}e^{it(-\Delta+V)}$$

exists by Cook's method. This in turn then implies completeness. $\square$

Proof. If $|t| \leqslant 1$ then we have

$$\left\|Ve^{it(-\Delta+V)}\varphi\right\|_{L^2} \leqslant \|V\|_{L^\infty}\left\|e^{it(-\Delta+V)}\varphi\right\|_{L^2} \leqslant \|V\|_{L^\infty}\|\varphi\|_{L^2} \leqslant \frac{C}{2}$$

Thus it suffices to consider $|t| \geqslant 1$ which we shall consider now.

We shall use Duhamel's formula: For $A = -\Delta + V$, $A_0 = -\Delta$

$$e^{-itA}\varphi = e^{-itA_0}\varphi + (-i)\int_0^t e^{-i(t-s)A_0}Ve^{-isA}\varphi\mathrm{d}s.$$

Indeed

$$e^{itA_0}e^{-itA}\varphi = e^{-itA_0}\varphi + (-i)\int_0^t e^{isA_0}Ve^{-isA}\varphi\mathrm{d}s$$

because

$$\frac{d}{dt}\left(e^{itA_0}e^{-itA}\varphi\right) = e^{itA_0}i(A_0 - A)e^{-itA}\varphi = -ie^{itA_0}Ve^{-itA}\varphi.$$

Consider

$$\left\|Ve^{-itA}\varphi\right\|_{L^2} \leqslant \left\|Ve^{-itA_0}\varphi + (-i)\int\limits_0^t Ve^{-i(t-s)A_0}Ve^{-isA}\varphi \mathrm{d}s\right\|_{L^2} \leqslant$$
$$\leqslant \left\|Ve^{-itA_0}\varphi\right\|_{L^2} + \int\limits_0^t \left\|Ve^{-i(t-s)A_0}Ve^{-isA}\varphi\right\|_{L^2}\mathrm{d}s$$

We know that

$$\left\|Ve^{-itA_0}\varphi\right\|_{L^2} \leqslant \|V\|_{L^2}\left\|e^{-itA_0}\varphi\right\|_{L^\infty} \leqslant \frac{C}{|t|^{3/2}}$$

and

$$\left\|Ve^{-i(t-s)A_0}Ve^{-isA}\varphi\right\|_{L^2} \leqslant \|V\|_{L^2}\left\|e^{-i(t-s)A_0}Ve^{-isA}\varphi\right\|_{L^\infty} \leqslant$$
$$\leqslant \frac{\|V\|_{L^2}}{|t-s|^{3/2}}\left\|Ve^{-isA}\varphi\right\|_{L^1}$$

However, the integral over s diverges thus it is only useful for $|s-t|$ not too small. On the other hand

$$\left\|Ve^{-i(t-s)A_0}Ve^{-isA}\varphi\right\|_{L^2} \leqslant \|V\|_{L^\infty}\left\|e^{-i(t-s)A_0}Ve^{-isA}\varphi\right\|_{L^2} =$$
$$= \|V\|_{L^\infty}\left\|Ve^{-isA}\varphi\right\|_{L^2} \leqslant \|V\|_{L^\infty}^2\left\|e^{-isA}\varphi\right\|_{L^2} = \|V\|_{L^\infty}^2\|\varphi\|_{L^2}$$

Define

$$f_t := \left(\left\|Ve^{-itA}\varphi\right\|_{L^1} + \left\|Ve^{-itA}\varphi\right\|_{L^2}\right)$$
$$M_t := \sup_{s\in[0,t]} f(t)$$

By Duhamel's formula we again have

$$\left\|Ve^{-itA}\varphi\right\|_{L^1} \leqslant \left\|Ve^{-itA_0}\varphi\right\|_{L^1} + \int\limits_0^t \left\|Ve^{-i(t-s)A_0}Ve^{-isA}\varphi\right\|_{L^1}\mathrm{d}s$$

The two terms can be estimated via

$$\left\|Ve^{-itA_0}\varphi\right\|_{L^1} \leqslant \|V\|_{L^1}\left\|e^{-itA_0}\varphi\right\|_{L^\infty} \leqslant C\frac{\|V\|_{L^1}\|\varphi\|_{L^1}}{t^{3/2}}$$

$$\left\|Ve^{-i(t-s)A_0}Ve^{-isA}\varphi\right\|_{L^1} \leqslant \|V\|_{L^1}\left\|e^{-i(t-s)A_0}Ve^{-isA}\varphi\right\|_{L^\infty} \leqslant \|V\|_{L^1}\frac{\left\|Ve^{-isA}\varphi\right\|_{L^1}}{|t-s|^{3/2}}$$

$$\left\|Ve^{-i(t-s)A_0}Ve^{-isA}\varphi\right\|_{L^1} \leqslant \|V\|_{L^2}\left\|e^{-i(t-s)A_0}Ve^{-isA}\varphi\right\|_{L^2} = \|V\|_{L^2}\left\|Ve^{-isA}\varphi\right\|_{L^2}$$

In summary

$$\begin{aligned} f_t &\leqslant \frac{C}{t^{3/2}} + \int_0^t \left(\left\|Ve^{-it(t-s)A_0}Ve^{-isA}\varphi\right\|_{L^2} + \left\|Ve^{-it(t-s)A_0}Ve^{-isA}\varphi\right\|_{L^1}\right)\mathrm{d}s \leqslant \\ &\leqslant \frac{C}{t^{3/2}} + \int_0^t \min\left\{\frac{f_s}{|t-s|^{3/2}}, f_s\right\}\mathrm{d}s \end{aligned}$$

Thus

$$M_t \leqslant \frac{C}{t^{\frac{3}{2}}} + M_t \underbrace{\int_0^t \min\left\{\frac{1}{|t-s|^{3/2}}, 1\right\}\mathrm{d}s}_{=:D<\infty}(\|V\|_{L^\infty} + \|V\|_{L^1}) = \frac{C}{t^{\frac{3}{2}}} + M_t D(\|V\|_{L^\infty} + \|V\|_{L^1})$$

If $D(\|V\|_{L^\infty} + \|V\|_{L^1}) < 1$ then $M_t \leqslant \frac{C'}{t^{3/2}}$, thus for all $t \in \mathbb{R}$

$$\|Ve^{-itA}\varphi\|_{L^2} + \|Ve^{-itA}\varphi\|_{L^1} \leqslant \frac{C}{1+|t|^{\frac{3}{2}}}$$

which ends the proof by Cook's theorem.

q.e.d.

Remark 8.22. In this case, i.e. $(\|V\|_{L^1} + \|V\|_\infty)$ being small, then for all $u \in L^2(\mathbb{R}^3)$

$$\left\|e^{-it(-\Delta+V)}u - e^{-it(-\Delta)}\varphi\right\|_{L^2} \xrightarrow{t\to\infty} \infty$$

for some $\varphi \in L^2$. Thus $u \in H_c(-\Delta+V)$. Consequently $H_p(-\Delta+V) = \{0\}$, i.e. $-\Delta+V$ has no eigenvalue. $\square$

Remark 8.23. Assume that the wave operators $\Omega_\pm = \text{s-lim}_{t\to\infty} e^{-itA}e^{itA_0}$ exist, $A_0 = -\Delta$ on $L^2(\mathbb{R}^d)$. Then $A\Omega_\pm = \Omega_\pm A_0$ which is equivalent to $A_0 = \Omega_\pm^{-1} A\Omega_\pm$. $\Omega_\pm : L^2(\mathbb{R}^d) \to \operatorname{ran}\Omega_\pm$ is unitary.
Take $\Omega_\pm(x,y)$ to be the kernel of $\Omega_\pm$. Then for all f

$$\begin{aligned}
&(A\Omega_\pm\overline{f})(x) = (\Omega_\pm A_0\overline{f})(x)\\
\implies &\int A_x\Omega_\pm(x,y)\overline{f}(y)\mathrm{d}y = \int \Omega_\pm(x,y)\overline{-\Delta f}(y)\mathrm{d}y\\
\implies &\int A_x\widehat{\Omega_\pm}(x,y)\overline{\hat{f}}(y)\mathrm{d}y = \int \Omega_\pm(x,k)|2\pi k|^2\overline{\hat{f}}(k)\mathrm{d}k\\
\implies &A_x\widehat{\Omega_\pm}(x,k)\overline{\hat{f}}(y)\mathrm{d}y = |2\pi k|^2\Omega_\pm(x,k)
\end{aligned}$$

for all x, k. Here $\hat{\Omega}_\pm(x,k)$ is the Fourier transform of $y \mapsto \Omega_\pm(x,y)$.
Thus for all $k \in \mathbb{R}^d$, $x \mapsto \widehat{\Omega}_\pm(x,k)$ is "like" an eigenfunction of A w.r.t. to the eigenvalue $|2\pi k|^2$. Here it might happen that $x \mapsto \Omega_\pm(x,k) \notin L^2(\mathbb{R}^d)$. □

Example 8.24. If $d = 1$ and $A = -\Delta + V(x)$ where

$$V(x) = \begin{cases} V_0 & \text{if } x > 0 \\ 0 & \text{if } x < 0 \end{cases}$$

then for all k

$$\Omega_\pm(x,k) = \begin{cases} Ae^{2\pi ikx} + Be^{-2\pi ikx}, & \text{if } x > 0 \\ Ce^{2\pi ikx} + De^{-2\pi ikx}, & \text{if } x < 0 \end{cases}$$

Remark 8.25 (Existence of Wave Operators)**.** By Cook's method $\Omega_\pm$ exist if

$$\int_{T_0}^{\infty} \|(A - A_0)e^{itA_0}\varphi\|_{L^2} < \infty$$

for φ in a dense set. Above we applied this to $A_0 = -\Delta$ and $A = -\Delta + V$. We can also apply this to $A_0 = -\Delta$ and $A = -\Delta + |v\rangle\langle v|$ or $A = -\Delta + B$ where B is trace class. One can also apply Kato's method: If $A - A_0$ is trace class, $\Omega_\pm = \text{s-lim}_{t\to\pm\infty} e^{-itA}e^{itA_0}$ exists. There are many extensions, e.g. assuming that $(A+i)^{-1} - (A_0+i)^{-1}$ is trace class. $\square$

Scattering

A scattering experiment is characterised by a set of ingoing particles with momenta and spins

$$\{\boldsymbol{k}_1, s_1, \ldots, \boldsymbol{k}_I, s_I\}$$

and and a set of outgoing particles

$$\{\boldsymbol{q}_1, \sigma_1, \ldots, \boldsymbol{q}_J, \boldsymbol{\sigma}_J\}$$

and the so-called scattering cross-section

$$\sigma(\boldsymbol{k}_1, s_1, \ldots, \boldsymbol{k}_I, s_I, \boldsymbol{q}_1, \sigma_1, \ldots, \boldsymbol{q}_J, \sigma_J) = \frac{N_e}{F_i}$$

where N_e is number of outgoing particles of a certain type and F_i is the ingoing flux, i.e. the number of particles coming in per unit time per unit area.

Lippmann-Schwinger Equation

We are looking for a scattering solution $\psi^{\pm}_{\boldsymbol{k}}$. The $\pm$ denotes the in/outgoing boundary condition and $\boldsymbol{k}$ the asymptotic momentum at large distances.

$$\psi^{\pm}_{\boldsymbol{k}} = \lim_{\varepsilon \downarrow 0} \varphi - \frac{1}{H_0 - \left(\frac{k^2}{2} \pm i\varepsilon\right)} \left(V \psi^{\pm}_{\boldsymbol{k}}\right)$$

This will deliver solution such that

$$H\psi^{\pm}_{\boldsymbol{k}} = \frac{k^2}{2} \psi^{\pm}_{\boldsymbol{k}}$$

where $H = H_0 + V$ and

$$H_0 \varphi = \frac{k^2}{2} \varphi.$$

In position space with $H_0 = -\frac{1}{2}\Delta$

$$\psi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} - \frac{1}{4\pi}\int \frac{e^{\mp i|\boldsymbol{k}||\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r}-\boldsymbol{r}'|} V(\boldsymbol{r}')\psi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}')\mathrm{d}r'$$

Modelling a (Simple) Scattering Experiment

We prepare a particle in a "free" state, wave packet

$$\varphi(\boldsymbol{r}, -t) = \frac{1}{(2\pi)^{3/2}}\int e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\psi(\boldsymbol{k})\mathrm{d}k$$

such that $\varphi(\boldsymbol{r}, -t)$ is outside the range of the potential.
Let $\varphi(\boldsymbol{r}, -t)$ evolve by e^{-iHt} (not H_0) to large times T and analyse $\varphi(\boldsymbol{r}, T)$ in terms of free wave packets.

(1) What does "prepare the wave packet" mean? Can we map any wave-packet of free mater (H_0), onto a scattering state of the free problem (H)? Is that mapping unique? (***Existence and Uniqueness of Scattering Theory***)

(2) What is the fate of the scattering state? Can the incoming packet en up as a bound state of H. (***Asymptotic Completeness of Scattering Theory***)

Point, Absolutely Continuous and Singular Spectrum

A Hilbert space is divided by a self-adjoint operator on it into the following spectral subspaces:

$$\mathscr{H}_p = \overline{\mathrm{span}(eigenvectors)}$$

the subspace of the pure-point spectrum,

$$\mathscr{H}_c = \mathscr{H}_p^{\perp}$$

the essential (continuous) subspace. One can further distinguish $\mathscr{H}_c$

$$\mathscr{H}_c = \mathscr{H}_{\mathrm{ac}} \oplus \mathscr{H}_s$$

where measure μ_u associated with $u \in \mathscr{H}_{\mathrm{ac}}$ is absolutely continuous w.r.t. the Lebesgue measure (i.e. there exists a measurable function f such that $\mu = f\lambda$, where λ is the Lebesgue

measure). The measure associated to the vectors in the complementary space is singular to λ but continuous (i.e. does not contain delta functions).
$\psi \in \mathscr{H}_{\mathrm{ac}}$ behave like wave packets, i.e.

$$\lim_{t\to\pm\infty} \left\langle e^{-itH}\psi \,\middle|\, \psi \right\rangle = 0$$

For $\psi \in \mathscr{H}_s$ only the corresponding time average decays.
A scattering experiment is composed of two dynamics: the free evolution H_0 and the interacting evolution H.

Theorem 8.26. *Let A be a self-adjoint operator and K relatively A-compact and denote by $P^{(c)}\mathscr{H} = \mathscr{H}_c$ and $P^{(ac)}\mathscr{H} = \mathscr{H}_{ac}$ the projection into the continuous and absolutely continuous subspaces respectively, ten*

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \left\| K e^{-itA} P^{(c)} \psi \right\|^2 \mathrm{d}t = 0$$
$$\lim_{T\to\infty} \left\| K e^{-itA} P^{(ac)} \psi \right\|^2 = 0$$

□

Remark 8.27 (Implications for Schrödinger Operators)**.** Let χ_R be the characteristic function of a sphere of radius R. Then χ_R is $(-\Delta)$-relatively compact.
In particular for any function $\psi \in \mathscr{H} = \mathscr{H}^{(\mathrm{ac}),-\Delta}$

$$\lim_{t\to\infty} \|\chi_R e^{it\Delta}\psi\| = 0$$

□

Theorem 8.28 (RAGE (Ruelle, Amrein, Georgescu, Enß) Theorem)**.** *Let A be a self-adjoint operator. Suppose there is a sequence of A-relatively compact operators $(K_n)_n$*

which converges strongly to the identity. Then

$$\mathscr{H}_c = \left\{ \psi \in \mathscr{H} \,\middle|\, \lim_{n\to\infty} \lim_{T\to\infty} \frac{1}{T} \int_0^T \|K_n e^{-itA}\psi\| \mathrm{d}t = 0 \right\}$$
$$\mathscr{H}_p = \left\{ \psi \in \mathscr{H} \,\middle|\, \lim_{n\to\infty} \sup_{t\geqslant 0} \|(1-K_n)e^{-itA}\psi\| = 0 \right\}$$

□

Scattering Operators $\Omega_\pm$ (Møller)

Let $U_0(t) = e^{-itH_0}$ and $U(t) = e^{-itH}$. Then the scattering operators are defined on $\mathscr{H}^{\mathrm{ac}}(H_0)$ via

$$\Omega_\pm := \operatorname*{s-lim}_{t\to\pm\infty} U(t)U_0(-t)$$

when they exist.

Definition 8.29 (Asymptotic Completeness)**.** If $\Omega_\pm$ are bijections $\mathscr{H}^{\mathrm{ac}}(H) \leftrightarrow \mathscr{H}^{\mathrm{ac}}(H_0)$ the scattering problem is said to be asymptotically complete. □

$\Omega_\pm$ exist and are complete for "short range potentials"

A potential V is called short ranged if

$$\int_0^\infty \left\| V(-\Delta+1)^{-1}\mathbf{1}_{B_r^C} \right\| \mathrm{d}r < \infty$$

and $V(-\Delta+1)^{-1}$ is relatively bounded. Here B_r denotes the ball of radius r.
For all $\varepsilon > 0$ the potentials $\frac{1}{r^{1+\varepsilon}}$ are short range, but the Coulomb potential is not.

Stationary Scattering Theory

$$\lim_{\varepsilon\downarrow 0} \varepsilon \int_0^\infty e^{-\varepsilon t} f(t)\mathrm{d}t = \lim_{t\to\infty} f(t).$$

Representing H_0 via its porjection valued measures

$$H_0 = \int_0^\infty \mathrm{d}P(E)$$

Then

$$e^{itH}e^{-itH_0} = e^{itH}\int_0^\infty e^{-itE}\mathrm{d}P(E)e^{itH} = \int_0^\infty e^{it(H-E)}\mathrm{d}P(E)$$

Then

$$\Omega_\pm = \lim_{\varepsilon\downarrow 0}\varepsilon\int_0^\infty e^{-\varepsilon t}\int_0^\infty e^{\pm it(H-E)}\mathrm{d}P(E)\mathrm{d}t = 1 - \lim_{\varepsilon\downarrow 0}\int_0^\infty (H-E\pm i\varepsilon)^{-1}V\,\mathrm{d}P(E)$$

which yields the Lippmann-Schwinger equation.

Asymptotic Completeness

A potential is called asymptotically complete if

$$\Omega_\pm P_{\mathrm{ac}}(H_0)\mathscr{H} = P_{\mathrm{ac}}(H)\mathscr{H}.$$

This is the case when the potential is short-range, i.e.

$$\int_0^\infty \|V(-\Delta+1)^{-1}\mathbf{1}_{B_r^C}\|\mathrm{d}r < \infty$$

or when Cook's criterion holds

$$\int_{t_0}^\infty \|Ve^{\pm itH_0}\varphi\|\mathrm{d}t < \infty$$

Consider the self-adjoint dilation operator

$$D = \frac{1}{2}(\boldsymbol{x}\cdot\boldsymbol{p} + \boldsymbol{p}\cdot\boldsymbol{x})$$

which generates the dilations

$$U_\lambda \psi(x) = \left(e^\lambda\right)^{\frac{3}{2}} \psi(e^\lambda x) = e^{i\lambda D}\psi(x)$$

Define the projectors onto the in- and out-going subspaces via

$$P_\pm := P_D(0, \pm\infty).$$

We also have Perry's estimate for any $n \in \mathbb{N}$

$$\left\| \mathbf{1}_{B_{2v|t|}} e^{-itH_0} f(h_0) P_D((\pm R, \pm\infty)) \right\| \leqslant \frac{C}{1+|t|^n} f$$

where f is differentiable function with support in $[v_0^2, v_1^2]$ where $v < v_0$.

Functions of the type

$$\psi = f(H_0) P_D((\pm R, \pm\infty))\varphi$$

are dense in $\mathscr{H}$.

By Cook's criterion $\Omega_\pm$ exists and thus $\Omega_\pm P_{\mathrm{ac}}\mathscr{H} \subset P_{\mathrm{ac}}\mathscr{H}$. The short range property enters as $(\Omega_\pm - 1) f(H_0) P_\pm$ being compact.

Final steps of the proof: Take $\psi(t) = e^{-itH}\psi$ from $P_{\mathrm{ac}}\mathscr{H}$. We need to show that $\psi \in \operatorname{ran}\Omega_\pm$. At large $t > 0$ $\psi(t)$ can be meaningfully decomposed into $\varphi_-(t) + \varphi_+(t)$ where $\varphi_\pm(t) \in P_{D,\pm}$.

In this step short range-ness is essential, i.e.e $f(H_0) - f(H)$ is compact.

Next we see that

$$\|\psi\|^2 = \cdots = \lim_{t\to\pm\infty} \langle \psi(t), \Omega_+\varphi_+(t) + \Omega_-\varphi_-(t)\rangle$$

Assume there exists $\psi_\perp$ which is orthogonal to $\operatorname{ran}\Omega_+$.

Teschl 12.43

$$\lim_{t\to+\infty} \left\langle P_\mp f(H_0)^* e^{-itH_0} \Omega_\mp^* \psi(t), \psi(t) \right\rangle = 0$$

Intertwining property: (bijective map between the dynamics of H_0 and the scattering dynamics of H)

$$\Omega_\pm f(H_0) = f(H)\Omega_\pm$$

at large t: $\varphi_+(t)$ is completely in $P_{\mathrm{ac}}\mathscr{H}$. At all times scattering wave packets are in $P_{\mathrm{ac}}(\mathscr{H})$.

Coulomb Scattering

Wave operators for $H_0 = -\Delta$, $H = -\Delta \mp \frac{1}{r}$ do not exists. Why? The classical trajectory of a particle moving classically, radially away then

$$r(t) = ct + d\log(t) + O(1)$$

never $\sim ct$.

There are three ways out:

(1) Exact solutions and eigenfunctions are known for $H = -\Delta \pm \frac{1}{r}$; hypergeometric functions

(1b) Cross-section formulae are known but they only contain information concerning the asymptotic momenta $\boldsymbol{p}_\pm$ (Rutherford formula).

(2) The Dollard Hamiltonian

$$H_D(t) = -\Delta - \frac{1}{2|t|\sqrt{-\Delta}}\vartheta(-4|t|\Delta - 1)$$

Then

$$\Omega_\pm^D = \operatorname*{s-lim}_{t\to\pm\infty} e^{it(-\Delta-\frac{1}{r})}e^{-i\int\limits_0^t H_D(s)\mathrm{d}s}$$

exists.

S-Matrix

We are interested in the transition probabilities

$$\left|\,\langle\Omega_+\varphi_i, \Omega_-\varphi_e\rangle\,\right|^2$$

or in other words

$$S := \Omega_-^\dagger\Omega_+$$

This is a unitary operator

$$S : P_{\mathrm{ac}}\mathscr{H} \longrightarrow P_{\mathrm{ac}}\mathscr{H}$$

S inherits all symmetries of H and H_0. In particular

$$[H_0, S] = 0$$

via the intertwining property. This means that "free" energy is conserved by S.

$$S = \lim_{\varepsilon \downarrow 0} \int \big(1 - 2\pi i \delta(H_0 - E)\big(V - V(H - E + i\varepsilon)^{-1}V\big)\delta(H_0 - E)\big)\mathrm{d}E$$

Abel limit.

For a rotationally symmetric potential the S matrix must commute with the angular momentum operators, i.e.

$$S\,|E, \ell, m\rangle = e^{i\delta_\ell(k)}\,|E, \ell, m\rangle$$

here $k^2 = 2E$. $\delta_\ell(k)$ is called the scattering phase.

Note that the 1 in the S-matrix formula above induces a singularity for transitions of the type $\langle \varphi, S\varphi\rangle$.

Thus we restrict our attention to the so-called T-matrix.

$$T(z) = V - V(H - z)^{-1}V.$$

We define the "on-shell" matrix element

$$t(\boldsymbol{k}, \boldsymbol{k}') = \lim_{\varepsilon \downarrow 0} \left\langle \boldsymbol{k} \,\middle|\, V - V(H - E - i\varepsilon)^{-1}V \,\middle|\, \boldsymbol{k} \right\rangle$$

where

$$|\boldsymbol{k}\rangle = (2\pi)^{-\frac{3}{2}} e^{i\boldsymbol{k}\cdot\boldsymbol{x}}, \qquad \langle \boldsymbol{k}, \boldsymbol{k}'\rangle = \delta(\boldsymbol{k} - \boldsymbol{k}')$$

Note that

$$\langle \boldsymbol{k} \,|\, V\Omega_- \,|\, \boldsymbol{k}'\rangle = \left\langle \boldsymbol{k} \,\middle|\, \Omega_+^* V \,\middle|\, \boldsymbol{k}' \right\rangle$$

Now defining for two unit vectors $\boldsymbol{n}, \boldsymbol{n}' \in \mathbb{R}^3$.

$$f(k, \boldsymbol{n}, \boldsymbol{n}') := -(2\pi)^2 t(k\boldsymbol{n}, t\boldsymbol{n}')$$

then

$$\sigma(k\boldsymbol{n}, k\boldsymbol{n}') = |f(k, \boldsymbol{n}, \boldsymbol{n}')|^2$$

Chapter 9

Many-Body Quantum Theory

Our Hilbert space in the following shall be $\mathscr{H} = L^2\Big((\mathbb{R}^3)^N\Big) = L^2(\mathbb{R}^{3N}) = \bigotimes^N L^2(\mathbb{R}^3)$.

Remark 9.1. In general we have for finite dimensional vector space H_1, H_2

$$L^2(H_1 \oplus H_2) \simeq L^2(H_1) \otimes L^2(H_2)$$

given by

$$u_i \otimes v_j \longmapsto u_i \otimes v_j$$

where $(u_i)_i$ is a basis for $L^2(H_1)$ and $(v_j)_j$ is one for $L^2(H_2)$ and

$$(u \otimes v)(x, y) = u(x)v(y)$$

Note that $L^2(H_1) \times L^2(H_2) \to L^2(H_1 \oplus H_2), (u, v) \mapsto u \otimes v$ is bilinear and thus has a unique lifting to $L^2(H_1) \otimes L^2(H_2)$. $\square$

The typical many-body Hamiltonian for N-particles is

$$H_N = \sum_{i=1}^{N} (-\Delta_{x_i} + V(x_i)) + \sum_{1 \leqslant i < j \leqslant N} W(x_i - x_j)$$

where $x_i \in \mathbb{R}^3$ is interpreted as the position i^{th} particle.

Example 9.2. A molecule with M nuclei at $(R_j)_{j=1}^N$ with charges $Z_j > 0$ then the

Hamiltonian of N-electrons is

$$H_N = \sum_{i=1}^{N} j\left(-\Delta_{x_i} - \sum_{j=1}^{M} \frac{Z_j}{x_i - R_j}\right) + \sum_{1\leqslant i<j\leqslant N} \frac{1}{|x_i - x_j|} + \underbrace{\sum_{1\leqslant j<k<\leqslant M} \frac{Z_j Z_k}{|R_j - R_k|}}_{\text{constant}}.$$

Remark 9.3 (Fundamental Questions). 1) When is H_N self-adjoint?

2) What does $\sigma(H_N)$ look like?

3) Dynamics (existence of wave operator, asymptotic completeness)

□

Remark 9.4. In one-body theory, $-\Delta + V(x)$, if $V(x) \xrightarrow{|x|\to\infty} 0$ "fast", then V is $(-\Delta)$-compact and thus $-\Delta + V$ is self-adjoint with domain $H^2(\mathbb{R}^d)$ and $\sigma_{\text{ess}}(-\Delta + V) = \sigma_{\text{ess}}(-\Delta) = [0, \infty)$.
In N-Body theory the interaction potential $W(x_1 - x_2)$ is never a compact perturbation of $(-\Delta)$ even if $W(x) \xrightarrow{|x|\to\infty} 0$ "fast". This is the case as $W(x_1 - x_2) \not\to 0$ as $|x_1|, |x_2| \to \infty$, i.e. by taking $x_2 = x_1 + k$ where k is some constant vector. □

Theorem 9.5 (Kato). *Let*

$$H_N = \sum_{i=1}^{N} (-\Delta_{x_i} + V(x_i)) + \sum_{1\leqslant i<j\leqslant N} W(x_i - x_j)$$

with $x_i \in \mathbb{R}^3$. Then this operator is self-adjoint on $L^2(\mathbb{R}^{3N})$ with domain $H^2(\mathbb{R}^{3N})$ provided that $V, W \in L^2(\mathbb{R}^3) + L^p(\mathbb{R}^3)$ for $2 \leqslant p \leqslant \infty$. □

Proof. This follows from Theorem 5.12, i.e. we have to prove that $V(x_i)mW(x_i - x_j)$ are bounded w.r.t. $-\sum_{i=1}^{N} \Delta_{x_i} = -\Delta_{\mathbb{R}^{3N}}$ with relative bound smaller than ε for any $\varepsilon > 0$, i.e.

$$\|V(x_i)\Psi\|_{L^2} \leqslant \varepsilon\|\psi\|_{H^2(\mathbb{R}^{3N})} + C_\varepsilon\|\psi\|_{L^2}$$
$$\|W(x_i - x_j)\Psi\|_{L^2} \leqslant \varepsilon\|\psi\|_{H^2(\mathbb{R}^{3N})} + C_\varepsilon\|\psi\|_{L^2}$$

The first case follows as in the one-body theory. Concerning the second suppose that $W \in L^2$, then

$$\|W(x-y)\Psi\|_{L^2}^2 = \int |W(x_i - x_j)|^2 |\Psi(x_1, \dots, x_N)|^2 \mathrm{d}x_1 \cdots \mathrm{d}x_N \leqslant$$
$$\leqslant \int \left(\int |W(x_i - x_j)|^2 \left(\sup_{x_i} |\Psi(x_1, \dots, x_N)|^2 \right) \mathrm{d}x_i \right) \prod_{j \neq i} \mathrm{d}x_j.$$

Here

$$\sup_{x_i} |\Psi(x_1, \dots, x_N)|^2 \leqslant C \|\Psi(x_1, \dots, x_N)\|_{H^2_{x_i}(\mathbb{R}^3)}^2$$

thus

$$\|W(x-y)\Psi\|_{L^2}^2 \leqslant C \int \left(\int |W(x_i - x_j)|^2 \|\Psi(x_1, \dots, x_N)\|_{H^2_{x_i}(\mathbb{R}^3)}^2 \mathrm{d}x_i \right) \prod_{j \neq i} \mathrm{d}x_j =$$
$$= C \int \left(\int \|W\|_{L^2}^2 \|\Psi(x_1, \dots, \widehat{x_i}, \dots, x_N)\|_{H^2_{x_i}(\mathbb{R}^3)}^2 \right) \prod_{j \neq i} \mathrm{d}x_j \leqslant$$
$$\leqslant \|W\|_{L^2(\mathbb{R}^3)}^2 \|\Psi\|_{H^2(\mathbb{R}^3)}^2$$

Note that if $W \in L^2(\mathbb{R}^3) + L^p(\mathbb{R}^3)$ then we can write it as $W = W_1 + W_2$ with $W_1 \in L^2, W_2 \in L^\infty$ and $\|W_1\|_{L^2} \leqslant \varepsilon$. Thus

$$\|W(x_i - x_j)\Psi\|_{L^2} \leqslant \|W_1(x_i - x_j)\Psi\|_{L^2} + \|W_2(x_i - x_j)\Psi\|_{L^2} \leqslant C\varepsilon \|\Psi\|_{H^2(\mathbb{R}^{3N})} + \|W_2\|_\infty \|\Psi\|_{L^2}$$

for all $\varepsilon > 0$.

q.e.d.

Remark 9.6. There is a nice story behind the proof of this theorem which can be found in the paper "Tosio Kato's Work on Non-Relativistic Quantum Mechanics" by Barry Simon `https://arxiv.org/pdf/1711.00528.pdf`. □

Now we shall consider what $\sigma(H_N)$ looks like. Note that $\sigma_{\text{ess}}(H_N) \neq \sigma_{\text{ess}}(-\Delta_{\mathbb{R}^{3N}}) = [0, \infty)$ except when $N = 1$ or $W \equiv 0$.
Assume that

$$H_N = \sum_{i=1}^{N} (-\Delta_{x_i} + V(x_i)) + \sum_{1 \leqslant i < j \leqslant N} W(x_i - x_j)$$

and $V, W \in L^2(\mathbb{R}^3) + L^p(\mathbb{R}^3)$ with $2 \leqslant p < \infty$. We know that H_N is self-adjoint and bounded from below, i.e.

$$E_N := \inf \sigma(H_N) > -\infty.$$

Theorem 9.7 (Humitzer, Van Winter, Zhislin (HVZ)). *Under these two assumptions and $W \geqslant 0$, then $\sigma_{ess}(H_N) = [E_{N-1}, \infty)$.* □

Example 9.8. Consider the Helium Hamiltonian

$$H_2 = -\Delta_{x_1} - \Delta_{x_2} - \frac{Z}{|x_1|} - \frac{Z}{|x_2|} + \frac{1}{|x_1 - x_2|}$$

with $Z > 0$. Then

$$\sigma_{\text{ess}}(H_2) = \left[\inf \sigma\left(-\Delta - \frac{Z}{|x|}\right), \infty\right) = \left[-\frac{Z^2}{4}, \infty\right)$$

since the spectrum of H_1 is given by

$$\sigma(H_1) = \left(-\frac{Z^2}{4n^2}\right)_{n=1}^{\infty} \cup [0, \infty)$$

where each eigenvalue has multiplicity n^2.

Proof. ($\supset$) The key point is that

$$H_N = H_{N-1} + (-\Delta_{x_N}) + V(x_N) + \sum_{i=1}^{N-1} V(x_i - x_N).$$

Take $\lambda \geqslant E_{N-1}$. We prove that $\lambda \in \sigma_{\text{ess}}(H_N)$ by constructing a singular Weyl sequence $\left(\psi^{(k)}\right)_k \subset L^2(\mathbb{R}^{3N})$ of unit vectors converging weakly to L^2 and

$$\|(H_N - \lambda)\psi_N^{(k)}\|_{L^2} \xrightarrow{k\to\infty} 0$$

We chose $\psi^{(k)} = \psi_{N-1}^{(k)} \otimes \varphi^{(k)}$, where $\psi_{N-1}^{(k)}$ is a Weyl sequence for $E_{N-1} = \inf \sigma(H_{N-1}) \in \sigma(H_{N-1})$, i.e. $\|\psi_{N-1}^{(k)}\|_{L^2} = 1$ and

$$\|(H_N - \lambda)\psi_{N-1}^{(k)}\|_{L^2} \xrightarrow{k\to\infty} 0$$

By a density argument, we can take $\psi_{N-1}^{(k)}$ such that $\operatorname{supp} \psi_{N-1}^{(k)} \subset B_{\mathbb{R}^{3(N-1)}}(0, R_k)$ with

$R_k \xrightarrow{k\to\infty} +\infty$

On the other hand, $\lambda - E_{N-1} \in \sigma_{\text{ess}}(-\Delta + V) = \sigma_{\text{ess}}(-\Delta) = [0,\infty)$. I.e. we can choose a Weyl sequence φ_k such that $\|\varphi^{(k)}\|_{L^2(\mathbb{R}^3)} = 1$, $\varphi^{(k)} \rightharpoonup 0$ in $L^2(\mathbb{R}^3)$ and

$$\|(-\Delta_{x_N} + V(x_N) - (\lambda - E_{N-1}))\varphi^{(k)}\|_{L^2} \xrightarrow{k\to\infty} .$$

In face wan choose φ^k such that $\operatorname{supp}\varphi^{(k)} \subset \big\{x \in \mathbb{R}^3 \,\big|\, |x| \geqslant 2R_k\big\}$.

With the choice $\psi_N^{(k)} = \psi_{N-1}^{(k)} \otimes \varphi^{(k)}$ then

$$\begin{aligned}\|(H_N - \lambda)\psi_N^{(k)}\| \leqslant{} & \|(H_{N-1} - E_{N-1})\psi_{N-1}^{(k)} \otimes \varphi^{(k)}\| + \\ & + \|(-\Delta_{x_N} + V(x_N) - (\lambda - E_{N-1}))\psi_{N-1}^{(k)} \otimes \varphi^{(k)}\| + \\ & + \left\|\sum_{i=1}^{N-1} W(x_i - x_N)\psi_{N-1}^{(k)} \otimes \varphi^{(k)}\right\|\end{aligned}$$

We have

$$\|(H_{N-1} - E_{N-1})\psi_{N-1}^{(k)} \otimes \varphi^{(k)}\| = \|(H_{N-1} - E_{N-1})\psi_{N-1}^{(k)}\| \underbrace{\|\varphi^{(k)}\|}_{=1} \xrightarrow{k\to\infty} 0$$

$$\|(-\Delta_{x_N} + V(x_N) - (\lambda - E_{N-1}))\psi_{N-1}^{(k)} \otimes \varphi^{(k)}\| = \underbrace{\|\psi_{N-1}^{(k)}\|}_{=1} \|(-\Delta_{x_N} + V(x_N) - (\lambda - E_{N-1}))\varphi^{(k)}\| \xrightarrow{k\to\infty} 0$$

$$\left\|\sum_{i=1}^{N-1} W(x_i - x_N)\psi_{N-1}^{(k)} \otimes \varphi^{(k)}\right\| = \Big\| \underbrace{\mathbf{1}_{\{|x_i - x_N| \geqslant R_k\}}}_{\xrightarrow{R_k\to\infty} 0} W(x_i - x_N)\psi_{N-1}^{(k)} \otimes \varphi^{(k)}\Big\|_{L^2} \xrightarrow{k\to\infty} 0$$

since $|x_i| \leqslant R_k, |x_N| \geqslant 2R_k$.

($\subset$) Here $W \geqslant 0$ is important. Take $\lambda \in \sigma_{\text{ess}}(H_N)$. Then we can find a Weyl sequence $\psi_N^{(k)}$ such that $\|\psi_N^{(k)}\|_{L^2} = 1$, $\psi_N^{(k)} \xrightharpoonup{k\to\infty} 0$ and

$$\|(H_N - \lambda)\psi_N^{(k)}\| \xrightarrow{k\to\infty} 0$$

Using the Lemma below we may choose a partition of unity as described therein and apply the IMS localisation formula

$$-\Delta = \sum_{i=0}^{N} \big(\varphi_i(-\Delta)\varphi_i - |\nabla\varphi_i|^2\big)$$

Now we have $\lambda = \lim_{k\to\infty} \left\langle \psi_N^{(k)}, H_N \psi_N^{(k)} \right\rangle$ and

$$\left\langle \psi_N^{(k)}, H_N \psi_N^{(k)} \right\rangle = \sum_{j=0}^{N} \left\langle \psi_N^{(k)}, \varphi_j H_N \varphi_j \psi_N^{(k)} \right\rangle - \sum_{j=0}^{N} \langle \psi_N^{(k)}, \underbrace{|\nabla \varphi_j|^2}_{\frac{C^2}{R^2}} \psi_N^{(k)} \rangle$$

The right-most term converges uniformly in k to 0 as $R \to \infty$.

Further

$$\left\langle \psi_N^{(k)}, \varphi_0 H_N \varphi_0 \psi_N^{(k)} \right\rangle \geqslant \underbrace{E_N}_{\leqslant 0} \int_{\mathbb{R}^{3N}} |\varphi_0|^2 |\psi_N^{(k))}| \xrightarrow{k\to\infty} 0$$

for fixed R since $\operatorname{supp} \varphi_0$ is bounded and $\psi_N^{(k)}$ converges strongly to 0 on bounded sets by the Sobolev embedding as $\psi_N^{(k)}$ is bounded in $H^1(\mathbb{R}^{3N})$ and converges weakly to 0.

If $j = 1, \dots, N$

$$\begin{aligned}
\left\langle \psi_N^{(k)}, \varphi_j H_N \varphi_j \psi_N^{(k)} \right\rangle &= \Bigg\langle \psi_N^{(k)}, \varphi_j \Bigg(\underbrace{H_{N-1}}_{\geqslant E_{N-1}} + (-\Delta_{x_N}) + V(x_N) + \\
&\qquad + \sum_{i=1}^{N} \underbrace{W(x_i - x_N)}_{\geqslant 0} \Bigg) \varphi_j \psi_N^{(k)} \Bigg\rangle \geqslant \\
&\geqslant \left\langle \psi_N^{(k)}, \varphi_j \big(E_{N-1} + \underbrace{(-\Delta_{x_N}) + V(x_N)}_{\substack{\gtrsim 0 \\ \text{as } R\to\infty}} \big) \varphi_j \psi_N^{(k)} \right\rangle \geqslant \\
&\geqslant E_{N-1} \int |\varphi_j|^2 |\psi_N^{(k)}|^2 + o(1)_{R\to\infty}
\end{aligned}$$

Thus

$$\begin{aligned}
\sum_{j=1}^{N} \left\langle \psi_N^{(k)}, \varphi_j H_N \varphi_j \psi_N^{(k)} \right\rangle &\geqslant E_{N-1} \Big(1 - \left\langle \psi_N^{(k)}, \varphi_0 H_N \varphi_0 \psi_N^{(k)} \right\rangle \Big) \geqslant \\
&\geqslant E_{N-1} (1 + o(1)_{k\to\infty}) + o(1)_{R\to\infty}
\end{aligned}$$

Altogether we may conclude

$$\lambda = \lim_{k\to\infty} \left\langle \psi_N^{(k)}, H_N \psi_N^{(k)} \right\rangle \geqslant E_{N-1}$$

thus $\sigma_{\mathrm{ess}}(H_N) \subset [E_N, \infty)$.

q.e.d.

Remark 9.9. Indeed, without the assumption $W \geqslant 0$, we still have $\sigma_{\text{ess}}(H_N) \supset [E_{N-1}, \infty)$. $\square$

Lemma 9.10. *There exists a partition of unity in $\mathbb{R}^{3N}$ such that $1 = \sum_{j=0}^{N} \varphi_j^2$, $\varphi_j \geqslant 0$ smooth such that*

1) $\operatorname{supp} \varphi_0 \subset \left\{ x = (x_1, \ldots, x_N) \in \mathbb{R}^{3N} \,\middle|\, \max |x_i| \leqslant 2R \right\}$

2) $\operatorname{supp} \varphi_j \subset \left\{ x = (x_1, \ldots, x_N) \in \mathbb{R}^{3N} \,\middle|\, |x_j| \geqslant R \right\}$

3) $|\nabla \varphi_0|, |\nabla \varphi_j| \leqslant \frac{C}{R}$ *where C is independent of R.*

$\square$

Proof. Exercise 14.2 *q.e.d.*

Theorem 9.11 (Zhislin)**.** *Consider the Hamiltonian*

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

with $x_i \in \mathbb{R}^3$. This describes an atom with Z protons at the origin and N electrons. We know that $H_{N,Z}$ is self-adjoint on $L^2(\mathbb{R}^{3N})$ with domain $H^2(\mathbb{R}^{3N})$ and $\sigma_{ess}(H_{N,Z}) = [E_{N-1,Z}, \infty)$.
If $N < Z+1$, then $E_{N,Z} < E_{N-1,Z}$ and $H_{N,Z}$ has infinitely many bound states below its essential spectrum. $\square$

Remark 9.12. The condition $N < Z + 1$ follows also on physical grounds as at large distance a nucleus with charge Z and $N-1$ electrons appears as a single charged particle with charge $Z - (N-1)$. A further electron will be attracted to this particle if the charge of the particle is positive, i.e. $Z - (N-1) > 0$.
However, it is an open conjecture, called the ***Ionisation Conjecture***, that if $N > Z+1$, then $E_{N,Z} = E_{N-1,Z}$ and $H_{N,Z}$ has no bound states below the essential spectrum. In fact we know that it fails for bosons, i.e. an atom has bound states for bosonic

electrons even for $N > Z+1$, but it is an open problem fro fermionic electrons. $\square$

Proof. We shall proceed by induction.

$(N=1)$ $H_{1,Z} = -\Delta - \frac{Z}{|x|}$ on $L^2(\mathbb{R}^3)$ has eigenvalues $-\frac{Z^2}{4n^2}$ with multiplicity n^2 for every $n = 1, 2, \dots$.

IS Assume that the theorem holds for $N-1$ and consider N. We know that $H_{N-1,Z}$ has a ground state $E_{N-1,Z}$, i.e. $E_{N-1,Z}$ is an eigenvalue

$$H_{N-1,Z}\Psi_{N-1} = E_{N-1,Z}\Psi_N$$

We wish to construct a sequence $\Psi_n^{(k)}$ of normalised functions with disjoint support and

$$\left\langle \Psi_N^{(k)}, H_{N,Z}\Psi_N^{(k)} \right\rangle < E_{N-1,Z}$$

for all $k = 1, 2, dots$. By the min-max principle then

$$\mu_k(H_{N-1,Z}) \leqslant \max_{1\leqslant i \leqslant k} \left\langle \Psi_N^{(i)}, H_{N,Z}\Psi_N^{(i)} \right\rangle < E_{N-1,Z} = \inf \sigma_{\text{ess}}(H_{N,Z})$$

Thus all $\mu_k(H_{N,Z})$ are eigenvalues and $\mu_1(H_{N,Z}) = E_{N,Z} < E_{N-1,Z}$.

We shall begin with a trial wave function $\Psi_N^{(k)} = \Psi_{N-1} \otimes \varphi^{(k)}$, i.e. $\Psi_N^{(k)}(x_1, \dots, x_N) = \Psi_{N-1}(x_1, \dots, x_{N-1})\varphi^{(k)}(x_N)$.

Then

$$\begin{aligned}
\left\langle \Psi_N^{(k)}, H_N\Psi_N^{(k)} \right\rangle - E_{N-1,Z} = \Bigg\langle \Psi_n^{(k)}, \Bigg(& (H_{N-1} - E_{N-1,Z}) + \\
& + \left(-\Delta - \frac{Z}{|x_N|} \sum_{i=1}^{N-1} \frac{1}{|x_i - x_N|} \right) \Bigg) \Psi_N^{(k)} \Bigg\rangle = \\
= 0 + \int_{\mathbb{R}^3} & |\nabla\varphi^{(k)}(x_N)|^2 - \int_{\mathbb{R}^3} \frac{Z}{|x_N|} |\varphi^{(k)}(x_N)|^2 + \\
& + \sum_{i=1}^{N-1} \int_{\mathbb{R}^{3N}} \frac{|\Psi_{N-1}(x_1, \dots, x_{N-1})|^2 |\varphi^{(k)}(x_N)|}{|x_i - x_N|} \mathrm{d}x_1 \cdots \mathrm{d}x_N
\end{aligned}$$

We will take $\varphi^{(k)}$ to be a radial function for in that case we may apply Newton's theorem to see

$$\int_{\mathbb{R}^3} \frac{|\varphi^{(k)}(x_N)|^2}{|x_i - x_N|} \mathrm{d}x_N = \int_{\mathbb{R}^3} \frac{|\varphi^{(k)}(x_N)|^2}{\max\{|x_i|, |x_N|\}} \mathrm{d}x_N \leqslant \int_{\mathbb{R}^3} \frac{|\varphi^{(k)}(x_N)|^2}{|x_N|} \mathrm{d}x_N$$

Thus we find

$$\sum_{i=1}^{N-1} \int_{\mathbb{R}^{3N}} \frac{|\Psi_{N-1}(x_1, \ldots, x_{N-1})|^2 |\varphi^{(k)}(x_N)|}{|x_i - x_N|} \mathrm{d}x_1 \cdot \mathrm{d}x_N \leqslant (N-1) \int_{\mathbb{R}^3} \frac{\varphi^{(k)}(x)}{|x|} \mathrm{d}x$$

We conclude that

$$\left\langle \Psi_N^{(k)}, H_N \Psi_N^{(k)} \right\rangle - E_{N-1,Z} \leqslant \int_{\mathbb{R}^3} |\nabla \varphi^{(k)}|^2 - \int_{\mathbb{R}^3} \frac{Z_0}{|x|} |\varphi^{(k)}(x)|^2 \mathrm{d}x$$

where $Z_0 = Z - (N-1) > 0$.

Here we can chose $\varphi^{(k)}(x) = R_k^{-\frac{3}{2}} \varphi_0\left(\frac{x}{R_k}\right)$ for some $\varphi_0 \in \mathscr{C}_c^\infty(\mathbb{R}^3)$, radial, $\|\varphi_0\|_{L^2} = 1$. Then

$$\int_{\mathbb{R}^3} |\nabla \varphi^{(k)}|^2 - \int_{\mathbb{R}^3} \frac{Z_0}{|x|} |\varphi(x)|^2 \mathrm{d}x = \frac{1}{R_k^2} \int_{\mathbb{R}^3} |\nabla \varphi^{(0)}|^2 - \frac{1}{R_k} \int_{\mathbb{R}^3} \frac{Z_0}{|x|} |\varphi^{(0)}(x)|^2 \mathrm{d}x < 0$$

If R_k large enough. We have to prove that $\left(\Psi_N^{(k)}\right)_k$ have disjoint support for which it is enough to establish that $\varphi^{(k)}$ have disjoint support, which we can do by choosing $\operatorname{supp} \varphi^{(0)} \subset \{1 < |x| < 2\}$ and $R_k = 4^k$.

q.e.d.

9.1 Particle Statistics

If we have a system of N identical particles with wave function $\Psi_N \in L^2(\mathbb{R}^{3N})$, then it has to satisfy one of the following two conditions

- Bosons: for all $\sigma \in \mathfrak{S}(N)$

$$\Psi_N(x_1, x_2, \ldots, x_N) = \Psi_N(x_{\sigma(1)}, x_{\sigma(2)}, \ldots, x_{\sigma(N)})$$

- Fermions: for all $\sigma \in \mathfrak{S}(N)$

$$\Psi_N(x_1, x_2, \ldots, x_N) = \operatorname{sgn}(\sigma)\Psi_N(x_{\sigma(1)}, x_{\sigma(2)}, \ldots, x_{\sigma(N)})$$

Example 9.13.
- Bosons: $\Psi_N(x_1, \ldots, x_N) = (u^{\otimes N})(x_1, \ldots, x_N) = u(x_1)\cdots u(x_N)$
- Fermions:

$$\begin{aligned}\Psi_N(x_1, \ldots, x_N) &= (u_1 \wedge \cdots \wedge u_N)(x_1, \ldots, x_N) = \\ &= \frac{1}{\sqrt{N!}} \det \begin{pmatrix} u_1(x_1) & u_2(x_1) & \cdots & u_N(x_1) \\ u_1(x_2) & u_2(x_2) & \cdots & u_N(x_2) \\ \vdots & & & \vdots \\ u_1(x_N) & u_2(x_N) & \cdots & u_N(x_N) \end{pmatrix}\end{aligned}$$

where $(u_i)_{i=1}^N$ is an orthonormal family in $L^2(\mathbb{R}^3)$. This is called the Slatter determinant.

Theorem 9.14. *The Kato theorem, HVZ theorem and Zhislin's theorem hold both for bosons and fermions, i.e. for*

$$H_N = \sum_{i=1}^N (-\Delta_{x_i} + V(x_i)) + \sum_{1 \leqslant i < j \leqslant N} W(x_i - x_j)$$

on $L^2_s(\mathbb{R}^3)$ and $L^2_a(\mathbb{R}^3)$. □

Theorem 9.15 (Ground State Energy of Non-Interacting System)**.** *Consider the Hamiltonian*

$$H_N = \sum_{i=1}^N h_{x_i}$$

on $L^2_s(\mathbb{R}^3)$ or $L^2_a(\mathbb{R}^3)$ where h is a self-adjoint operator on $L^2(\mathbb{R}^3)$ and h is bounded from below. Then

1) *For bosons, $\mu_1(H_N) = N\mu_1(h)$,*

2) *For fermions, $\mu_1(H_N) = \sum_{i=1}^N \mu_i(h)$.*

□

Proof.

Bosons Lower bound: $h \geqslant \mu_1(h)\mathbb{I}_{L^2(\mathbb{R}^3)}$. Then

$$H_N = \sum_{i=1}^{N} h_{x_i} \geqslant N\mu_1(h)\mathbb{I}_{L^2(\mathbb{R}^{3N})}$$

here

$$h_{x_i} = \mathbb{I}_{L^2(\mathbb{R}^3)} \otimes \cdots \otimes \underset{\substack{\uparrow \\ i^{\text{th}} \text{ variable}}}{h} \otimes \cdots \otimes \mathbb{I}_{L^2(\mathbb{R}^3)}$$

and

$$\mathbb{I}_{L^2(\mathbb{R}^{3N})} = \mathbb{I}_{L^2(\mathbb{R}^3)} \otimes \cdots \otimes \mathbb{I}_{L^2(\mathbb{R}^3)}$$

Thus $\mu_1(H_N) \geqslant N\mu_1(h)$. For the upper bound, per definitioenm $\mu_1(h) = \inf_{\|u\|_{L^2}=1} \langle u, hu \rangle$, $\mu_1(H_N) = \inf_{\|\Psi_N\|_{L^2}} \langle \Psi_N, H_N \Psi_N \rangle$.

If we choose $\Psi_N = u^{\otimes N}$, then

$$\langle \Psi_N, H_N\Psi_N \rangle = \left\langle u^{\otimes N}, \sum_{i=1}^{N} h_{x_i} u^{\otimes N} \right\rangle = \sum_{i=1}^{N} \|u\|_{L^2}^{N-1} \langle u, hu \rangle = N\|u\|_{L^2}^{N-1} \langle u, hu \rangle$$

thus

$$\mu_1(H_N) \leqslant \inf_{\|u\|_{L^2}=1} \left\langle u^{\otimes N}, hu^{\otimes N} \right\rangle = N\mu_1(h)$$

Fermions For this we need the two lemmas below. For the lower bound we have for a wave function Ψ_N, its density matrix $0 \leqslant$
$gamma_{\Psi_N} \leqslant 1$, $\operatorname{Tr} \gamma_{\Psi_N} = N$ and

$$\langle \Psi_N, H_N\Psi_N \rangle = \operatorname{Tr}[h\gamma_{\Psi_N}] \geqslant \sum_{i=1}^{N} \mu_i(h)$$

For the upper bound choose $\Psi_N = u_1 \wedge \cdots \wedge u_N$ with $(u_i)_i$ being an orthonormal family. Then

$$\gamma_{\Psi_N} = \sum_{i=1}^{N} |u_i\rangle \langle u_i|$$

Then

$$\langle \Psi_N, H_N\Psi_N \rangle = \operatorname{Tr}(h\gamma_{\Psi_N}) = \sum_{i=1}^{N} \langle u_i, hu_i \rangle$$

Minimising over all orthonormal families yields

$$\mu_1(H_N) \leqslant \sum_{i=1}^{N} \mu_i(h).$$

q.e.d.

Lemma 9.16 (Pauli-Exclusion Principle). *Take Ψ_N be an anti-symmetric wave function on $L^2(\mathbb{R}^{3N})$. Define the density matrix (one-body reduced density matrix) to be the positive, trace-class operator with trace N, $\gamma_{\Psi_N} : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ given by the kernel*

$$\gamma_{\Psi_N}(x;y) = N \int\limits_{\mathbb{R}^{3(N-1)}} \Psi_N(x, x_2, \ldots, x_N)\overline{\Psi_N(y, x_2, \ldots, x_N)}\mathrm{d}x_2 \cdots \mathrm{d}x_N$$

Indeed $\Psi_N \mapsto |\Psi_N\rangle \langle\Psi_N|$ is a projection on $L^2_a(\mathbb{R}^{3N})$ with kernel

$$(|\Psi_N\rangle \langle\Psi_N|)(X;Y) = \Psi_N(X)\overline{\Psi_N(Y)}$$

with $X, Y \in \mathbb{R}^{3N}$. Thus $\gamma_{\Psi_N} = N \operatorname{Tr}_{2\to N} |\Psi_N\rangle \langle\Psi_N|$.
Then $0 \leqslant \gamma_{\Psi_N} \leqslant \mathbb{I}_{L^2(\mathbb{R}^3)}$ as quadratic forms. □

Proof. It is easy to see that $\gamma_{\psi_N} \geqslant 0$ because $|\Psi_N\rangle \langle\Psi_N|$ and

$$\operatorname{Tr} \gamma_{\Psi_N} = \int\limits_{\mathbb{R}^3} \gamma_{\Psi_N}(x;x)\mathrm{d}x = N \int\limits_{\mathbb{R}^{3N}} |\Psi_N(x, x_2, \ldots, x_N)|^2 \mathrm{d}x\mathrm{d}x_2 \cdots \mathrm{d}x_N = N0$$

It is trivial that $0 \leqslant \gamma_{\Psi_N} \leqslant N$, but in fact $\gamma_{\Psi_N} \leqslant 1$.
From QFT we have $\langle f, \gamma_{\Psi_N} f\rangle = \left\langle \Psi_N, a^\dagger(f)a(f)\Psi_N \right\rangle$. By the CCR (canonical commutation relations)

$$\|f\|^2_{L^2} = \left\{a^\dagger(f), a(f)\right\} \geqslant a^\dagger(f)a(f) + a(f)a^\dagger(f) \geqslant a^\dagger(f)a(f)$$

Thus

$$\langle f, \gamma_{\Psi_N} f\rangle \leqslant \left\langle \Psi_N, \left\| f \right\|^2_{L^2} \Psi_N \right\rangle = \|f\|^2_{L^2}$$

for all $f \in L^2(\mathbb{R}^3)$. Thus $\gamma_{\Psi_N} \leqslant 1$.
A second proof of $\gamma_{\Psi_N} \leqslant 1$: We know that

$$\gamma_{\Psi_N} = \sum_{i=1}^{\infty} \lambda_i \, |f_i\rangle \langle f_i|$$

where λ_i are eigenvalues and $(f_i)_i$ is an orthonormal basis of $L^2(\mathbb{R}^3)$.
The inequality $\gamma_{\Psi_N} \leqslant 1$ is equivalent to $\lambda_i \leqslant 1$ for all i. Let us prove that $\lambda_1 \leqslant 1$. We know that $L^2(\mathbb{R}^{3N}) = L^2(\mathbb{R}^3) \otimes \cdots \otimes L^2(\mathbb{R}^3)$ has an orthonormal basis of the form

$$\{f_{i_1} \otimes \cdots \otimes f_{i_N}\}_{i_1,\ldots,i_N \geqslant}$$

Thus we can write

$$\Psi_N = \sum_{i_1,\ldots,i_N} c_{i_1,\ldots,i_N} f_{i_1} \otimes \cdots \otimes f_{i_N}.$$

Because Ψ_N is anti-symmetric it follows that $c_{i_1,\ldots,i_N}$ if some $i_j = i_k$ for $j \neq k$. Then we compute that

$$1 = \|\Psi_N\|_{L^2}^2 = \sum_{i_1,\ldots,i_N} |c_{i_1,\ldots,i_N}|^2$$

and

$$\begin{aligned}
\langle f, \gamma_{\Psi_N} f\rangle &= \int\limits_{\mathbb{R}^{3N}} \overline{f(x)} \Psi_N(x, x_2, \ldots, x_N) \overline{\Psi_N(y, x_2, \ldots, x_N)} f(y) \mathrm{d}x \mathrm{d}y \mathrm{d}x_2 \cdots \mathrm{d}x_N = \\
&= \sum_{i_1,\ldots,i_N} \sum_{j_1,\ldots,j_N} \int \overline{f(x)} f_{i_1}(x) \cdots f_{i_N}(x_N) \\
&\qquad\qquad \overline{f_{j_1}(y) \cdots f_{j_N}(x_N)} f(y) \mathrm{d}x \mathrm{d}y \mathrm{d}x_2 \cdots \mathrm{d}x_N c_{i_1,\ldots,i_N} \overline{c_{j_1,\ldots,j_N}} = \\
&= \sum_{i_1,\ldots,i_N} \sum_{j_1,\ldots,j_N} \overline{c_{j_1,\ldots,j_N}} \langle f, f_{i_1}\rangle \langle f_{j_1}, f\rangle \prod_{k=2}^N \overline{\langle f_{i_k}, f_{j_k}\rangle_{L^2_{x_k}}}
\end{aligned}$$

$\prod_{k=2}^N \overline{\langle f_{i_k}, f_{j_k}\rangle_{L^2_{x_k}}} \neq 0$ iff $i_k = j_k$ for all $k = 2, \ldots, N$ and this equal 1 in this case. Thus

$$\langle f, \gamma_{\Psi_N} f\rangle = \sum_{i_1,\ldots,i_N, j_1} \overline{c_{j_1, i_2, \ldots, i_N}} \langle f, f_{i_1}\rangle \langle f_{j_1}, f\rangle$$

Then by the Young inequality we have

$$|\langle f, \gamma_{\Psi_N} f\rangle| \leqslant \sum_{i_1,\ldots,i_N, j_1} \frac{|c_{i_1,\ldots,i_N}|^2 |\langle f_{i_1}, f\rangle|^2 + |c_{j_1, i_2, \ldots, i_N}|^2 |\langle f_{j_1}, f\rangle|^2}{2} \leqslant \|f\|_{L^2}^2$$

q.e.d.

Lemma 9.17. *If h is a self-adjoint operator on $L^2(\mathbb{R}^3)$, and $0 \leqslant \gamma \leqslant 1$, $\operatorname{Tr}\gamma = N$.*

Then

$$\inf_{\substack{0\leqslant\gamma\leqslant 1\\ \operatorname{Tr}\gamma=N}} \operatorname{Tr}[h\gamma] = \inf_{(\varphi_i)_{i=1}^N \ ONF} \sum_{i=1}^N \langle \varphi_i, h\varphi_i\rangle = \sum_{i=1}^N \mu_i(h)$$

□

Proof. First suppose that

$$h = \sum_{i=1}^\infty \mu_i \left|u_i\right\rangle \left\langle u_i\right|$$

Then

$$\operatorname{Tr}(h\gamma) = \sum_{i=1}^\infty \mu_i \underbrace{\langle u_i, \gamma u_i\rangle}_{=:\alpha_i}$$

with $0 \leqslant \alpha_i \leqslant 1$, $\sum_{i=1}^\infty \alpha_i = \operatorname{Tr}\gamma = N$.
The result follows from

$$\inf\left\{\sum_{i=1}^N \mu_i\alpha_i \,\middle|\, \sum_{i=1}^\infty \alpha_i = N\right\} = \mu_1 + \cdots + \mu_N$$

The general case is left as an exercise.

q.e.d.

Remark 9.18 (Real Calculations)**.** "Interaction" problem, use Density functional theory

$$\inf_{\|\Psi_N\|_{L^2}} \langle \Psi_N, H_N\Psi_N\rangle = \inf_{\substack{0\leqslant\gamma\leqslant 1\\ \operatorname{Tr}\gamma=N}} \inf_{\Psi_N\mapsto\gamma_{\Psi_N}=\gamma} \langle \Psi_N, H_N\Psi_N\rangle$$

If we know that $\mathcal{E}(\gamma) := \inf_{\Psi_N\mapsto\gamma_{\Psi_N}=\gamma} \langle \Psi_N, H_N\Psi_N\rangle$ then the problem

$$\inf_{\substack{0\leqslant\gamma\leqslant 1\\ \operatorname{Tr}\gamma=N}} \mathcal{E}(\gamma)$$

can be solved practically. However, computing $\mathcal{E}(\gamma)$ is impossible even by Quantum Computers.
However, we can approximate $\mathcal{E}(\gamma)$. □

Definition 9.19 (Hartree-Fock Approximation)**.** For fermions (electrons). Let $\Psi_N =$

$u_1 \wedge \cdots \wedge u_N$ and

$$H_N = \sum_{i=1}^{N}(-\Delta_{x_i} + V(x_i)) + \sum_{i<j}^{N} W(x_i - x_j).$$

Then

$$\langle \Psi_N, H_N \Psi_N \rangle = \mathrm{Tr}[(-\Delta + V)\gamma] + \frac{1}{2}\iint W(x-y)\big(\gamma(x,x)\gamma(y,y) - |\gamma(x,y)|^2\big)\mathrm{d}x\mathrm{d}y$$

with $\gamma = \gamma_{\Psi_N} = \sum_{i=1}^{N} |u_i\rangle \langle u_i|$. This is called the Hartree-Fock functional.
For bosons one takes $\Psi_N = u^{\otimes n}$ and

$$\langle \Psi_N, H_N \Psi_N \rangle = N \langle u, (-\Delta + V)u \rangle + \frac{N(N-1)}{2} \iint W(x-y)|u(x)|^2|u(y)|^2$$

the Hartree functional.

□

Remark 9.20. In the case of Bose-Einstein Condensation with very-short range potentials this can be further simplified to the Gross-Pitaevski functional

$$\mathcal{E}^{\mathrm{GP}}(u) = \langle u, (-\Delta + V)u \rangle + 4\pi a \int_{\mathbb{R}^3} |u(x)|^4 \mathrm{d}x$$

here

$$\frac{4\pi a}{N} := \inf\left\{ \int |\nabla f|^2 + \frac{1}{2}\int W(x)|f(x)|^2 \mathrm{d}x \,\middle|\, f(x) \xrightarrow{|x|\to\infty} 1 \right\}$$

In the exercises we consider the case

$$W = \begin{cases} +\infty, & \text{if } |x| < a \\ 0, & \text{if } |x| > a \end{cases}$$

□

Chapter 10

Entropy

Recall that for a mixed state γ in a Hilbert space, then $\gamma \geqslant 0$ and $\operatorname{Tr}[\gamma] = 1$. Thus $\gamma = \sum_i \lambda_i |u_i\rangle \langle u_i|$ and thus for any function defined on the spectrum

$$f(\gamma) = \sum_i f(\lambda_i) |u_i\rangle \langle u_i| \,.$$

Definition 10.1 (Von Neumann Entropy)**.** For a mixed state γ we define

$$S(\gamma) := -\operatorname{Tr}[\gamma \log(\gamma)] = -\sum_i \lambda_i \log \lambda_i$$

$\square$

Proposition 10.2. *1) $S(\gamma) \geqslant 0$, $\lambda_i \in [0,1]$, $S(\gamma) = 0$ iff γ is a pure state.*

2) If $\dim \mathscr{H} = N < \infty$, then $\max_\gamma S(\gamma) = \log N$, with optimiser $\gamma = \frac{1}{N}\sum_{i=1}^N |u_i\rangle \langle u_i|$

3) Gibbs Variational Principle: The ground state energy E_0 of a self-adjoint Hamiltonian A is given by

$$E_0 = \inf_{\substack{\gamma \geqslant 0 \\ \operatorname{Tr}\gamma = 1}} \operatorname{Tr}[A\gamma] = \mu_1(A)$$

(this is at zero temperature).

$\square$

Proof. 1) For $t \in (0,1)$ the function $t \mapsto -t \log t$ is positive and equal to 0 at $t = 0, 1$.

2) The function $f : t \mapsto t \log t$ is convex in $[0, \infty)$ as $f''(t) = \frac{1}{t} > 0$. Thus

$$-S(\gamma) = \sum_{i=1}^{N} f(\lambda_i) = N \sum_{i=1}^{N} \frac{f(\lambda_i)}{N} \geqslant N f\left(\sum_{i=1}^{N} \frac{\lambda_i}{N}\right) = N f\left(\frac{1}{N}\right) = -\log(N)$$

q.e.d.

If we are in positive temperature $T > 0$, then

Theorem 10.3 (Gibbs Variational Principal)**.** *The free energy F is given by*

$$F = \inf_{\substack{\gamma \geqslant 0 \\ \operatorname{Tr}\gamma = 1}} \left(\operatorname{Tr}[A\gamma] - TS(\gamma)\right) =: -log\operatorname{Tr}(e^{-A/T})$$

and there exists a minimiser $\gamma_A = \frac{e^{-A/T}}{Z_A}$ where $Z_A = \operatorname{Tr}[e^{-A/T}]$ provided that $e^{-A/T}$ is a trace class operator.

□

Theorem 10.4 (Klein Inequality)**.** *Given a function $F : \mathbb{R}^2 \to \mathbb{R}$ of the form*

$$F(x, y) = \sum_{i=1}^{N} f_i(x) g_i(y) \geqslant 0$$

Then for any self-adjoint trace class operator A, B (we do not require $A, B \geqslant 0$, $\operatorname{Tr}[A] = 1 = \operatorname{Tr}[B]$) then

$$\operatorname{Tr}[F(A, B)] \geqslant 0..$$

□

Remark 10.5. If we know that $A, B \geqslant 0$, then it suffices to assume $F(x, y) \geqslant 0$ for $x, y \geqslant 0$. More generally, all we need here is $F(x, y) \geqslant 0$ for $x \in \sigma(A), y \in \sigma(B)$. □

Proof. By the spectral theorem, $A = \sum_\alpha a_\alpha |u_\alpha\rangle \langle u_\alpha|$ and $B = \sum_\alpha b_\beta |v_\beta\rangle \langle v_\beta|$. Thus

$$F(A, B) = \sum_i f_i(A) g_i(B) = \sum_{i,\alpha,\beta} f_i(a_\alpha) g_i(b_\beta) |u_\alpha\rangle \langle u_\alpha| \, |v_\beta\rangle \langle v_\beta|$$

$$\operatorname{Tr}[F(A, B)] = \sum_{i,\alpha,\beta} f_i(a_\alpha) g_i(b_\beta) |\langle u_\alpha, v_\beta\rangle|^2 = \sum_{\alpha,\beta} |\langle u_\alpha, v_\beta\rangle|^2 \underbrace{\sum_i f_i(a_\alpha) g_i(b_\beta)}_{\geqslant 0} \geqslant 0$$

q.e.d.

Corollary 10.6. *If $f : \mathbb{R} \to \mathbb{R}$ is a convex function and A, B are self-adjoint trace-class operators, then*

$$\mathrm{Tr}[f(A) - f(B) - f'(B)(A - B)] \geqslant 0.$$

Moreover, if $A, B \geqslant 0$, we only need $f : \mathbb{R}_+ \to \mathbb{R}$ be convex. □

Proof. Let $F(x, y) = f(x) - f(y) - f'(y)(x - y)$. Then $F(x, y) \geqslant 0$ by convexity and the claim follows from Klein's inequality. (Note that $F(x, y) = \frac{1}{2} f(\vartheta)(x - y)^2$ for some ϑ in between x and y by Taylor's theorem if f is suitably differentiable). *q.e.d.*

Remark 10.7. In Klein's inequality

$$F(x, y) = \sum_i f_i(x) g_i(x) = \sum_i g_i(x) f_i(x)$$

but in general

$$\sum_i f_i(A) g_i(B) \neq \sum_i g_i(B) f_i(A)$$

However, by cyclicity of the trace

$$\mathrm{Tr}\left[\sum_i f_i(A) g_i(B)\right] = \mathrm{Tr}\left[\sum_i g_i(B) f_i(A)\right].$$

□

As consequence if $f(t) = t \log(t)$ and $A, B \geqslant 0$

$$\mathrm{Tr}[A \log A - B \log B - (1 + \log B)(A - B)] \geqslant 0$$

Thus

$$\mathrm{Tr}[A \log A - A \log B] \geqslant \mathrm{Tr}(A - B) = 1 - 1 = 0$$

for the penultimate equality holds for density matrices.

Definition 10.8 (Relative Entropy).

$$S(A|B) = \mathrm{Tr}[A\log A - A\log B].$$

□

Theorem 10.9 (Improved Klein Inequality for Relative Entropy). *If A, B are mixed states, then*

$$S(A|B) \geqslant \frac{1}{2}\mathrm{Tr}\left[|A-B|^2\right]$$

In particular, $S(A|B) = 0$ iff $A = B$. Thus $S(A|B)$ can be understood as a sort of distance between A and B. □

Proof. Using Klein's inequality for $f(t) = t\log(t)$ for

$$F(x,y) = f(x) - f(y) - f'(y)(x-y) - \frac{1}{2}(x-y)^2.$$

the result follows if we can prove that $F(x,y) \geqslant 0$ for all $x, y \in [0,1]$.
This follows from $F(x,y) = \left(\frac{1}{2}f''(\vartheta) - \frac{1}{2}\right)(x-y)^2$, for some ϑ in between x, y. Here $f''(\vartheta) = \frac{1}{\vartheta} \geqslant 1$. *q.e.d.*

Remark 10.10. We can check

$$\begin{aligned} F(x,y) &= x\log x - y\log y - (1+\log y)(x-y) - \frac{1}{2}(x-y)^2 = \\ &= x\log x - y\log y - (x-y) - \frac{1}{2}(x-y)^2 \geqslant 0 \end{aligned}$$

for all $x, y \in [0,1]$ and

$$\begin{aligned} \frac{d}{dy}F(x,y) &= -\frac{x}{y} + 1 + x - y = (1-\frac{x}{y})(1-y), \\ \frac{d^2}{dy^2}F(x,y) &= (1+\frac{x}{y^2})(1-y) - (1-\frac{x}{y}). \end{aligned}$$

Thus $y \mapsto F(x,y)$ has a minimum at $x = y$ for which $F(x,x) = 0$, i.e. $F(x,y) \geqslant 0$.

□

Proof of Theorem 10.3. Take A self-adjoint such that $e^{-\frac{A}{T}}$ is trace class. Let consider $T = 1$, otherwise rescale A. We check that

$$\begin{aligned}\operatorname{Tr}[A\gamma_A] - S(\gamma_A) &= \operatorname{Tr}(A\gamma_A) + \operatorname{Tr}[\gamma_A \log \gamma_A] = \operatorname{Tr}(A\gamma_A) - \operatorname{Tr}(\gamma_A \log Z_A) - \operatorname{Tr}(\gamma_A A) = \\ &= -\log Z_A \operatorname{Tr}(\gamma_A) = -\log Z_A.\end{aligned}$$

It remains to prove that for all mixed states γ

$$\operatorname{Tr}(A\gamma) - S(\gamma) \geqslant \operatorname{Tr}(A\gamma_A) - S(\gamma_A)$$

and equality only holds for $\gamma = \gamma_A$. Note that

$$\begin{aligned}S(\gamma|\gamma_A) &= \operatorname{Tr}[\gamma \log \gamma - \gamma \log(\gamma_A)] = \operatorname{Tr}[\gamma \log \gamma] + \operatorname{Tr}[\gamma(\log Z_A + A)] = \\ &= -S(\gamma) + \operatorname{Tr}(A\gamma) + \log Z_A = \operatorname{Tr}(A\gamma) - S(\gamma) - \operatorname{Tr}(A\gamma_A) + S(\gamma_A)\end{aligned}$$

and we know that $S(\gamma|\gamma_A) \geqslant 0$ and 0 iff $\gamma = \gamma_A$. *q.e.d.*

This implies that $\operatorname{Tr}(A\gamma) - S(\gamma) \geqslant -\log(\operatorname{Tr} e^{-A})$ and thus $S(\gamma) \leqslant \operatorname{Tr}(A\gamma) - log \operatorname{Tr} e^{-A}$. Indeed $S(\gamma) = \max_A \big(\operatorname{Tr}(A\gamma) - \log \operatorname{Tr}(e^{-A})\big)$. This expression tells us that $\gamma \mapsto S(\gamma)$ is concave. Because $\gamma \mapsto \operatorname{Tr}(A\gamma)$ is linear in γ (as the "maximum over linear/concave functions" is a concave function).

Definition 10.11 (Partial Trace)**.** Given a Hilbert space $\mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2$. Let ρ be a density matrix on $\mathscr{H}$. Then $\rho_1 = \operatorname{Tr}_2 \rho$ is a density matrix on $\mathscr{H}_1$ and $\rho_2 = \operatorname{Tr}_1 \rho$ is a density matrix on $\mathscr{H}_2$.
Here the partial trace Tr_i is defined as follows. We can write $\rho = \sum_i \rho_i^{(1)} \otimes \rho_i^{(2)}$ where $\rho_i^{(j)} : \mathscr{H}_j \to \mathscr{H}_j$. Then

$$\operatorname{Tr}_1(\rho) = \sum_i \operatorname{Tr}[\rho_i^{(1)}]\rho_i^{(2)}$$

and similarly for $\operatorname{Tr}_2 \rho$. □

Remark 10.12. It might happen that even if ρ is a pure state on $\mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2$ but ρ_1, ρ_2 are mixed states. □

Example 10.13. Let

$$\rho = \left| \sum_i \lambda_i u_i \otimes v_i \right\rangle \left\langle \sum_i \lambda_i u_i \otimes v_i \right| = \sum_{i,j} \lambda_i \overline{\lambda_j} \left| u_i \otimes v_i \right\rangle \left\langle u_j \otimes v_j \right| =$$
$$= \sum_{i,j} \lambda_i \overline{\lambda_j} \left| u_i \right\rangle \left\langle u_j \right| \otimes \left| v_i \right\rangle \left\langle v_j \right| .$$

Then

$$\rho_1 = \operatorname{Tr}_2 \rho = \sum_{ij} \lambda_i \overline{\lambda_j} \left| u_i \right\rangle \left\langle u_j \right| \langle v_i, v_j \rangle = \sum_i |\lambda_i|^2 \left| u_i \right\rangle \left\langle u_i \right|$$
$$\rho_2 = \operatorname{Tr}_1 \rho = \sum_i |\lambda_i|^2 \left| v_i \right\rangle \left\langle v_i \right|$$

Remark 10.14. If ρ is a pure state in $\mathscr{H}_1 \otimes \mathscr{H}_2$, then the eigenvalues of ρ_1 and ρ_2 are the same counting multiplicity (expect for 0). □

Remark 10.15. Given a mixed state ρ_1 on $\mathscr{H}_1$, then if $\dim \mathscr{H}_2 \geqslant \dim \mathscr{H}_1$ there exists a pure state ρ on $\mathscr{H}_1 \otimes \mathscr{H}_2$ such that $\rho_1 = \operatorname{Tr}_2 \rho$. □

Proposition 10.16. *5) Sub-Additivity: Given a mixed state ρ on $\mathscr{H}_1 \otimes \mathscr{H}_2$ with partial traces ρ_1, ρ_2. Then*

$$S(\rho) \leqslant S(\rho_1) + S(\rho_2).$$

□

Proof. We claim that

$$S(\rho_1) + S(\rho_2) - S(\rho) = S(\rho | \rho_1 \otimes \rho_2) \geqslant 0$$

from which the assertion follows. Noting that $\log(AB) = \log(A) + \log(B)$ for commuting operators A, B, in particular for

$$(rho_1 \otimes \mathbf{1}_{\mathscr{H}_2})(\mathbf{1}_{\mathscr{H}_1} \otimes \rho_2) = \rho_1 \otimes \rho_2$$

we have

$$\begin{aligned}S(\rho|\rho_1\otimes\rho_2) &= \mathrm{Tr}[\rho\log\rho-\rho\log(\rho_1\otimes\rho_2)] = \mathrm{Tr}[\rho\log\rho-\rho\log(\rho_1\otimes\mathbf{1}_{\mathscr{H}_2})-\rho\log(\mathbf{1}_{\mathscr{H}_1}\otimes\rho_2)] = \\ &= \mathrm{Tr}_{12}(\rho\log\rho)-\mathrm{Tr}_{12}(\rho\log\rho_1)-\mathrm{Tr}_{12}(\rho\log\rho_2) = \\ &= \mathrm{Tr}_{12}(\rho\log\rho)-\mathrm{Tr}_{1}(\rho_1\log\rho_1)-\mathrm{Tr}_{2}(\rho\log\rho_2) = -S(\rho)+S(\rho_1)+S(\rho_2).\end{aligned}$$

q.e.d.

Remark 10.17. In general there does not exist an inequality $S(\rho_{12})\geqslant S(\rho_1)$, e.g. it might happen that ρ_{12} is pure, i.e. $S(\rho_{12})=0$, but ρ_1 is not pure, $S(\rho_1)>0$. In this case

$$S(\rho_{12})\leqslant S(\rho_1)+S(\rho_2)$$

is trivial. What really happens here is the “cancelation of information” □

Theorem 10.18 (Araki-Lieb)**.**

$$S(\rho_{12})\geqslant|S(\rho_1)-S(\rho_2)|$$

□

Proof. Using sub-additivity we have $S(\rho 12)\leqslant S(\rho_1)+S(\rho_2)$. By the purification lemma, there exists a pure state ρ_{123} on $\mathscr{H}_1\otimes\mathscr{H}_2\otimes\mathscr{H}_3$ such that $\rho_{12}=\mathrm{Tr}_3\,\rho_{123}$. Then $S(\rho_1 2)=S(\rho_3)$ and $S(\rho_2)=S(\rho_{13})$ and thus

$$S(\rho_3)\leqslant S(\rho_1)+S(\rho_{13})$$

which implies that $S(\rho_{13})\geqslant S(\rho_3)-S(\rho_1)$ Similarly we find $S(\rho_{13})\geqslant|S(\rho_3)-S(\rho_1)|$. *q.e.d.*

Theorem 10.19 (Strong Sub-Additivity - SSA)**.** *If ρ_{123} is a mixed state in $\mathscr{H}_1\otimes\mathscr{H}_2\otimes\mathscr{H}_3$, then*

$$S(\rho_1)+S(\rho_{123})\leqslant S(\rho_{12})+S(\rho_{13}).$$

□

Remark 10.20 (Interpretation)**.** We can interpret sub-addivity as

$$S(A \cup B) \leqslant S(A) + S(B)$$

but SSA as

$$S(A \cup B) + S(A \cap B) \leqslant S(A) + S(B)$$

This deep result was proven by Lieb-Ruskai in 1973. □

SSA is equivalent to

Theorem 10.21 (Monotonicity of Relative Entropy)**.** *Let ρ_{12}, σ_{12} be density matrices on a Hilbert space $\mathscr{H}_1 \otimes \mathscr{H}_2$.*

$$S(\rho_{12}|\sigma_{12}) \geqslant S(\rho_1|\sigma_2).$$

□

Remark 10.22. This monotonicity implies SSA as follows:

$$S(\rho_{13}) + S(\rho_2) - S(\rho_{123}) = S(\rho_{123}|\rho_{13} \otimes \rho_2) \geqslant S(\rho_{12}|\rho_1 \otimes \rho_2) = S(\rho_1) + S(\rho_2) - S(\rho_{12})$$

Thus

$$S(\rho_{12}) + S(\rho_{13}) \geqslant S(\rho_1) + S(\rho_{123})$$

□

Remark 10.23. This is related to “quantum channels”. The partial trace is replaced by the “completed positive trace preserving maps”. □

Idea of Proof. The Golden-Thompsen inequality tells us that

$$\mathrm{Tr}(e^{A+B}) \leqslant \mathrm{Tr}(e^A e^B).$$

which is equivalent to

$$\mathrm{Tr}(e^{\ln A + \ln B}) \leqslant \mathrm{Tr}(AB)$$

Lieb's extension

$$\operatorname{Tr} e^{\ln A+\ln B-\ln C} \leqslant \operatorname{Tr}\left(\int_0^\infty A\frac{1}{C+t}B\frac{1}{C+t}\mathrm{d}t\right)$$

q.e.d.