Functional Analysis II
Prof. Phan Thành Nam

Unofficial Lecture Notes

Martin Peev

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Chapter 1

Hilbert Spaces & Operators

Definition 1.1 (Hilbert Space)**.** A space $\mathscr{H}$ is a Hilbert space iff

- $\mathscr{H}$ is a complex vector space.
- it is equipped with an inner product $\langle \cdot, \cdot \rangle$, where we shall assume that it is linear in the second argument and anti-linear in the first.
- it is complete w.r.t. the norm $\|x\| = \sqrt{\langle x, x \rangle}$, i.e. $(\mathscr{H}, \| \cdot \|)$ is a Banach space.

$\square$

Proposition 1.2 (Cauchy-Schwarz Inequality)**.** *For all* $x, y \in \mathscr{H}$

$$| \langle x, y \rangle | \leqslant \|x\| \|y\|.$$

$\square$

Corollary 1.3 (Triangle Inequality)**.** *For all* $x, y \in \mathscr{H}$

$$\|x + y\| \leqslant \|x\| + \|y\|.$$

$\square$

Theorem 1.4 (Pythagorean Theorem). *For all $x, y \in \mathscr{H}$ with $\langle x, y \rangle = 0$*

$$\|x + y\|^2 = \|x\|^2 + \|y\|^2.$$

□

Theorem 1.5 (Orthogonal Projection). *If V is a closed subspace of $\mathscr{H}$, then there exists an orthogonal subspace $V^\perp$ such that $\mathscr{H} = V \oplus V^\perp$, i.e. for all $x \in \mathscr{H}$ there exists a unique decomposition $x = y + z$ with $y \in V$ and $z \in V^\perp$ such that $\langle y, z \rangle = 0$. Indeed* $\inf_{a \in V} \|x - a\| = \|x - y\|$. □

Remark (Notation). We call $y = P_V(x)$, $z = P_{V^\perp}(x)$ the projections of x unto the respective subspaces. □

Definition 1.6 (Orthonormal Family). A set $(x_n)_n \subset \mathscr{H}$ is called an ONF iff for all n

- $\langle x_n, x_m \rangle = 0$ for $n \neq m$,
- $\|x_n\| = 1$.

□

Theorem 1.7. *If $(x_n)_{n \in \mathbb{N}}$ is an ONF then for all $x \in \mathscr{H}$ one can write*

$$x = \sum_{n=1}^{\infty} \langle x_n, x \rangle \, x_n + x^\perp$$

where $\left\langle x^\perp, x_n \right\rangle = 0$ for all n. Consequently

$$\|x\|^2 = \sum_{n=1}^{\infty} |\langle x_n, x \rangle|^2 + \|x^\perp\|^2.$$

□

Definition 1.8. $(x_n)_{n\in\mathbb{N}}$ is called an ***orthonormal basis (ONB)*** if for all $x \in \mathscr{H}$, one can write

$$x = \sum_{n=1}^{\infty} \langle x_n, x\rangle \, x_n$$

In this case

$$\|x\|^2 = \sum_{n=1}^{\infty} |\, \langle x_n, x\rangle \,|^2. \qquad \text{(Parseval Identity)}$$

□

Definition 1.9 (Separable Hilbert Space)**.** A Hilbert space $\mathscr{H}$ is called ***separable*** if there exists a countable ONB. □

Remark 1.10. All Hilbert spaces considered in this course will be separable.
All infinite dimensional separable Hilbert spaces are unitarily equivalent. □

Definition 1.11 (Weak Convergence)**.** We say that a sequence $(x_n)_n$ convergence weakly to x_∞ iff

$$\forall y \in \mathscr{H} : \langle x_n, y\rangle \xrightarrow{n\to\infty} \langle x_\infty, y\rangle$$

and we write

$$x_n \xrightharpoonup{n\to\infty} x_\infty.$$

□

Remark 1.12. Norm convergence implies weak convergence but the reverse is not true in infinite dimensions. □

Theorem 1.13 (Banach-Alaoglu)**.** *If $(x_n)_n$ is bounded in a Hilbert space $\mathscr{H}$, then there exists a subsequence $(x_{n_k})_k$ that converges weakly.* □

Proof. Because $\mathscr{H}$ is separable there exists an orthonormal basis $(u_i)_i$ of $\mathscr{H}$. Consider the sequence $(\langle x_n, u_1\rangle)_n$, which is a bounded sequence in $\mathbb{R}$ and thus contains a convergent subsequence $\left(\left\langle x_n^{(1)}, u_1\right\rangle\right)_n$. One now repeats this argument with u_2 and $\left(x_n^{(1)}\right)_n$ to get a subsequence $\left(x_n^{(2)}\right)_n$ and so forth. Thus we may define the sequence $y_n = x_n^{(n)}$ for which $\langle y_n, u_i\rangle$ converges for all $i \in \mathbb{N}$ by Cantor's diagonal argument.

We need to prove that y_n converges weakly. For any $u \in \mathscr{H}$ we have to consider to $\langle y_n, u\rangle$. We can prove that $\langle y_n, u\rangle$ converges as $n \to \infty$.

Define the linear operator $\mathscr{L} : \mathscr{H} \to \mathbb{C}$ by $\mathscr{L}(u) = \lim_{n\to\infty} \langle y_n, u\rangle$ for all $u \in \mathscr{H}$. Then $\mathscr{L}$ is linear and bounded since

$$|\mathscr{L}(u)| \leqslant \limsup |\langle y_n, u\rangle| \leqslant (\limsup \|y_n\|)\|u\| \leqslant Mu.$$

and thus $(y_n)_n$ converges weakly to the adjoint of $\mathscr{L}$ provided by the Riesz representation theorem. *q.e.d.*

Theorem 1.14 (Riesz Representation Theorem)**.** *For all $y \in \mathscr{H}$ there exists exactly one $\mathscr{L} \in \mathscr{H}^*$ such that for all $u \in \mathscr{H}$*

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

□

Definition 1.15 (Unbounded Operator)**.** We shall consider linear operator $A : D(A) \to \mathscr{H}$, with $\overline{D(A)} = \mathscr{H}$.

If $B : D(B) \to \mathscr{H}$ and $D(A) \subset D(B)$ and $B\big|_{D(A)} = A$, then we write $A \subset B$ and say that B is an ***extension*** of A. □

As in the finite dimensional case we want to consider how to define for a linear operator A the adjoint operator A^* such that

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

Definition 1.16 (Adjoint Operator)**.** Take $A : D(A) \to \mathscr{H}$. Define $A^* : D(A^*) \to \mathscr{H}$ to be the following

- $$D(A^*) = \left\{ x \in \mathscr{H} \;\middle|\; \sup_{\substack{y \in D(A) \\ \|y\| \leqslant 1}} |\langle x, Ay \rangle| < \infty \right\},$$

  i.e. we want $y \mapsto \langle x, Ay \rangle$ to be a bounded linear functional on $\mathscr{H}$ for x to be in $D(A^*)$.

- By the Riesz representation theorem, there exists then a unique z such that $\langle x, Ay \rangle = \langle z, y \rangle$ for all $y \in D(A)$. Define $A^* x = z$.

$\square$

Definition 1.17 (Symmetric Operator)**.** A linear operator $A : D(A) \to \mathscr{H}$ is symmetric iff

$$\forall x, y \in D(A) : \langle x, Ay \rangle = \langle Ax, y \rangle .$$

$\square$

Proposition 1.18. *The following are equivalent*

(i) $A : D(A) \to \mathscr{H}$ *is symmetric.*

(ii) $A \subset A^*$.

(iii) $\langle x, Ax \rangle \in \mathbb{R}$ *for all* $x \in D(A)$.

$\square$

Example 1.19. Consider the Hilbert space $\mathscr{H} = L^2(\mathbb{R}^d)$ with the standard inner product. Consider $A = -\Delta$ with $D(A) = \mathscr{C}_c^2(\mathbb{R}^d)$, then $Au \in \mathscr{H}$ for all $u \in D(A)$, i.e. A is well-defined.
We can check that A is symmetric by noting that

$$\langle u, Au \rangle = \int \overline{u}(-\Delta u) \mathrm{d}x = \int |\nabla u|^2 \mathrm{d}x \geqslant 0$$

However, one can prove that A cannot be extended to a bounded operator.

Definition 1.20 (Bounded Operator)**.** If $A : D(A) \to \mathscr{H}$ has domain $D(A) = \mathscr{H}$ and if there exists an $M \geqslant 0$ such that $\|Au\| \leqslant M\|u\|$ for all $u \in \mathscr{H}$, then A is called a bounded operator. □

Theorem 1.21 (B.L.T. Theorem)**.** *If $A : D(A) \to \mathscr{H}$ and if there exists an $M \geqslant 0$ such that $\|Au\| \leqslant M\|u\|$ for all $u \in D(A)$ then A can be uniquely extended to a bounded operator on $\mathscr{H}$.* □

Theorem 1.22 (Banach-Steinhaus)**.** *If $(x_n)_n$ converges weakly, then $(x_n)_n$ is bounded.* □

Definition 1.23 (Compact Operator)**.** A bounded operator A on $\mathscr{H}$ is a called a ***compact operator*** iff $A\left(\overline{B_1(0)}\right)$ is pre-compact in $\mathscr{H}$. Namely, if $(x_n)_n$ is a bounded sequence in $\mathscr{H}$, then there exists a subsequence $(x_{n_k})_k$ such that $(Ax_{n_k})_k$ converges strongly as $k \to \infty$. □

Proposition 1.24. *Let A be a bounded operator on $\mathscr{H}$. Then the following are equivalent*

(i) A is a compact operator.

(ii) for all weakly convergent sequences $(x_n)_n$, $(Ax_n)_n$ converges strongly.

□

Proof.

(ii)⇒(i) Assume that A maps weak convergence to strong convergence. If $(x_n)_n$ is bounded, then by Theorem 1.13 we can choose a subsequence that converges weakly, which we shall call again $(x_n)_n$ and $x_n \rightharpoonup x$. Then $Ax_n \to Ax$. Thus A is a compact operator.

(i)⇒(ii) Assume that A is compact and that $x_n \rightharpoonup x$ weakly. Then $(x_n)_n$ is bounded. Since A is compact there exists a subsequence $(x_{n_k})_k$ such that Ax_{n_k} converges strongly. The limit is Ax because for all $y \in \mathscr{H}$

$$\langle z, y\rangle \longleftarrow \langle Ax_n, y\rangle = \langle x_n, A^*y\rangle \longrightarrow \langle x, A^*y\rangle = \langle Ax, y\rangle .$$

We shall now prove that if $x_n \rightharpoonup x$, then $Ax_n \to x$ for the whole sequence by the "Argument of subsequences of subsequence". Assume by contradiction that $Ax_n \not\to Ax$ stronlgy. Then there exists a subsequence x_{n_l} such that

$$\liminf_{l\to\infty} \|Ax_{n_l} - Ax\| > 0.$$

On the other hand, by applying the above proof to the sequence x_{n_l}, we know that $x_{n_l} \rightharpoonup x$ which implies that there exists a subsequence $x_{n_{l_m}}$ such that $Ax_{n_{l_m}} \to Ax$ strongly. We get the contradiction

$$0 = \liminf_{m\to\infty} \left\|Ax_{n_{l_m}} - Ax\right\| \geqslant \liminf_{l\to\infty} \|Ax_{n_l} - Ax\| > 0.$$

q.e.d.

Theorem 1.25 (Spectral Theorem for Compact, Symmetric Operators)**.** *Let A be a compact, symmetric operator on $\mathscr{H}$. Then there exists a sequence $(\lambda_n)_n \subset \mathbb{R}$, $\lambda_n \xrightarrow{n\to\infty} 0$ and an ONB $(x_n)_n$ of $\mathscr{H}$ such that $Ax_n = \lambda_n x_n$ for all n. In particular*

$$Ax = \sum_{n=1}^{\infty} \lambda_n \langle x_n, x\rangle\, x_n$$

□

Proof.

Step 1 Define

$$a = \sup_{\substack{u\in\mathscr{H}\\ \|u\|=1}} |\langle u, Au\rangle|.$$

We prove that this there exists $u_1 \in \mathscr{H}$, $\|u_1\| = 1$ such that $a = |\langle u_1, Hu_1\rangle|$. Because A is bounded, we know that a is a finite, non-negative number and we can find a sequence of unit vectors $(x_n)_n \subset \mathscr{H}$ such that $|\langle x_n, Ax_n\rangle| \to a$. Since the sequence $(x_n)_n$ is bounded, we can go to a subsequence and assume that $x_n \rightharpoonup u_1$ weakly by Theorem 1.13. Because A is a compact operator $Ax_n \to Au_1$ strongly.

Using the fact that if $x_n \rightharpoonup x, y_n \to y$, then $\langle x_n, y_n\rangle \to \langle x, y\rangle$, we find that $\langle x_n, Ax_n\rangle \to \langle u_1, Au_1\rangle$ and thus $a = |\langle u_1, Au_1\rangle|$.

We only have to prove that $\|u_1\| = 1$. Using the lower semicontinuity of the norm we find that $\|u_1\| \leqslant 1$. For the converse assume that $\|u_1\| < 1$ then we can define $v_1 = \frac{u_1}{\|u_1\|}$ if $u_1 \neq 0$. Then

$$|\langle v_1, Av_1 \rangle| = \frac{|\langle u_1, Au_1 \rangle|}{\|u_1\|^2} = \frac{a}{\|u_1\|^2} > a$$

if $a > 0$ which is a contradiction. If $u_1 = 0$ or $a = 0$, then $a = 0$. This means that $\langle u, Au \rangle = 0$ for all $u \in \mathscr{H}$. Consider the function $\langle u + tv, A(u + tv) \rangle = 0$ for all $u, v \in \mathscr{H}$ and $t \in \mathbb{R}$. Then

$$0 = \langle u, Au \rangle + 2t\,\mathfrak{R}\,\langle u, Av \rangle + t^2 \langle v, Av \rangle = 2t\,\mathfrak{R}\,\langle u, Av \rangle$$

thus $\mathfrak{R}\,\langle u, Av \rangle = 0$ for all $u, v \in \mathscr{H}$. Replacing v by iv we get analogously $\mathfrak{I}\,\langle u, Av \rangle = 0$. This implies $\langle u, Av \rangle = 0$ for all $u, v \in \mathscr{H}$ which in turn implies that $A \equiv 0$ in which case the spectral theorem is trivial.

Step 2 We have already proven that there exists a unit vector u_1 such that $|\langle u_1, Au_1 \rangle| \geqslant |\langle u, Au \rangle|$ for all $u \in \mathscr{H}$. We shall now prove that u_1 is an eigenvector with eigenvalue $\langle u_1, Au_1 \rangle =: \lambda_1 \in \mathbb{R}$.

We know that

$$\begin{cases} \forall u \in \mathscr{H} : \langle u_1, Au_1 \rangle \geqslant \langle u, Au \rangle\,, & \text{if } \lambda_1 \geqslant 0 \\ \forall u \in \mathscr{H} : \langle u_1, Au_1 \rangle \leqslant \langle u, Au \rangle\,, & \text{if } \lambda_1 < 0 \end{cases}$$

Take an arbitrary $\varphi \in \mathscr{H}$ and define for $\varepsilon \in \mathbb{R}$ and small enough such that $u_1 + \varepsilon\varphi \neq 0$

$$f(\varepsilon) = \frac{\langle u_1 + \varepsilon\varphi, u_1 + \varepsilon\varphi \rangle}{\|u_1 + \varepsilon\varphi\|^2}$$

then either $\lambda_1 \geqslant 0$ and $f(\varepsilon) \leqslant f(0)$ or $\lambda_1 < 0$ and $f(\varepsilon) \geqslant 0$ for ε small enough. In both cases we conclude that

$$\frac{d}{d\varepsilon} f(\varepsilon)\bigg|_{\varepsilon=0} = 0,$$

i.e.

$$0 = \frac{d}{d\varepsilon} \frac{\langle u_1, Au_1 \rangle + 2\varepsilon \,\mathfrak{R} \langle \varphi, Au_1 \rangle + \varepsilon^2 \langle \varphi, A\varphi \rangle}{\|u_1\|^2 + 2\varepsilon \,\mathfrak{R} \langle \varphi, u_1 \rangle + \varepsilon^2 \|\varphi\|^2} \Bigg|_{\varepsilon=0} = 2 \,\mathfrak{R} \langle \varphi, Au_1 \rangle - 2 \,\mathfrak{R} \langle u_1, Au_1 \rangle \langle \varphi, u_1 \rangle =$$
$$= 2 \,\mathfrak{R} \langle \varphi, Au_1 - \lambda_1 u_1 \rangle$$

for all $\varphi \in \mathscr{H}$. Replacing φ by $i\varphi$ we get the imaginary part as above and therefore we can conclude that for all $\varphi \in \mathscr{H}$

$$\langle \varphi, Au_1 - \lambda_1 u_1 \rangle = 0,$$

i.e.

$$Au_1 = \lambda_1 u_1.$$

Step 3 Let $V_1 := \operatorname{span}(u_1)$. Then we can decompose $\mathscr{H} = V_1 \oplus V_1^{\perp}$. We want to prove that $A : V_1^{\perp} \to V_1^{\perp}$. Indeed, take $u \in V_1^{\perp}$, and we need to verify $Au \in V_1^{\perp}$ which follows from

$$\langle u_1, Au \rangle = \langle Au_1, u \rangle = \langle \lambda_1 u_1, u \rangle = \lambda_1 \langle u_1, u \rangle = 0$$

We can apply the results from Step 1 and Step 2 to $A\big|_{V_1^{\perp}}$. More precisely we can find $\lambda_2, u_2 \in V_1^{\perp}$ such that $Au_2 = \lambda_2 u_2$ and

$$|\lambda_2| = \sup_{\substack{u \in V_1^{\perp} \\ \|u\|=1}} \langle u, Au \rangle$$

Step 4 (Induction) For any $n \in \mathbb{N}$, assume that we already have $u_1, \ldots, u_n$ ONF and $\lambda_1, \ldots, \lambda_n$ such that $Au_i = \lambda_i u_i$ and $|\lambda_i| \geqslant |\langle u, Au \rangle|$ for all $u \in \{u_1, \ldots, u_{i-1}\}^{\perp}$. Define $V_n = \operatorname{span}(u_1, \ldots, u_n)$ and write $\mathscr{H} = V_n \oplus V_n^{\perp}$. We can show that $A : V_n \to V_n$ and $A : V_n^{\perp} \to V_n^{\perp}$ as in Step 3 and by applying Step 1 and 2 to $A\big|_{V_n^{\perp}}$ we can find u_{n+1} and λ_{n+1} satisfying the required properties.

Step 5 (Conclusion) Consider 2 cases. First assume that $\lambda_n = 0$ for some $n \in \mathbb{N}$ (note that $|\lambda_n|$ is a decreasing sequence in n). Then we have $Au_i = \lambda_i u_i$ for all $i = 1, \ldots, n$ and $A\big|_{V_n^{\perp}} \equiv 0$ as in Step 1. Then we only need to choose $\{u_{n+1}, \ldots\}$ to be an ONB for $V_n^{\perp}$. And we have $Au_i = \lambda_i u_i$ for all $i \in \mathbb{N}$ with $\lambda_i = 0$ for $i \geqslant 0$.

For the second case assume that $\lambda_n \neq 0$ for all $n \in \mathbb{N}$. We will prove that $(u_n)_{n\in\mathbb{N}}$ satisfies $\mathscr{H} = V \oplus \ker A$ with $V = \operatorname{span}((u_n)_n)$.

Take $u \in \mathscr{H}$ and assume that $\langle u, u_n \rangle = 0$ for all $n \in \mathbb{N}$, and prove $Au = 0$. Recall that $|\lambda_n| \geqslant |\langle \varphi, A\varphi \rangle|$ for all unit vectors $\varphi \in V_n^{\perp}$. Then $|\lambda_n| \geqslant \langle u, Au \rangle$ for all $n \in \mathbb{N}$ and thus $\lim |\lambda_n| \geqslant |\langle u, Au \rangle|$. We have to prove that $\lambda_n \to 0$. This is easy because $\lambda_n = \langle u_n, Au_n \rangle \to 0$ because $(u_n)_n$ is bounded and $Au_n \to 0$ strongly.

This follows from the fact that if $(x_n)_n$ is an ONF and A is a compact operator, then $Ax_n \to 0$ strongly as $n \to \infty$.

Thus $\langle u, Au \rangle = 0$ for all $u \in V^{\perp}$. Repeating this argument in Step 1, we get $Au = 0$ for all $u \in V^{\perp}$. Choosing $(\varphi_m)_{m\in\mathbb{N}}$ to be an ONB of $V^{\perp}$, then $(u_n)_{n\in\mathbb{N}} \cup (\varphi_m)_{m\in\mathbb{N}}$ forms an ONB of eigenvector of A for $\mathscr{H}$.

q.e.d.

Definition 1.26 (Schatten Spaces)**.** Consider a compact, symmetric operator A. We know that $A = \sum_{i=1}^{\infty} \lambda_i |u_n\rangle \langle u_n|$, where $Au_n = \lambda_n u_n$. We say that A is in the Schatten space S_p, with $1 \leqslant p < \infty$ if $(\lambda_n)_{n\in\mathbb{N}} \in \ell^p(\mathbb{N})$, i.e. if

$$\sum_{n=1}^{\infty} |\lambda_n|^p < \infty$$

and denote $\|A\|_{S_p} = \left(\sum_{n=1}^{\infty} |\lambda_n|^p\right)^{1/p}$. In particular we call

- $p = 1$ the trace class operators
- $p = 2$ the Hilbert-Schmidt operators
- $p = \infty$ the compact operators (formally)

□

Remark 1.27. $S_p \subset S_q$ if $p < q$ (because $\ell^p \subset \ell^q$). And thus

Trace class $\subset$ Hilbert-Schmidt $\subset$ compact $\subset$ bounded.

□

Theorem 1.28 (Trace Class Operators)**.** *Let A be a compact and symmetric operator. Then the following are equivalent*

(i) A is trace class

(ii) For all ONB $(\varphi_n)_n$

$$\sum_{n=1}^{\infty} |\langle \varphi_n, A\varphi_n \rangle| < \infty.$$

In this case $\operatorname{Tr}(A) = \sum_{n=1}^{\infty} \langle \varphi_n, A\varphi_n \rangle$ *is independent of the choice of ONB $(\varphi_n)_n$.*

□

Proof. Assume that $A\varphi = \sum_{n=1}^{\infty} \lambda_n \langle u_n, \varphi \rangle u_n$ for all $\varphi \in \mathscr{H}$, where $(\lambda_n)_n$, $(u_n)_n$ are eigenvalues and eigenfunctions of A. Then

$$\langle \varphi, A\varphi \rangle = \sum_{n=1}^{\infty} \langle \varphi, \lambda \langle \lambda_n, \varphi \rangle u_n \rangle = \sum_{n=1}^{\infty} \lambda_n |\langle u_n, \varphi \rangle|^2$$

(i)⇒(ii) Take ONB $(\varphi_n)_n$

$$\sum_{m=1}^{\infty} |\langle \varphi_m, A\varphi_m \rangle| = \sum_{m=1}^{\infty} \left| \sum_{n=1}^{\infty} \lambda_n |\langle \varphi_m, u_n \rangle|^2 \right| \leqslant \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} |\lambda_n| |\langle \varphi_m, u_n \rangle|^2 = \sum_{n=1}^{\infty} |\lambda_n| \underbrace{\sum_{m=1}^{\infty} |\langle \varphi_m, u_n \rangle|^2}_{=\|u_n\|^2=1} =$$

$$= \sum_n |\lambda_n| < \infty$$

(ii)⇒(i) Choosing $\varphi_n = u_n$ the eigenvectors of A then

$$\infty > \sum_{n=1}^{\infty} |\langle \varphi_n, A\varphi_n \rangle| = \sum_{n=1}^{\infty} |\lambda_n|$$

and thus A is trace class.

The last statement follows as in (i)⇒(ii) directly Fubini's theorem as the double sum is absolutely convergent

$$\sum_{m=1}^{\infty} \langle \varphi_m, A\varphi_m \rangle = \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} \lambda_n |\langle \varphi_m, u_n \rangle|^2 = \sum_{n=1}^{\infty} \lambda_n \underbrace{\sum_{m=1}^{\infty} |\langle \varphi_m, u_n \rangle|^2}_{=\|u_n\|^2=1} = \sum_n \lambda_n$$

q.e.d.

Remark 1.29 (Singular Value Decomposition). If A is a compact operator (not necessarily symmetric then we find ONBs $(u_n)_n, (v_n)_n$ and real numbers $\lambda_n \to 0$ such that for all $n \in \mathbb{N}$

$$Au_n = \lambda_n v_n$$

i.e.

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

for all $u \in \mathscr{H}$. □

Definition 1.30. In this general case, we say that $A \in S_p$ if

$$\sum_{n=1}^{\infty} |\lambda_n|^p < \infty$$

and we define

$$\|A\|_{S_p} = \left(\sum_{n=1}^{\infty} |\lambda_n|^p \right)^{1/p}.$$

□

Theorem 1.31 (Hilbert-Schmidt Operator). *The following are equivalent*

(i) A is a Hilbert-Schmidt operator, i.e. $A \in S_2$

(ii) $\sum_{n=1}^{\infty} \|A\varphi_n\|^2 < \infty$ for all ONBs $(\varphi_n)_n$. Moreover,

$$\|A\|_{S_2} = \left(\sum_{n=1}^{\infty} \|A\varphi_n\|^2 \right)^{1/2}$$

(independent of $(\varphi_n)_n$).

Moreover, if $\mathscr{H} = L^2(\Omega)$, then A is a Hilbert-Schmidt iff there exits a function $K(x,y) \in L^2(\Omega \times \Omega)$ such that

$$(Af)(x) = \int_{\Omega} K(x,y) f(y) \mathrm{d}y$$

for all $f \in L^2(\Omega)$. In this case, $K(x, y)$ is called the ***kernel*** *of A and*

$$\|A\|_{S_2} = \|K\|_{L^2(\Omega\times\Omega)}$$

$\square$

Proof.

(i)⇒(ii) Since A is Hilbert-Schmidt, it is compact with decomposition

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

for some ONBs $(u_n)_n, (v_n)_n$, for real numbers $\lambda_n \to 0$. Thus for all $u \in \mathscr{H}$

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

(by Parseval's identity as $(v_n)_n$ is an ONB). Thus by Fubini's theorem

$$\sum_m \|A\varphi_m\|^2 = \sum_m \sum_n |\lambda_n|^2 | \langle u_n, \varphi_m \rangle |^2 = \sum_n |\lambda_n|^2 \left(\sum_m | \langle u_n, \varphi_m \rangle |^2 \right) = \sum_n |\lambda_n|^2 < \infty$$

since A is Hilbert-Schmidt

(ii)⇒(i) Same as above.

Now let us assume that $\mathscr{H} = L^2(\Omega)$. Assume that $K(x, y) \in L^2(\Omega \times \Omega)$ and assume that $(Af)(x) = \int K(x, y)f(y)\mathrm{d}y$.

Take $(\varphi_n)_n$ to be an ONB for $L^2(\Omega)$. We have

$$\begin{aligned}\sum_{n=1}^{\infty} \|A\varphi_n\|^2 &= \sum_{m,n} | \langle \varphi_m, A\varphi_n \rangle |^2 = \sum_{m,n} \left| \int \overline{\varphi_m(x)} K(x, y) \varphi_n(y) \mathrm{d}x\mathrm{d}y \right|^2 = \\ &= \sum_{m,n} \left| \left\langle \varphi_m(x)\overline{\varphi_n(y)}, K(x, y) \right\rangle_{L^2(\Omega,\Omega)} \right|^2 = \|K(x, y)\|^2_{L^2(\Omega\times\Omega)}\end{aligned}$$

by Parseval's identity again. Here we used the fact $\left(\varphi_m(x)\overline{\varphi_n(y)}\right)_{m,n}$ is an ONB for $L^2(\Omega \times \Omega) = L^2(\Omega) \otimes L^2(\Omega)$.

This means that if $K \in L^2(\Omega \times \Omega)$, then A is Hilbert-Schmidt.

Conversely if A is Hilbert-Schmidt, then $K \in L^2$, where the kernel is defined as follows. Using the singular value decomposition of A we find for all $u \in L^2(\Omega)$

$$(Au)(x) = \sum_{n=1}^{\infty} \lambda_n \langle u_n, u \rangle v_n(x) = \sum_{n=1}^{\infty} \lambda_n \left(\int \overline{u_n(y)} u(y) \mathrm{d}y \right) v_n(x) = \int \left(\sum_{n=1}^{\infty} \lambda_n v_n(x) \overline{u_n(y)} \right) u(y) \mathrm{d}y$$

Thus

$$K(x,y) = \sum_{n=1}^{\infty} \lambda_n v_n(x) \overline{u_n(y)}$$

This belongs to $L^2(\Omega \times \Omega)$ (why?). *q.e.d.*

Remark 1.32. $Au = \sum_n \lambda_n \langle u_n, u \rangle v_n$ thus in Braket notation we have

$$A = \sum_n \lambda_n |v_n\rangle \langle u_n|$$

from which we can "directly" read off the kernel

$$\sum_n \lambda_n v_n(x) \overline{u_n(y)}.$$

□

Chapter 2

Self-Adjointness

Recall that for a densely defined unbounded operator $A : D(A) \to \mathscr{H}$ we can define $A^* : D(A^*) \to \mathscr{H}$ by

$$D(A^*) = \left\{ x \in \mathscr{H} \;\middle|\; \sup_{\substack{y \in D(A) \\ \|y\| \leqslant 1}} |\langle x, Ay \rangle| < \infty \right\} =$$
$$= \left\{ x \in \mathscr{H} \;\middle|\; \exists z \in \mathscr{H} : \forall y \in D(A)\, \langle x, Ay \rangle = \langle z, y \rangle \right\}$$

(by the Riesz representation theorem) and for all $x \in D(A^*)$ we then define $A^* x = z$, i.e. for all $y \in D(A)$ and $x \in D(A^*)$

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

Definition 2.1 (Self-Adjointness)**.** A is a self-adjoint operator iff

$$A = A^*$$

□

Remark 2.2. A is self-adjoint implies that A is symmetric, however, the converse does not hold. □

Example 2.3 (Multiplication Operator)**.** Consider $\mathscr{H} = L^2(\Omega)$, take $f : \Omega \to \mathbb{R}$ measurable. Define

$$A : \begin{array}{c} D(A) \longrightarrow \mathscr{H} \\ (Au)(x) = f(x)u(x) \end{array}$$

We can define

$$D(A) = \left\{ u \in L^2 \,\middle|\, fu \in L^2 \right\}$$

Why is self-adjointness relevant?

(Maths) We have the "spectral theorem" for self-adjoint operators.

$$\text{Self-Adjoint Operator} \overset{\text{unitary}}{\Longleftrightarrow} \text{Multiplication Operator on some } L^2(\Omega)$$

In particular, we can study spectra and actions of self-adjoint operators. E.g. if A_f is a multiplication operator associated with a function $f : \Omega \to \mathbb{R}$ then

$$\sigma(A) = \mathrm{ran}(f) = \left\{ f(x) \,\middle|\, x \in \Omega \right\}$$

and for all g real-valued function, we can define

$$g(A) = \text{multiplication operator associated with } g(f)$$

i.e.

$$(g(A)u)(x) = g(f(x))u(x)$$

for all $u \in D(g(A))$.

(Physics) In quantum mechanics, a particle is described by a wave function $\psi \in L^2(\mathbb{R}^d)$, with the interpretation

$$|\psi(x)|^2 = \text{ probability density of the particle}$$

i.e.

$$\int_\Omega |\psi(x)|^2 \mathrm{d}x = \text{probability of particle belonging to } \Omega.$$

For this quantum particle, we can consider a Hamiltonian

$$A : D(A) \longrightarrow \mathscr{H} = L^2(\mathbb{R}^d),$$

where the

$$\begin{aligned} \langle \psi, A\psi \rangle = &\ \text{the expected value of the the energy of the state } \psi \\ \sigma(A) = &\ \text{possible energy levels of the particle} \end{aligned}$$

and the excited state/ground state solves the Schrödinger equation

$$A\psi = \lambda\psi.$$

The evolution of a state $\psi(0)$ is governed by the time dependent Schrödinger equation

$$\partial_t \psi(t) = -\frac{i}{\hbar} A\psi(t)$$

with $\lim_{t\to 0} \psi(t) = \psi(0)$.

Theorem. *The time dependent Schrödinger equation has a unique solution $\psi(t)$ for all initial states $\psi(0) \in L^2(\mathbb{R}^d)$ satisfying $\|\psi(t)\|^2 = \|\psi(0)\|^2 = 1$ iff A is self-adjoint.* □

Remark. "Finding a self-adjoint extension of a symmetric operator is <u>tricky</u>." □

Example 2.4. Let $\mathscr{H} = L^2(0,1)$ and consider the operator $A = i\frac{d}{dx}$ with

$$D(A) = \mathscr{C}_c^1(0,1).$$

Then A is symmetric because for $g, f \in D(A)$

$$\langle g, Af \rangle = \int_0^1 \overline{g} i f' = -i \int_0^1 \overline{g'} f = \int_0^1 \overline{i g'} f = \langle Ag, f \rangle$$

But A is not self-adjoint. We have

$$\int_0^1 \overline{g} i f' = i\Big(\overline{g(1)}f(1) - \overline{g(0)}f(0)\Big) + \int_0^1 \overline{ig'} f$$

for general functions f, g.

We need to define A_0 of A such that for all $f, g \in D(A)$

$$\overline{g(1)}f(1) - \overline{g(0)}f(0) = 0$$

There are two possibilities.

$$\begin{aligned} D(A_0) &= \big\{ f \in H^1(0,1) \,\big|\, f(0) = 0 = f(1) \big\} \\ A_0 f &= i f' \end{aligned}$$

$$\begin{aligned} D(A_1) &= \big\{ f \in H^1(0,1) \,\big|\, f(0) = f(1) \big\} \\ A_1 f &= i f' \end{aligned}$$

where we define

$$H^1(0,1) := \big\{ f \in L^2 \,\big|\, f' \in L^2 \big\}$$

which is a Hilbert space.

A_0 is a self-adjoint extension of A whereas A_1 is not.

A_1 has the eigenvalues $2\pi n$ with eigenfunctions $\psi_n(x) = e^{i2\pi n x}$ for $n \in \mathbb{Z}$ but A_0 has no eigenvalue.

Example 2.5. Consider $H = L^2(0,1)$, $A = -\Delta = -d_x^2$ with $D(A) = \mathscr{C}_c^2(0,1)$. Then A is symmetric but not self-adjoint. There are three self-adjoint extensions of A.

(1) (Dirichlet Laplacian) $D(A_0) = \big\{ f \in H^2(0,1) \,\big|\, f(0) = f(1) = 0 \big\}$, $A_0 f = -\Delta f$.

(2) (Neumann Laplacian) $D(A_1) = \big\{ f \in H^2(0,1) \,\big|\, f'(0) = f'(1) = 0 \big\}$

(3) (Periodic Laplacian) $D(A_2) = \big\{ f \in H^2(0,1) \,\big|\, f(0) = f(1), f'(0) = f'(1) \big\}$

What is the "right" extension. For our purpose, we will focus on the ***Friedrich's***

extension.

An easy definition of a good extension would be to require

$$\inf_{\substack{u\in D(A)\\ \|u\|=1}} \langle u, Au\rangle = \inf_{\substack{v\in D(A_0)\\ \|v\|=1}} \langle v, Av\rangle$$

where $\geqslant$ is trivial but the reverse is not.

Definition 2.6 (Non-Negative Operator)**.** We say that A is non-negative/positive and write $A \geqslant 0$ if

$$\langle u, Au\rangle \geqslant 0$$

for all $u \in D(A)$. Similarly, we write $A \geqslant B$ if $A - B \geqslant 0$. If $A \geqslant -C\mathbb{I}$ for some constant C then A is called ***bounded from below***. □

Theorem 2.7 (Friedrich's Extension)**.** *If $A : D(A) \to \mathscr{H}$ is bounded from below, then there exists a unique self-adjoint extension A_0 such that*

$$\inf_{\substack{u\in D(A)\\ \|u\|=1}} \langle u, Au\rangle = \inf_{\substack{v\in D(A_0)\\ \|v\|=1}} \langle v, Av\rangle$$

□

Proof.

Step 1 W.l.o.g. we can assume that $A \geqslant \mathbb{I}$ (because we can replace A by A+const if necessary). Define the quadratic form

$$Q(u, v) = \langle u, Av\rangle$$

for all $u, v \in D(A)$. Thus $(u, v) \mapsto Q(u, v)$ is an inner product, i.e.

- $Q(u, v)$ is linear in v and anti-linear in u.
- $Q(u, v) = \overline{Q(v, u)}$
- $Q(u, u) \geqslant \|u\|^2$ for all $u \in D(A)$.

Define $\|u\|_Q = \sqrt{Q(u, u)} = \sqrt{\langle u, Au\rangle}$ for all $u \in D(A)$. This is a norm on $D(A)$. We define the quadratic form domain

$$Q(A) = \overline{D(A)}^{\|\cdot\|_Q}$$

as the completion of $D(A)$ with respect to $\|\cdot\|_Q$. $Q(A)$ is a Hilbert space with the inner product $Q(u,v)$.

In fact due to the inequality $\|u\|_Q \geqslant \|u\|$

$$D(A) \subset Q(A) \subset \mathscr{H}$$

and $D(A)$ is dense in either space with the respective norms.

Step 2 (Definition of Friedrich's Extension A_0) Let

$$D(A_0) = \left\{ x \in Q(A) \,\middle|\, \sup_{\substack{y \in Q(A) \\ \|y\| \leqslant 1}} |Q(x,y)| < \infty \right\}$$

We claim that

$$D(A_0) = \big\{ x \in Q(A) \,\big|\, \exists z \in \mathscr{H} : \forall y \in Q(A) : Q(x,y) = \langle z, y \rangle \big\}.$$

The reason for this is the Riesz representation theorem as for all $x \in Q(A)$ we can define

$$\mathscr{L}_x : \begin{array}{c} Q(a) \longrightarrow \mathbb{C} \\ y \longmapsto Q(x,y) \end{array}$$

Then $\mathscr{L}_x$ is a linear functional, and

$$\sup_{\substack{y \in Q(A) \\ \|y\| \leqslant 1}} |\mathscr{L}_x(y)| < \infty \iff \mathscr{L}_x \text{ is } \textbf{\textit{continuous}} \iff \exists z \in \mathscr{H} : \forall y \in Q(A) : \mathscr{L}_x(y) = \langle z, y \rangle$$

as $Q(A)$ is dense in $\mathscr{H}$. Thus we can define for $x \in D(A_0)$

$$A_0 x_0 := z$$

We now prove that A_0 is a self-adjoint operator. First, we can show that A_0 is symmetric. In fact for all $x, y \in D(A_0)$,

$$\langle x, A_0 y \rangle = Q(x,y) = \overline{Q(y,x)} = \overline{\langle y, A_0 x \rangle} = \langle A_0 x, y \rangle$$

Thus $A_0 \subset A_0^*$. It remains to prove that $D(A_0^*) \subset D(A_0)$. In fact

$$x \in D(A_0^*) \iff \sup_{\substack{y \in D(A_0) \\ \|y\| \leqslant 1}} |\langle x, A_0 y \rangle| < \infty \iff \sup_{\substack{y \in D(A_0) \\ \|y\| \leqslant 1}} |Q(x,y)| < \infty \iff x \in D(A_0)$$

Why is $x \in Q(A)$ (exercise using $Q(A) = \overline{D(A)}^{\|\cdot\|_Q}$)?

q.e.d.

Example 2.8. Let us consider $\mathscr{H} = L^2(0,1)$, $A = -\Delta = -d_x^2$ and

$$D(A) = \left\{ \mathscr{C}^2(0,1) \,\middle|\, u(0) = u(1) = 0 \right\}.$$

Then A is symmetric and $A \geqslant 0$, but A is not self-adjoint.
The quadratic form of A is

$$Q(u,v) = \langle u, Av \rangle = \int \overline{u}(-v'') = \int \overline{u}' v'$$

the quadratic form domain thus is

$$Q(A) = \overline{D(A)}^{\|\cdot\|_Q} = H_0^1(0,1) = \left\{ f \in L^2(0,1) \,\middle|\, f' \in L^2(0,1), f(0) = f(1) = 0 \right\}$$

and the Friedrich's extension is $A_0 = -\Delta$ with $D(A_0) = H_0^2(0,1)$.

Theorem 2.9 (Min-Max-Principle)**.** *Let $A : D(A) \to \mathscr{H}$ be bounded from below and let A_0 be the Friedrich extension of A. For $n = 1, 2, \ldots,$ we can define the* $\min - \max$*-value*

$$\mu_n(A) = \inf_{\substack{M \subset D(A) \\ \dim M = n}} \sup_{\substack{u \in M \\ \|u\| = 1}} \langle u, Au \rangle$$

and we define

$$\mu_\infty(A) = \lim_{n \to \infty} \mu_n(A) \qquad \textit{(finite or } +\infty\textit{)}$$

If $\mu_n(A) < \mu_\infty(A)$, then $\mu_1, \ldots, \mu_n$ are the lowest eigenvalues of A_0. In this case μ_∞ is called the bottom of the essential spectrum. □

Remark 2.10. All of the min − max-values are well-defined by A, and there is no need to consider A_0, but the when we talk about the eigenvalues, then A_0 should appear. □

Proof. We shall prove the following for the case $A = A_0$. The general assertion then follows from the fact that

$$\mu_n(A) = \mu_n(A_0)$$

for all $n \in \mathbb{N}$ which is left as an exercise.

Step 1 Assume that $\mu_1 < \infty$, then there exists a $m \in \mathbb{N}$ such that $\mu_1 = \mu_2 = \cdots = \mu_m < \mu_\infty$ (since $(\mu_n)_n$ is increasing in n). In this case, we prove that $\mu_1 = \cdots = \mu_m$ are eigenvalues of A (i.e. this is an eigenvalue of multiplicity m).

We claim that there exists a $u \in Q(A)$, such that

$$Q(u) = \inf_{\substack{\varphi \in Q(A) \\ \|\varphi\|=1}} Q(\varphi)$$

To prove this note that since $\mu_1 = \cdots = \mu_m$ we can find a sequence of subspaces M_k such that

- $\dim M_k = m$
- For all $k \in \mathbb{N}$
$$\max_{\substack{\varphi \in M_k \\ \|\varphi\|=1}} \langle \varphi, A\varphi \rangle \leqslant \mu_1 + 2^{-k}.$$

We prove that there exist $u_k \in M_k$ for all $k \in \mathbb{N}$ such that $\|u_k\| = 1$, $\|u_k - u_{k+1}\| \leqslant C\sqrt{2}^{-k}$ (with C independent of k). We find $(u_k)_k$ by induction. First, u_1 can be chosen freely, ($u_1 \in M_1$, $\|u_1\| = 1$). Assume that we can already chose u_k. Now we want to find $u_{k+1} \in M_{k+1}$, $\|u_{k+1}\| = 1$, $\|u_k - u_{k+1}\| \leqslant C\sqrt{2}^{-k}$. If $u_k \in M_{k+1}$, then $u_{k+1} = u_k$. If $u_k \notin M_{k+1}$, then $\operatorname{span}(M_{k+1} \cup \{u_k\})$ has $(m+1)$-dimensions. By the definition of μ_{m+1} we know

$$\max_{\substack{\varphi \in \operatorname{span}(M_{k+1} \cup \{u_k\}) \\ \|\varphi\|=1}} \langle \varphi, A\varphi \rangle \geqslant \mu_{m+1} > \mu_1$$

Thus there exists a $\varphi \in \operatorname{span}(M_{k+1} \cup \{u_k\})$ such that $\langle \varphi, A\varphi \rangle \geqslant \mu_{m+1}$. Let us write

$\varphi = a + b$ with $a \in \operatorname{span}\{u_k\}$ and $b \in M_{k+1}$. We have

$$\begin{aligned}\mu_{m+1} &\leqslant Q(\varphi) = Q(a+b) = 2Q(a) + 2Q(b) - Q(a-b) \leqslant \\ &\leqslant 2(\mu_1 + 2^{-k})\|a\|^2 + 2(\mu_1 + 2^{-(k+1)})\|b\|^2 - \mu_1\|a-b\|^2 \leqslant 2 \cdot 2^{-k}\|a\|^2 + 2 \cdot 2^{-(k+1)}\|b\|^2 + \mu_1\end{aligned}$$

where we used that $\|a-b\|^2 = 2\|a\|^2 + 2\|b\|^2 - \|a+b\|^2$ and $\|a+b\| = 1$. This yields

$$\mu_{m+1} - \mu_1 \leqslant 2^{-k+1}(\|a\|^2 + \|b\|^2) \quad \therefore \quad \|a\|^2 + \|b\|^2 \geqslant \frac{\mu_{m+1} - \mu_1}{2} 2^k$$

Noting that for $a, b \in \mathscr{H}$, $a, b \neq 0$

$$\left\| \frac{a}{\|a\|} + \frac{b}{\|b\|} \right\| \leqslant \frac{2\|a+b\|}{\max\{\|a\|, \|b\|\}}$$

Thus

$$\left\| \frac{a}{\|a\|} + \frac{b}{\|b\|} \right\| \leqslant \frac{2}{\max\{\|a\|, \|b\|\}} \leqslant \frac{2\sqrt{2}}{\sqrt{\|a\|^2 + \|b\|^2}} \leqslant \frac{2\sqrt{2}}{\sqrt{\frac{m_{k+1} - \mu_1}{2} 2^k}} = C\sqrt{2}^{-k}$$

Since $a \in \operatorname{span}\{u_k\}$, i.e. $a = \lambda u_k$, for some $\lambda \in \mathbb{C}$, then we can choose $u_{k+1} \in \operatorname{span}\{b\}$ such that

$$\|u_k - u_{k+1}\| = \left\| \frac{a}{\|a\|} + \frac{b}{\|b\|} \right\| \leqslant C\sqrt{2}^{-k}$$

Using this, wee see that $(u_k)_k$ is a Cauchy sequence in $\mathscr{H}$, and hence there exists a $\lim u_k = u$ in $\mathscr{H}$. In particular $\|u\| = 1$. It remains to prove that $u \in Q(A)$ and $Q(u) \leqslant \mu_1$.

We know that $u_k \in M_k \subset Q(A)$, $\|u_k\| = 1$ and $Q(u_k) \leqslant \mu_1 + 2^{-k}$ for all k. In the Hilbert space $(Q(A), \|\cdot\|_Q)$, u_k is a bounded sequence, and by Theorem 1.13 there exists a subsequence that converges weakly to some $v \in Q(A)$. Since $u_k \to u$ in $\mathscr{H}$, we can conclude that $u = v$. And by lower semi-continuity

$$Q(u) = \|u\|_Q^2 \leqslant \liminf_{k\to\infty} \|u_k\|_Q^2 = \lim Q(u_k) \leqslant \mu_1$$

Concluding $\|u\| = 1$ and $Q(u) = \mu_1$. Take any $\varphi \in Q(A)$, then

$$f(\varepsilon) = Q(u + \varepsilon\varphi) - \mu_1\|\varepsilon + \varphi\|^2 \geqslant 0 = f(0)$$

Thus $f'(0) = 0$ which yields

$$\Re\, Q(u,\varphi) = \Re\, \mu_1 \langle u, \varphi\rangle$$

for all $\varphi \in Q(A)$ and replacing φ by $i\varphi$ we get the same equality for the imaginary part, i.e.

$$Q(u,\varphi) = \mu_1 \langle u, \varphi\rangle \quad \therefore \quad \sup_{\|\varphi\|\leqslant 1} Q(u,\varphi) \leqslant \mu_1 \|u\|$$

Thus $u \in D(A)$, hence $Q(u,\varphi) = \langle Au, \varphi\rangle$ for all $\varphi \in Q(A)$. Thus we have $Au = \mu_1 u$.

Step 2 Define V_m to be the eigenspace of A with eigenvalues $\mu_1 = \cdots = \mu_m$ and define $A_m = A\big|_{V_m^\perp \cap D(A)}$. Then $\mu_n(A_m) = \mu_{m+n}(A)$ for all $n \in \mathbb{N}$.

By the definition:

$$\mu_n(A_m) = \inf_{\substack{M \subset V_m^\perp \cap D(A)\\ \dim M = n}} \sup_{\substack{u \in M\\ \|u\|=1}} \langle u, A_m u\rangle \leqslant \inf_{\substack{M \subset V_m^\perp \cap D(A)\\ \dim M = n}} \sup_{\substack{u \in M \oplus V_m\\ \|u\|=1}} \langle u, Au\rangle$$

We claim that for $M \subset V_m^\perp$ then

$$\sup_{\substack{u \in M\\ \|u\|=1}} \langle u, Au\rangle = \sup_{\substack{u \in M\oplus V_m\\ \|u\|=1}} \langle u, Au\rangle .$$

In fact ($\leqslant$) is trivial; to prove the converse we use that $A_0 v = \mu_1(A) v$ for all $v \in V_m$. Indeed, for every $u \in M \oplus V_m$ we can write $u = \varphi + v$ with $\varphi \in V_m^\perp$ and $v \in V_m$. Then we have

$$\langle u, Au\rangle = \langle \varphi + v, A(\varphi + v)\rangle = \langle \varphi, A\varphi\rangle + \mu_1(A)\|v\|^2 \geqslant \|\varphi\|^2 \left\langle \frac{\varphi}{\|\varphi\|}, A\frac{\varphi}{\|\varphi\|}\right\rangle + \|v\|^2 \mu_1(A)$$

Then for $\varphi_1 := \frac{\varphi}{\|\varphi\|}$

$$\sup_{\substack{u \in M\oplus V_m\\ \|u\|=1}} \langle u, Au\rangle = \sup_{\substack{\varphi \in M \subset V_m^\perp\\ v \in V_m\\ \|\varphi\|^2 + \|v\|^2 = 1}} \big(\langle \varphi_1, A\varphi_1\rangle + \|v\|^2\mu_1(A)\big) \leqslant$$

$$\leqslant \big(1 - \|v\|^2\big)\left(\sup_{\substack{\varphi_1 \in M\oplus V_m\\ \|\varphi_1\|=1}} \langle \varphi_1, A\varphi_1\rangle\right) + \|v\|^2 \mu_1(A) \leqslant \sup_{\substack{\varphi_1 \in M\oplus V_m\\ \|\varphi_1\|=1}} \langle \varphi_1, A\varphi_1\rangle$$

because $\mu_1(A) \leqslant \langle \varphi_1, A\varphi_1\rangle$.

By the claim,

$$\mu_n(A_m) = \inf_{\substack{M \subset V_m^\perp \\ \dim M = n}} \sup_{\substack{\varphi_1 \in M \oplus V_m \\ \|\varphi_1\|=1}} \langle u, Au \rangle$$

Defining $N = M \oplus V_m$, we have $\dim N = n + m$, and

$$\mu_n(A_m) = \inf_{\substack{M \subset V_m^\perp \\ \dim M = n}} \sup_{\substack{u \in N \\ \|u\|=1}} \langle u, Au \rangle \geqslant \inf_{\substack{N_1 \subset \mathscr{H} \\ \dim N_1 = n+m}} \sup_{\substack{u \in N_1 \\ \|u\|=1}} \langle u, Au \rangle = \mu_{m+n}(A)$$

The other inequality is similar and uses the fact that if $N \subset \mathscr{H}$, with $\dim N = m + n$, then $\dim\big(N \cap V_m^\perp\big) \geqslant n$. For this reason

$$\mu_{m+n}(A) \geqslant \mu_n(A_m).$$

q.e.d.

Theorem 2.11 (Max-Min Theorem)**.** *Let $A : D(A) \to \mathscr{H}$ bounded from below. Then*

$$\mu_m(A) = \sup_{\dim N = n-1} \inf_{\substack{u \perp N \subset D(A) \\ \|u\|=1}} \langle u, Au \rangle$$

□

The problem with the Friedrich's extension is that we do not know the domain of $D(A_0)$

$$D(A_0) = \left\{ x \in Q(A) \;\middle|\; \sup_{\substack{y \in D(Q) \\ \|y\| \leqslant 1}} |Q(x, y)| < \infty \right\}$$

and $Q(x, y) = \langle A_0 x, y \rangle$ for all $y \in Q(A)$.

Theorem 2.12 (Kato-Rellich)**.** *Assume that $A : D(A) \to \mathscr{H}$ is self-adjoint and $B : D(B) \to \mathscr{H}$ is symmetric and $D(A) \subset D(B)$, and $\varepsilon > 0$*

$$\|Bx\| \leqslant (1 - \varepsilon)\|Ax\| + C_\varepsilon \|x\|$$

for all $x \in D(A)$. Then $A + B$ is a self-adjoint operator on the domain $D(A + B) = D(A)$. □

Lemma 2.13. *Let $A : D(A) \to \mathscr{H}$ be symmetric. Then the following are equivalent*

(i) A is self-adjoint.

(ii) both $\operatorname{ran}(A \pm i) = \mathscr{H}$.

□

Proof.

(i)⇒(ii) We prove that $\operatorname{ran}(A \pm i)$ is closed, i.e. if $x_n \in D(A)$, then $Ax_n + ix_n \to y$, then $y \in \operatorname{ran}(A + i)$. We have

$$\|Ax + ix\|^2 = \|Ax\|^2 + \|x\|^2$$

for all $x \in D(A)$. Thus $\|(A + i)(x_m - x_n)\|^2 = \|A(x_m - x_n)\|^2 + \|x_m - x_n\|^2$. Since $(A + i)x_m$ is a Cauchy sequence, Ax_n and x_n are Cauchy sequences, i.e. $Ax_n \to a$ and $x_n \to b$. But we know that A is closed, i.e. $a = Ab$ and $b \in D(A)$. Thus $Ax_n + ix_n \to Ab + ib = y$ which implies that $y \in \operatorname{ran}(A + i)$.

We now prove that $\operatorname{ran}(A + i) = \mathscr{H}$. If $\operatorname{ran}(A + i) \subsetneq \mathscr{H}$, then there exists a $z \in \mathscr{H}$ such that $z \notin \operatorname{ran}(A + i)$ and

$$\langle z, (A + i)x\rangle = 0$$

for all $x \in D(A)$ (by closedness of the range). Thus $\langle z, Ax\rangle = -i \langle z, x\rangle$. This in turn implies that $z \in D(A^*) = D(A)$ by Cauchy Schwartz, thus

$$0 = \langle z, (A + i)x\rangle = \langle (A - i)z, x\rangle$$

for all $x \in D(A)$, hence $(A - i)z = 0$, $Az = iz$ which implies

$$\underbrace{\langle z, Az\rangle}_{\in \mathbb{R}} = i\|z\|^2 \quad \therefore \quad z = 0$$

which is a contradiction.

(ii)⇒(i) We need to prove $D(A^*) \subset D(A)$. Take $x \in D(A^*)$. Since $\operatorname{ran}(A + i) = \mathscr{H}$, there exists $a \in D(A)$ such that

$$(A + i)a = A^*x - ix$$

Thus

$$\langle (A+i)a, y\rangle = \langle A^*x - ix, y\rangle = \langle x, (A-i)y\rangle$$

and because A is symmetric $\langle (A+i)a, y\rangle = \langle a, (A-i)y\rangle$ and therefore for all $y \in D(A)$

$$\langle x, (A-i)y\rangle = \langle a, (A-i)y\rangle$$

however as $\operatorname{ran} A - i = \mathscr{H}$ it follows that $x = a \in D(A)$.

q.e.d.

Proof of Theorem 2.12. Note that

$$A + B + in = \big(\mathbb{I} + B(A+in)^{-1}\big)(A+m)$$

$\operatorname{ran}(A+in) = \mathscr{H}$, $\operatorname{ran}(\mathbb{I} + B(A+in)^{-1}) = \mathscr{H}$ is $\|B(A+in)^{-1}\| < 1$ for n large enough and $\operatorname{ran}(A+B\pm in) = \mathscr{H}$. *q.e.d.*

Lemma 2.14. *Let B be a bounded operator and $\|B\| < 1$, then $(\mathbb{I} - B)^{-1}$ is a bounded operator (in particular $\mathbb{I} - B$ is bijective) and $\|(\mathbb{I}-B)^{-1}\| \leqslant (1 - \|B\|)^{-1}$.* □

Proof. Per the assumption we have that

$$(\mathbb{I} - B)^{-1} = \sum_{n=0}^{\infty} B^n$$

converges in the operator topology (why?). Consequently

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

q.e.d.

Proof of Theorem 2.12. First, it is obvious that $A + B : D(A) \to \mathscr{H}$ is symmetric. Thus we need to prove $\operatorname{ran}(A+B\pm in) = \mathscr{H}$ for some $n \in \mathbb{N}$.
Let us consider

$$A + B + in = \big(\mathbb{I} + B(A+in)^{-1}\big)(A+in)$$

because $\operatorname{ran}(A+in) = \mathscr{H}$ because of the Lemma (and $A = A^*$).

So it suffices to show that $\operatorname{ran}(\mathbb{I} + B(A+in)^{-1}) = \mathscr{H}$. By the lemma it suffices to verify that

$$\|B(A+in)^{-1}\| < 1.$$

Take $x \in \mathscr{H}$, we have per the assumption of the theorem that

$$\|B\underbrace{(A+in)^{-1}x}_{\in D(A)\subset D(B)}\| \leqslant (1-\varepsilon)\|A(A+in)^{-1}x\| + C_\varepsilon\|(A+in)^{-1}x\|$$

and for all $y \in D(A)$

$$\|(A+in)y\|^2 = \|Ay\|^2 + n^2y^2 \quad \therefore \quad \|(A+in)y\| \geqslant n\|y\|.$$

Choose $y = (A+in)^{-1}x$ for all $x \in \mathscr{H}$

$$\|x\| \geqslant n\|(A+in)^{-1}x\|$$

thus

$$C_\varepsilon\|(A+in)^{-1}x\| \leqslant \frac{C_\varepsilon}{n}\|x\|$$

and therefore

$$\|A(A+in)^{-1}x\| \leqslant \|x\|$$

as for all $a \in \mathbb{R}$, $\left|\frac{a}{a+in}\right| \leqslant 1$. Thus

$$\|B(A+in)^{-1}x\| \leqslant (1-\varepsilon)\|x\| + \frac{C_\varepsilon}{n}\|x\| = \left(1-\varepsilon+\frac{C_\varepsilon}{n}\right)\|x\| < \|x\|$$

for n large enough, hence also $\|B(A+in)^{-1}\| < 1$.

q.e.d.

Chapter 3

Spectrum

Definition 3.1. For an operator $A : D(A) \to \mathscr{H}$. We define the ***Resolvent Set***

$$\rho(A) := \left\{ z \in \mathbb{C} \,\middle|\, (A - z)^{-1} \text{ is bounded} \right\}$$

and the ***Spectrum***

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

□

Example 3.2. If $Au = \lambda u$ for some $u \neq 0$ then $\lambda \in \sigma(A)$. But in general the spectrum is much larger than the set of eigenvalues.

Definition 3.3.

- ***Discrete Spectrum***

$$\sigma_{\text{dis}}(A) := \{\text{Isolated eigenvalues of } A \text{ with finite multiplicity}\}$$

- ***Essential Spectrum***

$$\sigma_{\text{ess}}(A) := \sigma(A) \setminus \sigma_{\text{dis}}(A)$$

□

Theorem 3.4. *$\sigma(A)$ is always a closed set.* □

Proof. We show that $\rho(A)$ is open. Take $z \in \rho(A)$. We prove that if $|z' - z| < \varepsilon$ small enough

$$A - z' = A - z + z - z' = (A - z)(\mathbb{I} + (z - z')(A - z)^{-1}).$$

Since $(A - z)^{-1}$ is bounded, we can conclude that $(A - z')^{-1}$ bounded iff

$$(1 + (z - z')(A - z)^{-1})^{-1}$$

is bounded. This holds because

$$\|(z - z')(A - z)^{-1}\| \leqslant \varepsilon \|(A - z)^{-1}\| < 1$$

if $\varepsilon > 0$ small enough. The conclusion follows from Lemma 2.14. *q.e.d.*

Theorem 3.5 (Self-Adjointness vs. Spectrum)**.** *Let $D(A) \to \mathscr{H}$ be symmetric. Then*

$$A \textit{ is self-adjoint} \iff \sigma(A) \subset \mathbb{R}$$

$\square$

Proof. $(\Rightarrow)$ Assume that A is self-adjoint. Take $z = a + ib$ for $a, b \in \mathbb{R}$ and $b \neq 0$. We prove that $z \in \rho(A)$. Consider

$$A - z = A - a - ib = b\left(\frac{A - a}{b} - i\right).$$

Because A is self-adjoint, $B = \frac{A-a}{b}$ is also self-adjoint and $\operatorname{ran}(B - i) = \mathscr{H}$. Moreover

$$\|(B - i)x\|^2 = \|Bx\|^2 + \|x\|^2 \geqslant \|x\|^2$$

hence $(B - i)^{-1}$ is a bounded operator and $\|(B - i)^{-1}\| \leqslant 1$. Thus $(A - z)^{-1}$ is bounded with

$$\|(A - z)^{-1}\| \leqslant \frac{1}{|b|} = \frac{1}{|\Im z|}.$$

$(\Leftarrow)$ Assume that $\sigma(A) \subset \mathbb{R}$. Then $\pm i \in \rho(A)$ hence $(A \pm i)^{-1}$ is bounded and therefore $\operatorname{ran}(A \pm i) = \mathscr{H}$ hence A is self-adjoint.

q.e.d.

Theorem 3.6 (Semi-Boundedness of Operators & its Spectrum)**.** *Let A be self-adjoint. Then*

$$\inf_{\substack{x\in D(A)\\ \|x\|=1}} \langle x, Ax\rangle = \inf \sigma(A).$$

$\square$

Proof. Assume that $\langle x, Ax\rangle \geqslant E\|x\|^2$ for all $x \in D(A)$. Then we have to prove $\sigma(A) \geqslant E$. This will tell us that

$$\inf_{\substack{x\in D(A)\\ \|x\|=1}} \langle x, Ax\rangle \leqslant \sigma(A).$$

We know that $\sigma(A) \subset \mathbb{R}$. To prove that $\inf \sigma(A) \geqslant E$ we need to show that for all $\varepsilon > 0$

$$E - \varepsilon \in \rho(A).$$

Consider for all $x \in D(A)$ with $\|x\| = 1$

$$\|(A - E + \varepsilon)x\| \geqslant \langle x, (A - E + \varepsilon)x\rangle \geqslant \varepsilon$$

hence $(A - E + \varepsilon)^{-1}$ is bounded and $\|(A - E + \varepsilon)^{-1}\| \leqslant \frac{1}{\varepsilon} < \infty$.
Now we prove that

$$\inf_{\substack{x\in D(A)\\ \|x\|=1}} \langle x, Ax\rangle \geqslant \inf \sigma(A)$$

Assuming that $\inf \sigma(A) \geqslant E$ we shall prove that $A \geqslant E$. Since $E - \varepsilon \in \rho(A)$ for $\varepsilon > 0$ we have

$$f(\varepsilon) = \left\langle x, (A - E + \varepsilon)^{-1}x\right\rangle$$

for some $x \in \mathscr{H}$. We will prove that $f(\varepsilon) \geqslant 0$ for all $\varepsilon > 0$. If this is true, then for all $\varepsilon > 0$

$$(A - E + \varepsilon)^{-1} \geqslant 0 \implies (A - E + \varepsilon) \geqslant 0 \implies A - E \geqslant 0$$

For $\|x\| = 1$, and $\varepsilon > 0$ we have (why?)

$$f'(\varepsilon) = -\left\langle x, (A - E + \varepsilon)^{-2}x\right\rangle = -\|(A - E + \varepsilon)x\|^2 \leqslant -\left\langle x, (A - E + \varepsilon)^{-1}\right\rangle^2 = -f(\varepsilon)^2$$

hence

$$-\frac{f'(\varepsilon)}{f(\varepsilon)^2} = \left(\frac{1}{f(\varepsilon)}\right)' \geqslant 1 \qquad (*)$$

hence for $a > b > 0$

$$\frac{1}{f(a)} - \frac{1}{f(b)} \geqslant a - b \tag{$**$}$$

We assume that $f(b) < 0$ for some $b > 0$. From $(*)$ we have $f' \leqslant 0$ thus f is decreasing and therefore $f(a) \leqslant f(b) < 0$ for $a > b$. From $(**)$

$$\frac{f(b)}{f(a)} - 1 \leqslant (a-b)f(b) \implies 0 < \frac{f(b)}{f(a)} \leqslant 1 + (a-b)f(b)$$

for $a > b$, i.e.

$$0 < 1 + (a-b)f(b)$$

which yields a contradiction for a large. *q.e.d.*

Example 3.7 (Multiplication Operators)**.** Take f to be a measurable function on (Ω, μ). Define A_f on $H = L^2(\Omega, \mu)$ by

$$(A_f u)(x) = f(x)u(x)$$

for $u \in L^2(\Omega, \mu)$. A_f is a self-adjoint operator on

$$D(A_f) := \big\{ u \in L^2 \,\big|\, fu \in L^2 \big\}.$$

Take $z \in \mathbb{C}$. Then

$$\big((A_f - z)^{-1} u\big)(x) = \frac{1}{f(x) - z} u(x)$$

is well-defined if $f(x) \neq z$ for a.e. $x \in \Omega$. Moreover $(A_f - z)^{-1}$ is bounded iff for all $u \in L^2$.

$$\int \left| \frac{1}{f(x) - z} u(x) \right|^2 \mathrm{d}\mu(x) \leqslant C \int |u(x)|^2 \mathrm{d}\mu(x) \iff \frac{1}{|f(x) - z|^2} \leqslant C \quad \text{a.e.}$$

This requires that $z \notin \operatorname{ess\,ran}(f)$, where

$$\operatorname{ess\,ran}(f) = \big\{ z \in \mathbb{C} \,\big|\, \forall \varepsilon > 0 : \mu\big(\big\{ x \in \Omega \,\big|\, |f(x) - z| < \varepsilon \big\}\big) > 0 \big\}$$

Thus $\sigma(A_f) = \operatorname{ess\,ran}(f)$. In particular, if there exists $z \in \mathbb{C}$ such that $\mu(f^{-1}(z)) > 0$ then z is an eigenvalue A_f with the eigenfunction $u(x) = \mathbf{1}_{f^{-1}(z)}(x)$.

Going back to the discrete spectrum and essential spectrum

$$A_f \text{ is self-adjoint } \iff f \text{ is real-valued}$$

with the discrete spectrum being

$$\sigma_{\text{dis}}(A_f) := \left\{\lambda \in \mathbb{R} \,\middle|\, \mu(f^{-1}(\lambda)) > 0 \text{ and the eigenvalue has finite multiplicity}\right\}$$

and the essential spectrum is

$$\begin{aligned}\sigma_{\text{ess}}(A_f) := \big\{\lambda \in \sigma(A) \,\big|\, &\text{eigenvalues with infinite multiplicity or there exists} \\ &(\lambda_n)_n \subset \sigma(A), \lambda_n \neq \lambda, \lambda_n \to \lambda\big\}\end{aligned}$$

Similar things hold true for general self-adjoint operators but we need Spectral theorem for this.

Chapter 4

Spectral Theorem

Remark 4.1 (Motivation: Functional Calculus)**.** For an operator A we want to define $f(A)$, where f is a given function. In the case, $f(t) = t^2$, $f(A) = A^2$, but in general $f(A)$ is not trivial! If $A : D(A) \to \mathscr{H}$, then $A^2 : D(A^2) \to \mathscr{H}$ but it is not obvious that $D(A^2)$ is dense. $\square$

Theorem 4.2 (Spectral Theorem for Unbounded Self-Adjoint Operators)**.** *Let $A : D(A) \to \mathscr{H}$ be self-adjoint operator. Then there exists a Borel subset $\Omega \subset \mathbb{R}^n$ for some $d \in \mathbb{N}$, a Borel measure μ on Ω which is locally bounded, and a function $a : \Omega \to \mathbb{R}$ which is locally bounded an μ-measurable, such that*

$$UAU^* = M_a$$

where M_a is the multiplication operator associated with a, i.e.

$$D(M_a) = \left\{ u \in L^2 \,\middle|\, au \in L^2 \right\}$$

and $M_a(u)(x) = a(x)u(x)$.
Here U is a unitary transformation $L^2(\Omega, \mu) \to \mathscr{H}$ and $UD(M_a) = D(A)$.
In fact, we can choose $\Omega = \sigma(A) \times \mathbb{N} \subset \mathbb{R}^2$ and $a(\lambda, n) = \lambda$. $\square$

Remark 4.3.

- Cauchy 1826 (matrices), Stone, von Neumann 1930s (motivated by QM)

- For $A = -\Delta$ in $\mathscr{H} = L^2\big(\mathbb{R}^d\big)$. Under the Fourier transform we have

$$\widehat{Af}(k) = |k|^2 \hat{f}(k)$$

Thus A is self adjoint on the space

$$D(A) = H^2(\mathbb{R}^d) = \left\{ f \in L^2 \,\middle|\, |k|^2 \hat{f}(k) \in L^2 \right\}$$

- For a compact operator

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

with $\sigma(A) = \left(\lambda_n\right)_n \subset \mathbb{R}$ and $\left(u_n\right)_n \subset \mathscr{H}$ ONB. Then

$$a(\lambda, n) = \lambda, \qquad \mu(\lambda, n) = \begin{cases} 0, & \text{if } \lambda \notin \sigma(A) \\ \text{multiplicity of } \lambda, & \text{if } \lambda \in \sigma(A) \end{cases}$$

□

Theorem 4.4 (Spectral Theorem, Functional Calculus Form)**.** *Let $A : D(A) \to \mathscr{H}$ be self-adjoint. Then there exists a unique linear map*

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

where $B(\mathbb{R}, \mathbb{C})$ are the bounded Borel (measurable) functions on $\mathbb{R}$ and $B(\mathscr{H})$ such that

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

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

3) $\|f(A)\| = \|f\|_{L^\infty(\sigma(A))}$

4) $f(A) = 0$ iff f is supported outside of $\sigma(A)$.

5) $\sigma(f(A)) = f(\sigma(A))$. Consequently if $f \geqslant 0$ then $f(A) \geqslant 0$.

6) If $f_n \uparrow f$ then $\|f_n(A)u - f(A)u\| \to 0$.

$\square$

Theorem 4.5 (Spectral Theorem, Projection-Valued Form)**.** *Let $A : D(A) \to \mathscr{H}$ be self-adjoint. Then there exist a unique family of projection valued measures P_A such that*

$$A = \int\limits_{\sigma(A)} \lambda \mathrm{d}P_A(\lambda)$$

Here P is a family of projection-valued measures if

- $P(\Omega) = P(\Omega)^2$
- $P(\mathbb{R}) = P(\sigma(A)) = 1$
- *If $\Omega = \bigcup_{n=1}^{\infty} \Omega_n$ where Ω_n are disjoint, then*

$$\left\| \sum_{n=1}^{N} P(\Omega_n)u - P(\Omega)u \right\| \xrightarrow{n\to\infty} 0.$$

$\square$

Remark 4.6 (Explanation)**.** Assume the "multiplication version". Thus we may assume that $A = M_a$ on $L^2(\Omega, \mu)$. Then we can define the functional calculus via

$$f(A) := M_{f(a)}.$$

And for the "projection-valued measure version"

$$P_A(B) := \mathbf{1}_B(A)$$
$$\int\limits_{\sigma(A)} \lambda \mathrm{d}P_A(\lambda).$$

$\square$

Our strategy will be to prove the theorem first for bounded operators, then for unbounded operators (whose resolvent is bounded), e.g. $A \geqslant 1 \rightsquigarrow A^{-1}$ is bounded, if A is not bounded from below then $(A \pm i)^{-1}$ is bounded.

4.1 Step 1 (Continuous Functional Calculus for Bounded Self-Adjoint Operators)

Theorem 4.7. *Let $A = A^*$ be bounded. Then there exists a unique linear mapping*

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

such that

- *if $f(t) = \sum_{j=0}^{n} = \alpha_j t^j$ is a polynomial then $f(A) = \sum_{j=1}^{n} \alpha_j A^j$*
- $f(A)g(A) = (fg)(A)$
- $\|f(A)\| = \|f\|_\infty$.

□

Proof. We define $f(A) = \sum \alpha_j A^j$ if f is a polynomial. Now we want to extend this definition to $\mathscr{C}(\mathbb{R})$. Since A is bounded, $\sigma(A)$ is a compact set, so $\mathscr{C}(\mathbb{R})$ can be reduced to $\mathscr{C}(\sigma(A))$. Now we prove that if f is a polynomial, then

$$\sigma(f(A)) = f(\sigma(A))$$

For every $\lambda \in \mathbb{C}$ we can write

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

then

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

and

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

Further we have

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

Now we have defined an operator $\mathscr{L}$ from the set of polynomials into the bounded operators which satisfies

$$\begin{aligned}
\mathscr{L}(f)\mathscr{L}(g) &= f(A)g(A) = (fg)(A) = \mathscr{L}(fg) \\
\|\mathscr{L}(f)\| &= \|f(A)\| = \|f\|_\infty
\end{aligned}$$

This means that $\mathscr{L}$ is an isometry of a dense subset the C^*-algebra $\mathscr{C}(\sigma(A))$. Thus by continuity we can extend it to the whole space.

q.e.d.

4.2 Step 2 (Spectral Measure for Bounded Self-Adjoint Operators)

Theorem 4.8. *Let $A = A^*$ be bounded in $\mathscr{H}$. For every $v \in \mathscr{H}$, there exists a unique Borel measure μ_v on $\sigma(A)$ such that*

$$\langle v, f(A)v\rangle = \int f(t)\mathrm{d}\mu_v(t)$$

for every function $f \in \mathscr{C}(\sigma(A))$. □

Proof. Using the linear map $\mathscr{L}$ from the previous section we can define

$$\varphi : \begin{aligned} \mathscr{C}(\sigma(A)) &\longrightarrow \mathbb{R} \\ f &\longmapsto \varphi(f) = \langle v, f(A)v \rangle \end{aligned}$$

Then φ is linear and it is positive, i.e. $f \geqslant 0$ implies that $\varphi(f) \geqslant 0$. Indeed, if $f \geqslant 0$ then $f = g^2$ hence

$$\varphi(f) = \left\langle v, g^2(A)v \right\rangle = \left\langle v, (g(A))^2 v \right\rangle = \|g(A)v\|^2 \geqslant 0$$

We can apply the Riesz-Markov theorem for functionals on the continuous functions which gives us a unique measure μ_v such that

$$\varphi(f) = \int\limits_{\sigma(A)} f(t) \mathrm{d}\mu(t)$$

for all $f \in \mathscr{C}(\sigma(A))$ *q.e.d.*

4.3 Step 3 (Spectral Theorem for Bounded Self-Adjoint Operators)

Observe that for $f \in \mathscr{C}(\sigma(A))$

$$\|f(A)v\|^2 = \langle v, f(A)^* f(A)v \rangle = \int\limits_{\sigma(A)} \overline{f(t)} f(t) \mathrm{d}\mu(t) = \|f\|^2_{L^2(\sigma(A))}$$

hence our mapping $f \mapsto f(A)v$ is isometric and therefore we may extend it to all of $L^2(\sigma(A), \mu)$ as the continuous functions are dense, i.e. we may define

$$U : \begin{aligned} L^2(\sigma(A), \mu_v) &\longrightarrow \mathscr{H}_v \subset \mathscr{H} \\ f &\longmapsto f(A)v \end{aligned}$$

If $\mathscr{H}_v := \left\{ f(A)v \,\middle|\, f \in L^2(\sigma(A), \mu_v) \right\} = \mathscr{H}$ then we are done, because we now have

$$\langle v, f(A)v \rangle = \int\limits_{\sigma(A)} f(t) \mathrm{d}\mu_v(t)$$

for all $f \in L^2(\sigma(A), \mu_v)$. We can define $\mu = \mu_v$. But in general $\mathscr{H}_v \subsetneq \mathscr{H}$.

Lemma 4.9. *There exists a family $(v_n)_n$ (at most countable) such that*

$$\mathscr{H} = \bigoplus_{n=1}^{\infty} H_{v_n}$$

and $\{H_{v_n}\}$ orthogonal. □

Proof. Noting that $A : H_v \to H_v$ one can either use induction or Zorn's Lemma. Consider the set of $I = (v_i)_i$ such that

$$H_I = \bigoplus_i H_{v_i}$$

with H_{v_i} being orthogonal. Then Zorn's lemma provides us with an I such that X_I is maximal w.r.t. "$\subset$". Thus $H_I = \mathscr{H}$, because if $H_I \subsetneq \mathscr{H}$, then $H_I^\perp \neq \{0\}$ and since A is self-adjoint $A : H_{V_I} \to H_{V_I}$, $A : H_I^\perp \to H_I^\perp$ thus there exists $v_0 \in H_I^\perp$ such that $H_{V_0} \subset H_I^\perp$. Then $I' := I \cup \{v_0\}$ has $H_I' = H_I \oplus H_{v_0} \supsetneq H_I$ which is a contradiction. *q.e.d.*

Proposition 4.10. *Then*

$$U^{-1}AU : \begin{array}{c} L^2(\sigma(A), \mu_v) \longrightarrow L^2(\sigma(A), \mu_v) \\ f(x) \longmapsto xf(x) \end{array}$$

□

Proof. We check that $A : H_v \to H_v$

$$U^{-1}AUf = U^{-1}Af(A)v = U^{-1}g(A)v$$

Here if $f \in L^2$, then $g = xf(x) \in L^2$ because $\sigma(A)$ is bonded and

$$\mu_v(\sigma(A)) = \int 1 \mathrm{d}\mu_v(x) = \mathscr{L}(1) = \|v\|^2 < \infty$$

Here $A : H_v \to H_v$ because if $f(A)v \in H_v$ then

$$Af(A) = g(A)v \in H_v.$$

q.e.d.

Remark 4.11. If $H_v = \mathscr{H}$, then v is called ***cyclical***. □

To conclude the proof. Let $\mathscr{H} = \bigoplus_i H_{v_i}$ with $A : H_{v_i} \to H_{v_i}$.
So we can write $A = \bigoplus_{i\in I} A_i$, $A_i := A\big|_{H_{v_i}}$. Now for every $i \in I$ there exists a μ_{v_i} on $\sigma(A)$ such that there exists an isometry $U : L^2(\sigma(A), \mu_{v_i}) \to H_{v_i}$ and

$$U_i^{-1} A_i U_i = M_x \quad \text{on } L^2(\sigma(A), \mu_{v_i})$$

Now define $\Omega = \sigma(A) \times \mathbb{N}$ and μ onΩ, via

$$\mu(B, n) = \mu_{v_n}(B)$$

for some Borel set B and $n \in \mathbb{N}$. Then we can define $U : L^2(\Omega, \mu) \to \mathscr{H}$ by $U = \bigoplus_i U_i$ where $L^2(\Omega, \mu) = \bigoplus_i L^2(\sigma(A), \mu_{v_i})$. Then $U^{-1}AU = M_a$ on $L^2(\Omega, \mu)$ with $a(\lambda, n) = \lambda$.

4.4 Step 4 (Spectral Theorem for Unbounded Self-Adjoint Operators)

Let $A : D(A) \to \mathscr{H}$ be self-adjoint. Then $\operatorname{ran}(A \pm i) = \mathscr{H}$ and $(A \pm i)^{-1}$ is bounded.

Lemma 4.12. $S = (A + i)^{-1}$. *Then* $S^* = (A - i)^{-1}$ *and* $S^*S = SS^*$ *(i.e.* S *is normal).* □

Proof. Let $x_1 := Sx = (A + i)^{-1}x \in D(A)$ and $y_1 := (A - i)^{-1}y \in D(A)$, then

$$\langle Sx, y\rangle = \langle x_1, (A - i)y_1\rangle = \langle (A - i)x_1, y_1\rangle = \langle (A - i)x_1, y_1\rangle = \langle x, y_1\rangle = \left\langle x, (A - i)^{-1}y\right\rangle.$$

q.e.d.

Now define $B_1 := \frac{1}{2}(S + S^*)$, $B_2 := \frac{1}{2i}(S - S^*)$, then

$$B_1^* = \frac{S^* + S}{2} = B_1, \qquad B_2^* = -\frac{S^* - S}{2i} = B_2$$

So $S = B_1 + iB_2$ with B_1 and B_2 being self-adjoint and bounded, and $B_1B_2 = B_2B_1$.

By the spectral theorem for bounded (normal) operators, there exists a unitary $U : L^2(\sigma(S), \mu) \to \mathscr{H}$ and a function $f \in L^2$ such that

$$U^{-1}SU = M_f \quad \text{on } L^2(\sigma(S), \mu)$$

We want to prove that $U^{-1}AU = M_g$. What is g? Since $S = (A+i)^{-1}$ we might guess that $g = \frac{1}{f} - i$.

To prove that g is well-defined, we have to check that $f \neq 0$ a.e. Assume that $f = 0$ on a set $\mathcal{O}$ with $\mu(O) > 0$. Then $0 \not\equiv \mathbf{1}_O \in \ker(M_f)$ and since $U^{-1}SU = M_f$ it follows that $\ker S \neq \{0\}$ which is a contradiction. Since $Sx = 0$ implies

$$\forall y \in \mathscr{H} : \langle Sx, y\rangle = 0 \quad \therefore \quad \langle x, S^* y\rangle = 0 \quad \therefore \quad \forall z \in D(A)\, \langle x, z\rangle = 0$$

since $S^* : \mathscr{H} :\to D(A)$, hence $x = 0$.

Thus $f \neq 0$ a.e. and therefore we can define $g = \frac{1}{f} - i$. Consider $M_{(g+i)^{-1}} = M_f = U^{-1}SU$, then

$$M_{g+i} = \left(M_{(g+i)^{-1}}\right)^{-1} = (U^{-1}SU)^{-1} = U^{-1}S^{-1}U = U^{-1}(A+i)U \quad \therefore \quad M_g = U^{-1}AU$$

We also have $D(M_g) = U^{-1}(D(A))$ (which is easy to check).

4.5 Applications of the Spectral Theorem

4.5.1 Schrödinger Equation

Given $A : D(A) \to \mathscr{H}$ self-adjoint then we are interested in the solutions of

$$\begin{aligned} i\partial_t \psi(t) &= A\psi(t), \qquad \text{for } t \in \mathbb{R} \\ \psi(0) &= \psi_0 \end{aligned}$$

Theorem 4.13. *For all $\psi_0 \in \mathscr{H}$, then there exists a unique solution to the Schrödinger equation*

$$\psi(t) = e^{-itA}\psi_0$$

for all $t \in \mathbb{R}$ with e^{-itA} being bounded and unitary. □

Proof. By the spectral theorem, up to a unitary transformation we have $\mathscr{H} = L^2(\Omega, \mu)$ and $A = M_a$. Then the equation becomes

$$\begin{aligned} i\partial_t \psi(t) &= a(x)\psi(t,x), \qquad \text{for } t \in \mathbb{R} \\ \psi(0,x) &= \psi_0(x) \end{aligned}$$

and this has the unique solution

$$\psi(t,x) = e^{-ita(x)}\psi_0(x)$$

q.e.d.

4.5.2 Spectrum of Self-Adjoint Operators

Let $A : D(A) \to \mathscr{H}$ be self-adjoint. Then

$$\begin{aligned} \sigma(A) &= \left\{\lambda \in \mathbb{C} \,\middle|\, (A-\lambda)^{-1} \text{ is not bounded}\right\} \\ \sigma_{\text{disc}}(A) &= \left\{\lambda \in \sigma(A) \,\middle|\, H_\lambda = \left\{u \,\middle|\, Au = \lambda u\right\} = \ker(A-\lambda) \neq \{0\} \text{ and } \dim H_\lambda < \infty\right\} \end{aligned}$$

Theorem 4.14. *If λ is an isolated point in $\sigma(A)$, then λ is an eigenvalue of $\sigma(A)$, i.e. there exists an $\varepsilon > 0$ such that $(\lambda - \varepsilon, \lambda + \varepsilon) \cap \sigma(A) = \{\lambda\}$.* □

Proof. By the spectral theorem $H = L^2(\Omega, \mu)$ and $A = M_a$. Then $\sigma(A) = \sigma(M_a) = \operatorname{ess\,ran}(a)$ and λ is an isolated point of $\sigma(A)$ iff λ is an isolated point of $\operatorname{ess\,ran}(a)$. Recall that $\lambda \in \operatorname{ess\,ran}(a)$ iff for every $\varepsilon > 0$

$$\mu(a^{-1}(\lambda - \varepsilon, \lambda + \varepsilon)) > 0$$

When $\varepsilon > 0$ is small enough then $a^{-1}(\lambda - \varepsilon, \lambda + \varepsilon) = a^{-1}(\lambda)$ per the assumption, i.e.

$$\mu(a^{-1}(\lambda)) > 0$$

Then define $f := \mathbf{1}_{a^{-1}(\lambda)} \in L^2(\Omega, \mu)$. Then $f \neq 0$ and $af = \lambda f$ thus f is an eigenvalue of M_a. *q.e.d.*

4.5.3 Another Proof of $\min - \max$-Principle

Let $A : D(A) \to \mathscr{H}$ be self-adjoint and bounded from below then

$$\mu_n(A) = \inf_{\substack{M \subset D(A) \\ \dim M = n}} \max_{\substack{u \in M \\ \|u\|=1}} \langle u, Au \rangle .$$

The Min-Max-principle asserts that if $\mu_n < \mu_\infty = \lim_{k\to\infty} \mu_k$, then μ_n is an eigenvalue.

Let us prove that $\mu_1 = \mu_2 = \cdots = \mu_k < \mu_{k+1}$, then $\mu_1 = \cdots = \mu_k$ are eigenvalues. We know that $\mu_1 = \inf \sigma(A)$ (exercise!).

There are two possiblities

- If μ_1 is an isolated point of $\sigma(A)$ or $a^{-1}(\mu_1)$ has positive measure then μ_1 is an eigenvalue.

- If μ_1 is not an isolated point and has zero measure then for for all $\varepsilon > 0$

  $$(\mu_1 - \varepsilon, \mu_2 + \varepsilon) \cap \sigma(A) \supsetneq \{\mu_1\}$$

  Up to a unitary transformation we may assume that $\mathscr{H} = L^2(\Omega, \mu)$, $A = M_a$. We know that for every $\varepsilon > 0$

  $$\mu(a^{-1}(\mu_1 - \varepsilon, \mu_1 + \varepsilon)) > 0$$

  This means that we can find a sequence $\varepsilon_n \downarrow 0$ such that

  $$\mu\big(a^{-1}([\mu_1 + \varepsilon_{n+1}, \mu_1 + \varepsilon_n])\big) > 0$$

  This is obtained by induction and the fact that μ_1 is not an isolated point and

  $$\lim_{\varepsilon \downarrow 0} \mu\big(a^{-1}(\mu_1 - \varepsilon, \mu_1 + \varepsilon)\big) = \mu\big(a^{-1}(\{\mu_1\})\big) = 0$$

  Define $f_n = \mathbf{1}_{a^{-1}([\mu_1+\varepsilon_{n+1}, \mu_1+\varepsilon_n])}$. Then for all $n \in \mathbb{N}$

  $$\frac{\langle f_n, Af_n \rangle}{\|f_n\|} = \frac{\int a|f_n|^2}{\int |f_n|^2} \leqslant \mu_1 + \varepsilon_n$$

Observe that $f_n \perp f_m$ if $n \neq m$. Thus for $M_n := \operatorname{span}(f_n, \dots, f_{2n-1})$. Then

$$\mu_n \leqslant \sup_{\substack{u \in M_n \\ \|u\|=1}} \langle u, Au \rangle \leqslant \mu_1 + \varepsilon_n$$

and therefore $\mu_\infty \leqslant \mu_1$ which is a contradiction.

4.5.4 Weyl's Criterion

Theorem 4.15 (Weyl's Criterion)**.** *Let $A : D(A) \to \mathscr{H}$ be self-adjoint. Then*

- *$\lambda \in \sigma(A)$ iff there exists a Weyl sequence $(x_n)_n \subset D(A)$ such that $\|x_n\| = 1$, $\|(A - \lambda)x_n\| \xrightarrow{n\to\infty} 0$*
- *$\lambda \in \sigma_{ess}(A)$ iff there exits a Weyl sequence $(x_n)_n \subset D(A)$ such that $\|x_n\| = 1$, $\|(A - \lambda)x_n\| \to 0$ as $x_n \rightharpoonup 0$ iff $(x_n)_n$ is an ONF.*
- *$\lambda \in \sigma_{dis}(A)$ iff $\lambda \in \sigma(A)$ but for all $\|x_n\| = 1$, $\|(A - \lambda)x_n\| \to 0$ there exists a subsequence $x_{n_k} \to x_\infty$ strongly and $x_\infty \in D(A)$, $Ax_\infty = \lambda x_\infty$.*

□

Proof. (i) By the spectral theorem we may assume that $\mathscr{H} = L^2(\Omega, \mu)$ and $A = M_a$. Then let us assume

$$\lambda \in \sigma(A) = \sigma(M_a) = \operatorname{ess\,ran} a \iff \forall \varepsilon > 0 : \mu\big(a^{-1}(\lambda - \varepsilon, \lambda + \varepsilon)\big) > 0$$

For a sequence $\varepsilon_n \downarrow 0$ define $f_n := \mathbf{1}_{a^{-1}(\lambda-\varepsilon_n,\lambda+\varepsilon_n)} \neq 0$ and $x_n := \frac{f_n}{\|f_n\|}$. Then

$$\|(A - \lambda)x_n\| = \left\|(a - \lambda)\frac{f_n}{\|f_n\|}\right\| \leqslant \varepsilon_n \xrightarrow{n\to\infty} 0$$

because $|(a - \lambda)f_n| \leqslant \varepsilon_n |f_n|$ pointwise.

Conversely, assume that there exists a Weyl sequence, $(x_n)_n \subset D(A)$, $\|x_n\| = 1$ and $\|(A - \lambda)x_n\| \to 0$.

We shall prove $(A - \lambda)^{-1}$ is not bounded by contradiction, i.e. assume that $(A - \lambda)^{-1}$ is bounded. Then $1 = \|x_n\| = \|(A - \lambda)^{-1}(A - \lambda)x_n\| \leqslant \|(A - \lambda)^{-1}\|\|(A - \lambda)x_n\| \to 0$.

(ii) Assume that $\lambda \in \sigma_{\text{ess}}(A)$. Then for all $\varepsilon > 0$

$$\mu(a^{-1}(\lambda - \varepsilon, \lambda + \varepsilon)) > 0.$$

Let us consider $\mu(a^{-1}(\lambda))$.

- If $\mu(a^{-1}(\lambda)) > 0$ then λ is an eigenvalue of A with eigenfunction $\sim \mathbf{1}_{a^{-1}(\lambda)}$.
- If λ has infinite multiplicity, $\dim(\ker(A - \lambda)) = \infty$, then we can choose $(x_n)_n$ ONB for $\ker(A - \lambda)$ and $(A - \lambda)x_n = 0$ for all $n \in \mathbb{N}$.
- If λ has finite multiplicity, then it is ***not*** an isolated point of $\sigma(A)$, then we can define $\Omega_n = a^{-1}(\lambda - \varepsilon_n, \lambda + \varepsilon_n)$ for $\varepsilon_n \downarrow 0$ and (by going to be a subsequence if necessary), $\mu(\Omega_n \setminus \Omega_{n+1}) > 0$ for all $n \in \mathbb{N}$.

  Define $f_n := \mathbf{1}_{\Omega_n \setminus \Omega_{n+1}}$ and $x_n = \frac{f_n}{\|f_n\|}$. We have

  $$\|(A - \lambda)x_n\| \leqslant \varepsilon_n \xrightarrow{n \to \infty} 0$$

  similarly to (i) and $(x_n)_n$ is an ONF because $\Omega_n \setminus \Omega_{n+1}$ and $\Omega_m \setminus \Omega_{m+1}$ are disjoint if $n \neq m$.
- If $\mu(a^{-1}(\lambda)) = 0$, then $\bigcap \Omega_n = a^{-1}(\lambda)$ and therefore

  $$\lim_{n \to \infty} \mu(\Omega_n) = \mu(a^{-1}(\lambda)) = 0$$

  Thus up to a subsequence we can assume that $\mu(\Omega_n \setminus \Omega_{n+1}) > 0$ for all $n \in \mathbb{N}$ and proceed similarly.

In summary we proved that if $\lambda \in \sigma_{\text{ess}}(A)$, then there exists an ONF $(x_n)_n$ in $D(A)$ such that $\|x_n\| = 1$, $\|(A - \lambda)x_n\| \to 0$. Then in particular $x_n \rightharpoonup 0$ weakly.

It remains to prove that if there exists a Weyl sequence $(x_n)_n$, $x_n \rightharpoonup 0$ weakly, then $\lambda \in \sigma_{\text{ess}}(A)$.

To do this assume (iii) for the moment. Since λ has a Weyl sequence, by (i) $\lambda \in \sigma(A)$. We check that $\lambda \notin \sigma_{\text{dis}}(A)$. Assume that $\lambda \in \sigma_{\text{dis}}(A)$. By (iii), there exists a subsequence x_{n_k} that converges strongly in $\mathscr{H}$, but this is impossible as $x_n \rightharpoonup 0$ weakly.

(iii) Assume that $\lambda \in \sigma_{\text{dis}}(A)$, i.e. λ is an isolated eigenvalue with $\dim(\ker(A - \lambda)) < \infty$. Because λ is an isolated point of $\sigma(A)$ there exists an $\varepsilon > 0$ such that $|t - \lambda| > \varepsilon$ for all $t \in \sigma(A) \setminus \{\lambda\}$.

Thus $\|(A-\lambda)u\| \geqslant \varepsilon\|u\|$ for all $u \in \ker(A-\lambda)^\perp$. Now take a Weyl sequence (x_n). We may decompose it as $x_n = Px_n + P^\perp x_n$, where P is the projection onto $\ker(A-\lambda)$ and $P^\perp = \mathbf{1} - P$. Then

$$\|(A-\lambda)x_n\| = \|\underbrace{(A-\lambda)Px_n}_{=0} + (A-\lambda)P^\perp x_n\| \geqslant \varepsilon\|P^\perp x_n\| \quad \therefore \quad P^\perp x_n \xrightarrow{n\to\infty} 0 \quad \therefore$$

$$\therefore \quad \|x_n - Px_n\| \xrightarrow{n\to\infty} 0$$

Since P is a projection onto a finite-dimensional space it is compact. Thus Px_n is pre-compact, i.e. we can go to a subsequence and assume that $Px_n \to x_\infty$ strongly. $x_n \to x_\infty$ and

$$Ax_n = (A-\lambda)x_n + \lambda x_n \xrightarrow{n\to\infty} \lambda x_\infty$$

Since A is closed, $x_\infty \in D(A)$, $Ax_\infty = \lambda x_\infty$.

Conversely, assume that every Weyl sequence there exists a subsequence such that $x_n \to x_\infty \in D(A)$. We have to prove that $\lambda \in \sigma_{\text{dis}}(A)$. If $\lambda \in \sigma_{\text{ess}}(A)$, then by (ii) there exists a Weyl sequence $(x_n)_n$ such that $x_n \rightharpoonup 0$ weakly. But then x_n cannot converge strongly.

q.e.d.

From the proof we get

Lemma 4.16 (Spectral Gap). *If λ is an isolated point of $\sigma(A)$, then there exists $\varepsilon > 0$ such that for all $u \in \ker(A-\lambda)^\perp$*

$$\|(A-\lambda)u\| \geqslant \varepsilon\|u\|$$

This holds even if λ has infinite multiplicity. □

4.5.5 Weyl Theory

A corollary to Theorem 2.12 which we can now prove is

Lemma 4.17. *Let $A : D(A) \to \mathscr{H}$ be self-adjoint, B be a compact self-adjoint operator.*

Then $A+B$ is self-adjoint (by Theorem 2.12) and

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

□

Proof. Assume that $\lambda \in \sigma_{\text{ess}}(A)$. Then there exists a Weyl sequence $(x_n)_n \subset D(A)$, $\|x_n\| = 1$, $\|(A-\lambda)x_n\| \to 0$ and $x_n \rightharpoonup 0$. Then x_n is also a Weyl sequence for $A+B$ because $Bx_n \to 0$ strongly as B is compact. *q.e.d.*

Definition 4.18. $A : D(A) \to \mathscr{H}$ be self-adjoint. $B : D(B) \to \mathscr{H}$ symmetric and $D(A) \subset D(B)$.
Then we call B "***A-compact***" (relatively compact w.r.t. A) if $B(A+i)^{-1}$ is a compact operator. □

Remark 4.19. If we know that $A \geqslant 1$, then B is A-compact iff BA^{-1} is compact.

Proof. If B is A-compact, then

$$BA^{-1} = \underbrace{B(A+i)^{-1}}_{\text{compact}}\underbrace{(A+i)A^{-1}}_{\text{bounded}}$$

where the last follows from the inequality $\left|\frac{a+i}{a}\right| = \frac{\sqrt{a^2+1}}{a^2} \leqslant \sqrt{2}$ if $a \geqslant 1$. Thus BA^{-1} is compact as the compact operators are a double-sided ideal. Conversely, if BA^{-1} is compact then

$$B(A+i)^{-1} = \underbrace{BA^{-1}}_{\text{compact}}\underbrace{A(A+i)^{-1}}_{\text{bounded}}.$$

□

□

Lemma 4.20. *Assume that B is A-compact. Then for all $\varepsilon > 0$ there exists $C_\varepsilon > 0$ such that for all $x \in D(A)$*

$$\|Bx\| \leqslant \varepsilon\|Ax\| + C_\varepsilon\|x\|.$$

□

Proof. Assume that $B(A+in)^{-1}$ as in the proof of Theorem 2.12. We have for all $x \in \mathscr{H}$

$$\|B(A+in)^{-1}x\| = \|\underbrace{B(A+i)^{-1}}_{\text{compact}}\underbrace{(A+i)(A+in)^{-1}}_{\text{bounded}}x\| \leqslant \varepsilon_n\|x\|.$$

with $\varepsilon_n \downarrow 0$ (exercise).

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

$$\|Bx\| = \|B(A+in)^{-1}(A+in)x\| \leqslant \varepsilon_n\|(A+in)x\| \leqslant \varepsilon\sqrt{\|Ax\|^2+n^2\|x\|^2} \leqslant$$
$$\leqslant \varepsilon_n\|Ax\| + (\varepsilon_n n)\|x\|.$$

q.e.d.

Theorem 4.21 (Weyl)**.** *If B is A-compact, then*

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

□

Proof. Let $\lambda \in \sigma_{\mathrm{ess}}(A)$, then there exists a Weyl sequence $(x_n)_n \subset D(A)$, $\|x_n\| = 1$, such that $\|(A-\lambda)x_n\| \to 0$ and $x_n \rightharpoonup 0$.

Then we prove that x_n is also a Weyl sequence for $A+B$, i.e. $Bx_n \to 0$. To see this note that

$$1 = \frac{A+i}{A+i} = \frac{A-\lambda}{A+i} + \frac{\lambda+i}{A+i} = (A+i)^{-1}(A-\lambda+\lambda+i)$$

then

$$Bx_n = \underbrace{B(A+i)^{-1}}_{\text{compact}}\Big(\underbrace{(A-\lambda)x_n}_{\to 0} + \underbrace{(\lambda+i)x_n}_{\rightharpoonup 0}\Big) \xrightarrow{n\to\infty} 0.$$

q.e.d.

Remark 4.22 (Spectral Theorem)**.** 1) Multiplication $U^{-1}AU = M_a$ on $L^2(\Omega,\mu)$.

2) Functional Calculus: $f(A)$ can be defined such that

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

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

Multiplication is useful to study the spectrum of one operator. However, if A, B are self-adjoint operators (that might not even commute), then the multiplication version is not useful to study $A + B$, as $U_A \neq U_B$.

We may use the functional calculus. If A and B commute, then $f(A)$ and $g(B)$ commute. When f, g are polynomials this is obvious and may be generalised $\square$

Chapter 5

Free Schrödinger Operator $-\Delta$

Theorem 5.1. *Define $A = -\Delta$ on $\mathscr{C}_c^\infty\big(\mathbb{R}^d\big)$. Then there exists a self-adjoint extension of A to the Sobolev space*

$$D(A) = H^2(\mathbb{R}^d) = \left\{f \in L^2(\mathbb{R}^d) \,\middle|\, \forall |\alpha| \leqslant 2 : D^\alpha f \in L^2\right\} = \left\{f \in L^2(\mathbb{R}^d) \,\middle|\, |k|^2 \hat{f}(k) \in L^2\right\}$$

In fact for all $u \in D(A)$

$$\overline{Au}(k) = 4\pi^2 |k|^2 \hat{u}(k).$$

□

Definition 5.2 (Fourier Transform)**.** For $f, g \in L^1(\mathbb{R}^d)$, define

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

$$\check{g}(k) = \int\limits_{\mathbb{R}^d} g(x) e^{2\pi i k\cdot x} \mathrm{d}x$$

□

Theorem 5.3.

- *For all $f \in L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$*

$$\|\hat{f}\|_{L^2} = \|f\|_{L^2}. \qquad \text{(Placherl Identity)}$$

This allows one to extend the Fourier transform to an isometry in $L^2(\mathbb{R}^d)$.

- *Inverse Fourier transform@*

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

- *Duality*

$$\left\langle \hat{f}, \hat{g} \right\rangle_{L^2} = \langle f, g \rangle_{L^2}$$

□

Definition 5.4. For $\alpha = (\alpha_1, \dots, \alpha_d) \in \mathbb{N}^d$ and $k \in \mathbb{R}^d$ we define

$$(D^\alpha u)(x) = \left(\partial_{x_1}^{\alpha_1} \cdots \partial_{x_n}^{\alpha_n} u\right)(x)$$
$$(ck)^\alpha = c^|\alpha| \prod_{j=1}^{d} k_j^{\alpha_j}, \quad |\alpha| = \sum_{j=1}^{d} \alpha_j$$

□

Theorem 5.5. *If $f \in \mathscr{C}_c^\infty\left(\mathbb{R}^d\right)$, then for all $\alpha \in \mathbb{N}^d$*

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

□

Proof.

$$\begin{aligned}
\overline{\partial_{x_i} f}(k) &= \int\limits_{\mathbb{R}^d} \partial_{x_j} f(x) e^{-2\pi i k\cdot x} \mathrm{d}x = \\
&= -\int\limits_{\mathbb{R}^d} f(x) \partial_{x_j} e^{-2\pi i k\cdot x} \mathrm{d}x = \\
&= (2\pi i k_j) \int\limits_{\mathbb{R}^d} f(x) e^{-2\pi i k\cdot x} \mathrm{d}x = (2\pi i k_j) \hat{f}(k)
\end{aligned}$$

q.e.d.

Proof of Theorem 5.1. Let $u \in \mathscr{C}_c^\infty(\mathbb{R}^d)$. Denote $\mathscr{F} u = \hat{u}$ then

$$\mathscr{F}(Au)(k) = \widehat{-\Delta u}(k) = -(2\pi i k)^2 \hat{u}(k) = 4\pi^2 |k|^2 \hat{u}(k)$$

Since $\mathscr{F} : L^2 \to L^2$ is a unitary transformation we see that

$$\mathscr{F} A \mathscr{F}^{-1} = M_{4\pi^2|k|^2}.$$

Here $M_{4\pi^2|k|^2}$ can be extended to a self-adjoint operator on

$$D(M_{4\pi^2|k|^2}) = \left\{ g \in L^2 \,\middle|\, 4\pi^2|k|^2 g \in L^2 \right\}$$

A can thus be extended to a self-adjoint operator on

$$D(A) = \left\{ f \in L^2 \,\middle|\, 4\pi|k|^2 \hat{f} \in L^2 \right\} =: H^2(\mathbb{R}^d)$$

q.e.d.

Remark 5.6. $A = -\Delta$ in $D(A) = H^2\big(\mathbb{R}^d\big)$ is the Friedrich's extension of A defined on $\mathscr{C}_c^\infty(\mathbb{R}^d)$. $\square$

Definition 5.7 (Sobolev Spaces)**.**

$$H^s(\mathbb{R}^d) := \left\{ f \in L^2(\mathbb{R}^d) \,\middle|\, |k|^s \hat{f}(k) \in L^2(\mathbb{R}^d) \right\}$$

This is a Hilbert space with the inner product

$$\langle f, g \rangle_{H^s} = \int\limits_{\mathbb{R}^d} \overline{\hat{f}(k)} \hat{g}(k) (1 + |2\pi k|^2)^s \mathrm{d}k$$

$\square$

Definition 5.8 (Weak Derivative)**.** If $f \in L^1_{\mathrm{loc}}$, i.e. $f \in L^1(K)$ for all $K \subset \mathbb{R}^d$ compact and $g \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$, then for $\alpha \in \mathbb{N}^d$ we call $D^\alpha f = g$ in the weak sense (or g the weak derivative of f) if for all $\varphi \in \mathscr{C}_c^\infty(\mathbb{R}^d)$

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

$\square$

Remark 5.9 (Motivation)**.** If $f \in \mathscr{C}_c^\infty$ then

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

Thus the strong (or usual) derivative agrees with the weak derivative if the former exists. However even if $f \notin \mathscr{C}$, we can still define its weak derivative. □

Theorem 5.10.

$$H^s(\mathbb{R}^d) = \left\{ f \in L^2(\mathbb{R}^d) \,\middle|\, \forall \alpha \in \mathbb{N}^d |\alpha| \leqslant s \implies D^\alpha f \in L^2(\mathbb{R}^d) \right\}$$

□

Proof. Assume that $f \in H^s$, i.e. $f \in L^2$, $|k|^s \hat{f}(k) \in L^2$. Take α such that $|\alpha| \leqslant s$. We prove that $D^\alpha f$ exists and belongs to L^2. For all $\varphi \in \mathscr{C}_c^\infty(\mathbb{R}^d)$

$$\int f D^\alpha \varphi = \langle D^\alpha \overline{\varphi}, f \rangle_{L^2} = \left\langle \widehat{D^\alpha \overline{\varphi}}, \hat{f} \right\rangle_{L^2} = \int \overline{(2\pi i k)^\alpha \hat{\overline{\varphi}}} \hat{f}(k) \mathrm{d}k$$

thus

$$\left| \int f D^\alpha \varphi \right| \leqslant \int \overline{|2\pi k|^{|\alpha|} |\hat{\overline{\varphi}}|} |\hat{f}(k)| \mathrm{d}k \leqslant \left\| |2\pi k|^{|\alpha|} \hat{f}(k) \right\|_{L^2} \underbrace{\left\| \hat{\overline{\varphi}} \right\|_{L^2}}_{= \|\varphi\|_{L^2}} < \infty$$

where we used that $|k|^s \hat{f}(k) \in L^2$ and $|k|^{|\alpha|} \leqslant C(1 + |k|^s)$.

Thus $\mathscr{L}(\varphi) = \int f D^\alpha \varphi$ is a continuous functional on $\mathscr{C}_c^\infty(\mathbb{R}^d)$ and therefore L^2. By the Riesz representation theorem we now prove that there exists a unique $g \in L^2$ such that $g = D^\alpha f$. By Riesz there exists an $h \in L^2$ such that $\mathscr{L}(\varphi) = \langle h, \varphi \rangle$ for all $\varphi \in \mathscr{C}_c^\infty$. thus we can choose $g = (-1)^{|\alpha|} \overline{h}$.

Conversely, assume that $f \in L^2$ and for $|\alpha| \leqslant s$ $D^\alpha f \in L^2$. We need to prove that $f \in H^s(\mathbb{R}^d)$, i.e. $|k|^s \hat{f}(k) \in L^2$.

Again, take $\varphi \in \mathscr{C}_c^\infty(\mathbb{R}^d)$. Then we compute

$$\begin{aligned} \langle \overline{\varphi}, D^\alpha f \rangle &= \int (D^\alpha f)\varphi = (-1)^{|\alpha|} \int f D^\alpha \varphi = (-1)^{|\alpha|} \int \overline{(2\pi i k)^\alpha \hat{\overline{\varphi}}(k)} \hat{f}(k) \mathrm{d}k = \\ &= \left\langle \hat{\overline{\varphi}}, (-1)^{|\alpha|} \overline{(2\pi i k)^\alpha} \hat{f}(k) \right\rangle \end{aligned} \tag{$*$}$$

Using

$$\|g\|_{L^2} = \sup_{\substack{\varphi \in \mathscr{C}_c^\infty(\mathbb{R}^d) \\ \|phi\|_{L^2} \leqslant 1}} |\langle \varphi, g \rangle_{L^2}| = \|g\|_{L^2}$$

we find by $(*)$ that

$$\|D^\alpha f\|_{L^2} = \|(-1)^\alpha (2\pi i \cdot)^\alpha \hat{f}\|_{L^2} \quad \therefore \quad \forall \alpha \in \mathbb{N}^d : |\alpha| \leqslant s \implies |k^\alpha| \hat{f}(k) \in L^2$$

and therefore also $|k|^s \hat{f}(k) \in L^2$.

q.e.d.

Remark 5.11. $\|\hat{f}\|_{L^2} = \|f\|_{L^2}$ and $\|\hat{f}\|_{L^\infty} \leqslant \|f\|_{L^1}$ for all $f \in L^1$. The second claim follows from

$$|\hat{f}(k)| = \left| \int f(x) e^{-2\pi i k \cdot x} \mathrm{d}x \right| \leqslant \int |f(x)| \mathrm{d}x = \|f\|_{L^1}.$$

□

Theorem 5.12 (Hausdorff-Young)**.** *If $f \in L^p(\mathbb{R}^d)$, $1 \leqslant p \leqslant 2$, then $\hat{f} \in L^{p'} \in \mathbb{R}^d$ with $\frac{1}{p} + \frac{1}{p'} = 1$ and $\|\hat{f}\|_{L^{p'}} \leqslant \|f\|_{L^p}$.* □

Theorem 5.13 (Riesz-Thorrin Interpolation Theorem)**.** *If we define a linear operator $\mathscr{L}$ such that*

$$\begin{aligned} \mathscr{L} : L^{p_0} &\longrightarrow L^{q_0}, \qquad \|\mathscr{L}\|_{p_0,q_0} \leqslant 1 \\ \mathscr{L} : L^{p_1} &\longrightarrow L^{q_1}, \qquad \|\mathscr{L}\|_{p_1,q_1} \leqslant 1 \end{aligned}$$

Then $\mathscr{L}$ can be extended to $L^{p_s} \to L^{q_s}$ with $\|\mathscr{L}\|_{p_s,q_s} \leqslant 1$ where

$$\frac{1}{p_s} = \frac{1-s}{p_0} + \frac{s}{p_1}, \quad \frac{1}{q_s} = \frac{1-s}{q_0} + \frac{s}{q_1}$$

for all $x \in [0,1]$. □

Proof of Theorem 5.12. Define $\mathscr{L} u = \hat{u}$, then $\mathscr{L}$ is linear and $\|L\|_{2,2} \leqslant 1$ $(p_0 = q_0 = 2)$ and $\|\mathscr{L}\|_{1,\infty} \leqslant 1$ $(p_1 = 1, q_1 = \infty)$.

Thus by the Riesz-Thorrin theorem we have $\|\mathscr{L}\|_{p_s,q_s}$ with

$$\frac{1}{p_s} = \frac{1-s}{2} + \frac{s}{1} = \frac{1+s}{2}$$
$$\frac{1}{q_s} = \frac{1-s}{2} + \frac{s}{\infty} = \frac{1-s}{2}$$

for all $s \in [0,1]$, i.e. $p_s^{-1} + q_s^{-1} = 1$. In particular $p_s \in [1,2]$. *q.e.d.*

Definition 5.14 (Convolution)**.** We define for suitably integrable functions f, g

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

For such functions

- $f * g = g * f$
- $(f * g) * h = f * (g * h)$.

□

Remark 5.15. Observe that if $f \in L^p, g \in L^q$ with $\frac{1}{p} + \frac{1}{q} = 1$ then

$$|(f*g)(x)| = \left|\int f(x-y)g(y)\mathrm{d}y\right| \leqslant \left(\int |f(x-y)|^p \mathrm{d}y\right)^{1/p} \left(\int |g(y)|^q \mathrm{d}y\right)^{1/q} = \|f\|_p \|g\|_q.$$

□

Theorem 5.16 (Convolutions)**.** *If $f \in L^p, g \in L^q$ then $f * g \in L^r$ and*

$$\|f * g\|_{L^r} \leqslant \|f\|_p \|g\|_q$$

where

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

□

Proof.

- If $r = \infty$ then this is the case from above.

- If $r = p$, $q = 1$ and we have

$$|(f * g)(x)| = \left| \int f(x-y)g(y)\mathrm{d}y \right| \leqslant \left(\int |g(y)|\mathrm{d}y \right)^{1/p'} \left(\int |f(x-y)|^p |g(y)| \, dy \right)^{1/p}$$

and therefore

$$\int |(f * g)(x)|^p \mathrm{d}x \leqslant \|g\|_1^{\frac{p}{p'}} \iint |f(x-y)|^p |g(y)| \mathrm{d}y\mathrm{d}x = \|g\|_1^{1+\frac{p}{p'}} \|f\|_p^p = (\|g\|_1 \|f\|_p)^p$$

as $1 + \frac{p}{p'} = p$.

- For all other r, $p \leqslant r \leqslant \infty$, we can use the Riesz-Thorin theorem.

q.e.d.

Theorem 5.17. *If $p^{-1} + q^{-1} = 1 + r^{-1}$ and $r \in [1,2]$, then for all $f \in L^p$, $g \in L^q$, $f * g \in L^r$ and $\widehat{f * g} \in L^{r'}$ where $r^{-1} + r'^{-1} = 1$ and*

$$\widehat{f * g} = \hat{f}\hat{g}.$$

□

Proof.

$$\widehat{f * g}(k) = \int \left(\int f(x-y)g(y)\mathrm{d}y \right) e^{-2\pi i k \cdot x} \mathrm{d}x = \iint f(x-y)g(y)e^{-2\pi i k \cdot y} e^{-2\pi i k(x-y)} \mathrm{d}x\mathrm{d}y =$$
$$= \iint f(x-y)e^{-2\pi i k \cdot (x-y)} \mathrm{d}x g(y) e^{-2\pi i k \cdot y} \mathrm{d}y = \hat{f}(k)\hat{g}(k)$$

q.e.d.

Theorem 5.18 (Fundamental Theorem of Calculus of Variations)**.** *If $f \in L^1_{loc}(\mathbb{R}^d)$ and*

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

for all $\varphi \in \mathscr{C}_c^\infty(\mathbb{R}^d)$. Then $f = 0$ a.e. □

Theorem 5.19 (Approximation of δ by convolution)**.** *For any $g \in L^1(\mathbb{R}^d)$, $\int g = 1$ define*

$$g_n(x) = n^d(gnx)$$

(such that $\int g_n = 1$). Then for all $f \in L^p(\mathbb{R}^d)$ with $1 \leqslant p < \infty$

$$g_n * f \xrightarrow[L^p]{n\to\infty} f.$$

$\square$

Proof.

Step 1 Assume that $f \in \mathscr{C}_c^\infty(\mathbb{R}^d)$. Then

$$(g_n * f)(x) - f(x) = \int g_n(x-y)f(y)\mathrm{d}y - \int g_n(x-y)f(x)\mathrm{d}y = \int g_n(x-y)(f(y)-f(x))\mathrm{d}y.$$

Let us assume that g has compact support, e.g. $\operatorname{supp} g \subset B_R(0)$ thus $\operatorname{supp} g_n \subset B_{\frac{R}{n}}(0)$.

Thus

$$|(g_n * f)(x) - f(x)| \leqslant \left(\int |g_n(x-y)|\mathrm{d}y\right) \sup_{|z-x|\leqslant \frac{R}{n}} |f(z)-f(x)| \leq \|g\|_{L^1} \sup_{|z-x|\leqslant \frac{R}{n}} |f(z)-f(x)| \xrightarrow{n\to\infty} 0$$

Step 2 Now let $f \in L^p(\mathbb{R}^d)$. Using the denseness of $\mathscr{C}_c^\infty(\mathbb{R}^d)$ in $L^p(\mathbb{R}^d)$ we can find $f_\varepsilon \in \mathscr{C}_c^\infty$ such that $\|f - f_\varepsilon\|_p \leqslant \varepsilon$.

We have

$$\|g_n * f - f\|_p = \|g_n * (f - f_\varepsilon) + g_n * f_\varepsilon - f_\varepsilon + f_\varepsilon - f\|_p\| \leqslant \underbrace{\|g_n * (f - f_\varepsilon)\|_p}_{\|g_n\|_1 \|f - f_\varepsilon\|_p} + \|g_n * f_\varepsilon - f_\varepsilon\|_p + \|f_\varepsilon - f\|_p \leqslant$$

thus we have by Step 1

$$\limsup_{n\to\infty} \|g_n * f - f\|_p \leqslant (\|g\|_1 + 1)\|f_\varepsilon - f\|_p + 0 \leqslant \varepsilon \xrightarrow{\varepsilon\to 0} 0.$$

Step 3. For the general case $g \in L^1(\mathbb{R}^d)$ one has to approximate g by functions with compact support.

q.e.d.

Proof of Theorem 5.18.

Step 1 Assume that $f \in L^1(\mathbb{R}^d)$. Choose $g \in \mathscr{C}_c^\infty(\mathbb{R}^d)$, $\int g = 1$ and $g_n(x) := n^d g(nx)$.

By the previous theorem $g_n * f \to f$ strongly in $L^1(\mathbb{R}^d)$. On the other hand $g_n(x-y) = \varphi(y) \in \mathscr{C}_c^\infty$ thus

$$(g_n * f)(x) = \int g_n(x-y)f(y)\mathrm{d}y = 0$$

for a.e. x. Thu $f = 0$ in L^1, i.e. $f = 0$ a.e.

Step 2 Let $f \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$. Choose $h \in \mathscr{C}_c^\infty$. It follows that $fh \in L^1(\mathbb{R}^d)$ and for all $\varphi \in \mathscr{C}_c^\infty(\mathbb{R}^d)$

$$\int f \underbrace{h\varphi}_{\in \mathscr{C}_c^\infty} = 0$$

Applying Step 1 with fh implies that $fh = 0$. This is true for all $h \in \mathscr{C}_c^\infty$ thus $f = 0$.

q.e.d.

5.1 Sobolev Inequality

Theorem 5.20 (Standard Sobolev Inequality)**.** *For $d \geqslant 3$ and $f \in H^1(\mathbb{R}^d)$, we have*

$$\|\nabla f\|_2 \geqslant C_d \|f\|_{p^*}$$

with $p^* = \frac{2d}{d-2}$, where the constant C_d is independent of f. □

Theorem 5.21 (Hardy-Littlewood-Sobolev Inequality)**.** *For $d \geqslant 1$, $0 < \alpha < d$, $\frac{1}{p} + \frac{1}{q} + \frac{\alpha}{d} = 2$*

$$\left| \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{f(x)g(y)}{|x-y|^\alpha} \mathrm{d}x\mathrm{d}y \right| \leqslant C \|f\|_p \|g\|_q$$

□

Proof. Assume that $f, g \geqslant 0$ and $\|f\|_p = \|g\|_q = 1$. Using the Layered-Cake representation for $f \geqslant 0$

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

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

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

Then

$$E := \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{f(x)g(y)}{|x-y|^\alpha} \mathrm{d}x\mathrm{d}y = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \int_0^\infty \int_0^\infty \int_0^\infty \mathbf{1}_{\{f(x)>a\}} \mathbf{1}_{\{g(y)>b\}} \mathbf{1}_{\{|x-y|<c\}} \alpha c^{-\alpha-1} \mathrm{d}a\, \mathrm{d}b\, \mathrm{d}c\, \mathrm{d}x\mathrm{d}y$$

We can ignore of the three characteristic functions to get an upper bound. Defining

$$I(a,b,c) = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \mathbf{1}_{\{f(x)>a\}} \mathbf{1}_{\{g(y)>b\}} \mathbf{1}_{\{|x-y|<c\}} \alpha c^{-\alpha-1} \mathrm{d}x\mathrm{d}y$$

we can use Tonelli's theorem to rewrite

$$E = \int_0^\infty \int_0^\infty \int_0^\infty I(a,b,c) \mathrm{d}a\, \mathrm{d}b\, \mathrm{d}c$$

Ignoring one of the three characterstic functions we can estimate

$$I(a,b,c) \leqslant h_1(a) h_2(b) \alpha c^{-\alpha-1}$$

where

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

$$h_2(b) := \int_{\mathbb{R}^d} \mathbf{1}_{\{g(y)>b\}} \mathrm{d}y$$

Similarly

$$I(a,b,c) \leqslant h_2(b) h_3(c) \alpha c^{-\alpha-1}$$

where

$$h_3(c) = \int_{\mathbb{R}^d} \mathbf{1}_{\{|x-y|<c\}} \mathrm{d}x = |B_1| c^d$$

also $I(a,b,c) \leqslant h_1(a) h_3(c) \alpha c^{-\alpha-1}$.

Thus

$$I(a,b,c) \leqslant \min\{h_1(a)h_2(b), h_1(a)h_3(c), h_2(b)h_3(c)\}\alpha c^{-\alpha-1}.$$

We estimate

$$\begin{aligned}
\int_0^\infty I(a,b,c)\mathrm{d}c = \int_{h_3(c)<h_1(a)} I(a,b,c)\mathrm{d}c + \int_{h_3(c)>h_1(a)} I(a,b,c)\mathrm{d}c \leqslant \\
\leqslant C \int_{h_3(c)<h_1(a)} h_2(b)c^d c^{-\alpha-1}\mathrm{d}c + C \int_{h_3(c)>h_1(a)} h_1(a)h_2(b)c^d c^{-\alpha-1}\mathrm{d}c = \\
= C' h_2(b) h_1(a)^{\frac{d-\alpha}{d}} + C'' h_2(b) h_1(a)^{\frac{d-\alpha}{d}} = C h_2(b) h_1(a)^{1-\frac{\alpha}{d}}
\end{aligned}$$

By the same argument we can also show that

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

Combining these two

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

Integrating over a, b we find that

$$\int_0^\infty\int_0^\infty\int_0^\infty I(a,b,c)\mathrm{d}c\mathrm{d}b\mathrm{d}a \leqslant C \iint_{b\leqslant a^{\frac{p}{q}}} h_1(a)h_2(b)^{1-\frac{\alpha}{d}} + C \iint_{b>a^{\frac{p}{q}}} h_2(b)h_1(a)^{1-\frac{\alpha}{d}} = A + B$$

Using the identities

$$\begin{aligned}
1 = \int |f(x)|^p \mathrm{d}x = p \int h_1(a) a^{p-1} \mathrm{d}a \\
1 = \int |g(y)|^q \mathrm{d}x = q \int h_2(b) b^{q-1} \mathrm{d}b
\end{aligned}$$

We find

$$A \leqslant C \iint\limits_{b \leqslant a^{\frac{p}{q}}} h_1(a)h_1(a)h_2(b)^{1-\frac{\alpha}{d}} \mathrm{d}a\mathrm{d}b = C \int h_1(a)a^{p-1} \int\limits_{b \leqslant a^{\frac{p}{q}}} a^{-(p-1)} h_2(b)^{1-\frac{\alpha}{d}} \mathrm{d}b\mathrm{d}a$$

If we bound can bound

$$\int\limits_{b \leqslant a^{\frac{p}{q}}} a^{-(p-1)} h_2(b)^{1-\frac{\alpha}{d}} \mathrm{d}b \leqslant C$$

(independently of a) then we can estimate A. Indeed

$$\int\limits_{b \leqslant a^{\frac{p}{q}}} h_2(b)^{1-\frac{\alpha}{d}} \mathrm{d}b \leqslant \left(\int\limits_{b \leqslant a^{\frac{p}{q}}} h_2(b) b^{q-1} \mathrm{d}b \right)^{1-\frac{\alpha}{d}} \left(\int\limits_{b \leqslant a^{\frac{p}{q}}} b^{-\xi} \mathrm{d}b \right)$$

here $(q-1)(1-\frac{\alpha}{d}) - \xi\frac{\alpha}{d} = 0$. We have $0 < \xi < 1$, then

$$\int\limits_{b \leqslant a^{\frac{p}{q}}} b^{-\xi} \mathrm{d}b = C \left(a^{\frac{p}{q}} \right)^{-\xi+1}$$

Thus

$$\int\limits_{b \leqslant a^{\frac{p}{q}}} a^{-(p-1)} h_2(b)^{1-\frac{\alpha}{d}} \mathrm{d}b \leqslant C a^{-(p-1)} a^{\frac{p}{q}(-\xi+1)} = C$$

since $-(p-1) + \frac{p}{q}(-\xi+1) = 0$ as $\frac{1}{p} + \frac{1}{q} + \frac{\alpha}{d} = 2$.
For the second term we have

$$B = \iint\limits_{b > a^{\frac{p}{q}}} h_2(b)h_1(a)^{1-\frac{\alpha}{d}} = \iint\limits_{a < b^{\frac{q}{p}}} h_2(b)h_1(a)^{1-\frac{\alpha}{d}} \leqslant C$$

analogously to A. *q.e.d.*

Theorem 5.22 (Fourier Transform of $\frac{1}{|x|^\alpha}$). *Defining $c_\alpha := \pi^{-\frac{\alpha}{2}}\Gamma\left(\frac{\alpha}{2}\right)$ where Γ is the Gamma function. Then for $0 < \alpha < d$*

$$c_\alpha \widehat{\frac{1}{|x|^\alpha}} = c_{d-\alpha} \frac{1}{|k|^{d-\alpha}}$$

in the sense that

$$c_\alpha \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \frac{\overline{f(x)}g(y)}{|x-y|^\alpha}\mathrm{d}x\mathrm{d}y = c_{d-\alpha}\int_{\mathbb{R}^d} \frac{\overline{\hat{f}(k)}\hat{g}(k)}{|k|^{d-\alpha}}\mathrm{d}k$$

for all $f, g \in \mathscr{C}_c^\infty(\mathbb{R}^d)$. □

Remark 5.23.

- The left-hand-side is well-defined if $f \in L^p$, $g \in L^q$ by the HLS inequality, if $\frac{1}{p} + \frac{1}{q} = 2 - \frac{s}{d}$.
- The right-hand-side is well-defined by the generalised Hausdorff-Young inequality (see Chapter IX.4 of Simon and Reed, Methods of Mathematical Physics).
- In general, for a function w nice enough we have

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \overline{f(x)}g(y)w(x-y)\mathrm{d}x\mathrm{d}y = \int_{\mathbb{R}^d} \overline{f(x)}(g*w)(x)\mathrm{d}x = \langle f, g*w\rangle = \left\langle \hat{f}, \widehat{g*w}\right\rangle =$$
$$= \left\langle \hat{f}, \hat{g}\hat{w}\right\rangle = \int_{\mathbb{R}^d} \overline{\hat{f(k)}}\hat{g}(k)\hat{w}(k)\mathrm{d}k$$

Consequently, if $\hat{w} \geqslant 0$ then

$$\int\int \overline{f(x)}f(y)w(x-y)\mathrm{d}x\mathrm{d}y = \int |\hat{f}(k)|\hat{w}(k)\mathrm{d}k \geqslant 0$$

In particular

$$\int\int \frac{\overline{f(x)}f(y)}{|x-y|^s}\mathrm{d}x\mathrm{d}y \geqslant 0$$

for all f nice enough.

□

Lemma 5.24 (Fourier Transform of Gaussians)**.**

$$\widehat{e^{-\pi x^2}} = e^{-\pi k^2} \quad \textit{in } \mathbb{R}^d$$

More generally for $\lambda > 0$

$$\widehat{e^{-\pi\lambda x^2}} = \frac{1}{\lambda^{d/2}} e^{-\pi\frac{k^2}{\lambda}}.$$

□

Proof. We have for $x, k \in \mathbb{R}^d$

$$\widehat{e^{-\pi\cdot^2}}(k) = \int_{\mathbb{R}^d} e^{-\pi x^2} e^{-2\pi i k x} \mathrm{d}x = \int_{\mathbb{R}^d} e^{-\pi(x_1^2+\cdots+x_d^2)} e^{-2\pi i(k_1x_1+\cdots+k_dx_d)} \mathrm{d}x = \prod_{j=1}^{d} \int_{\mathbb{R}} e^{-\pi x_j^2} e^{-2\pi i k_j x_j} \mathrm{d}x_j$$

Thus we can restrict to $d = 1$. In this case

$$\int_{\mathbb{R}} e^{-\pi x^2} e^{-2\pi i k x} \mathrm{d}x = \int_{\mathbb{R}} e^{-\pi(x^2+2ikx)} \mathrm{d}x = e^{-\pi k^2} \int_{\mathbb{R}} e^{-\pi(x+ik)^2} \mathrm{d}x$$

We only need to prove $\int_{\mathbb{R}} e^{-\pi(x+ik)^2} \mathrm{d}x = 1$ for all k. Obviously this holds for $k = 0$ and

$$\frac{d}{dk} \int_{\mathbb{R}} e^{-\pi(x+ik)^2} \mathrm{d}x = \int_{\mathbb{R}} \frac{d}{dk} e^{-\pi(x+ik)^2} \mathrm{d}x = \int_{\mathbb{R}} (-2\pi i(x+ik)) e^{-\pi(x+ik)^2} \mathrm{d}x = i \int_{\mathbb{R}} \frac{d}{dx} e^{-\pi(x+ik)^2} \mathrm{d}x =$$
$$= i\, e^{-\pi(x+ik)^2}\Big|_{x=-\infty}^{\infty} = 0$$

thus the integral is independent of k and therefore is equal to 1 for all k. *q.e.d.*

Proof of Theorem 5.22.

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

Thus we have

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

Taking the Fourier transform of both sides

$$c_s \widehat{|x|^{-s}} \text{``}=\text{''} \int_0^\infty \widehat{e^{-\pi\lambda x^2}} \lambda^{\frac{s}{2}-1} \mathrm{d}\lambda = \int_0^\infty \frac{1}{\lambda^{\frac{d}{2}}} e^{-\pi\frac{k^2}{\lambda}} \lambda^{\frac{s}{2}-1} \mathrm{d}\lambda \overset{\lambda=t^{-1}}{=\!=\!=} \int_0^\infty t^{\frac{d}{2}} e^{-\pi t k^2} t^{1-\frac{s}{2}} \frac{\mathrm{d}t}{t^2} = \int_0^\infty e^{-\pi t k^2} t^{\frac{d-s}{2}-1} \mathrm{d}t =$$
$$= c_{d-s} |k|^{-(d-s)}$$

q.e.d.

Proof of Theorem 5.20.

$$\int \overline{f}g = \int \overline{\hat{f}}\hat{g} = \int |k|\overline{\hat{f}(k)}\frac{\hat{g}(k)}{|k|}\mathrm{d}k \leqslant \left(\int |k|^2|\hat{f}(k)|^2\mathrm{d}k\right)^{1/2}\left(\int \frac{|\hat{g}(k)|^2}{|k|^2}\mathrm{d}k\right)^{1/2} =$$
$$= C\left(\int |\nabla f|^2\right)^{1/2}\left(\int\int \frac{\overline{g(x)}g(y)}{|x-y|^{d-2}}\right)^{1/2} \leqslant C\|\nabla f\|_2\|g\|_q$$

where $\frac{1}{q}+\frac{1}{q}+\frac{d-2}{d}=2$, hence $\frac{2}{q}=1+\frac{2}{d}$, $\frac{1}{p^*}+\frac{1}{q}=1$. Finally

$$\|f\|_{p^*} = \sup_{\|g\|_q\leqslant 1} |\langle f,g\rangle| \leqslant C\|\nabla f\|_2$$

q.e.d.

Remark 5.25 (Fractional Sobolev Space)**.** Recall that $H^s(\mathbb{R}^d) = \left\{f \in L^2 \,\middle|\, |k|^s\hat{f}(k) \in L^2\right\}$. This definition is good for all $s > 0$. When $s \notin \mathbb{N}$, $H^s(\mathbb{R}^d)$ is called a fractional Sobolev space. This is relevant in "relativistic physics". In this case the Kinetic energy operator then

$$\sqrt{-\Delta + c^4m^2} - c^2m = \frac{-\Delta}{\sqrt{-\Delta+c^4m^2}+c^2m} \approx \begin{cases} -\frac{\Delta}{2c^2m}, & \text{if } -\Delta \ll c^2m \\ \sqrt{-\Delta}, & \text{if } -\Delta \gg c^2m \end{cases}$$

where m is the mass of the particle under consideration and c is the speed of light. □

Theorem 5.26 (Fractional Sobolev Inequality)**.** *Take* $0 < s < \min\{1, \frac{d}{2}\}$ *and* $p = \frac{2d}{d-2s}$. *Then for all* $f \in H^s(\mathbb{R}^d)$

$$\langle f, (-\Delta)^s f\rangle \geqslant C\|f\|_p^2.$$

The constant $C > 0$ *is independent of* f.

Here

$$\langle f, (-\Delta)^s f\rangle = \int_{\mathbb{R}^d} |\hat{f}(k)|^2(4\pi^2|k|^2)^s\mathrm{d}k$$

□

Proof. Analogous to the integer case. *q.e.d.*

Returning to H^1 does a version of the Sobolev Inequality hold for $d = 1, 2$. It does not hold that

$$\|\nabla f\|_2 \geqslant C\|f\|_p$$

for $d = 1, 2$ for any p.

Theorem 5.27 (Full Sobolev inequality for $H^1(\mathbb{R}^d)$)**.** *We have*

$$\|f\|_{H^1(\mathbb{R}^d)} \geqslant C\|f\|_p$$

where

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

in the last case f is even continuous. Heuristically, the Sobolev inequality is stronger in lower dimensions. $\square$

Proof.

($d \geqslant 3$) We know that

$$\|f\|_{H^1} \geqslant \|\nabla f\|_{L^2} \geqslant C\|f\|_{L^{p^*}}$$
$$\|f\|_{H^1} \geqslant \|f\|_2$$

where $p^* = \frac{2d}{d-2}$. By Hölder's inequality we know that for $2 \leqslant p \leqslant p^*$

$$\|f\|_p \leqslant \max\{\|f\|_2, \|f\|_{p^*}\}.$$

($d \geqslant 2$)

$$\|f\|_{H^1}^2 = \int_{\mathbb{R}^2} (1 + 4\pi^2 k^2)|\hat{f}(k)|^2 \mathrm{d}k$$

Take $1 < q < 2$. Then

$$\|\hat{f}\|_q^q = \int_{\mathbb{R}^2} |\hat{f}(k)|^q \mathrm{d}k \leqslant \left(\int_{\mathbb{R}^2} |\hat{f}(k)|^2 \big(1 + 4\pi^2|k|^2\big) \mathrm{d}k\right)^{\frac{q}{2}} \left(\int_{\mathbb{R}^2} \frac{1}{(1 + 4\pi^2|k|^2)^\eta} \mathrm{d}k\right)^{1-\frac{q}{2}}$$

where $\frac{q}{2} - \eta(1-\frac{q}{2}) = 0$ hence $\eta = \frac{\frac{q}{2}}{1-\frac{q}{2}} = \frac{q}{2-q} > 1$ which implies that

$$\int\limits_{\mathbb{R}^2} \frac{1}{(1+4\pi^2|k|^2)^\eta} \mathrm{d}k = C < \infty$$

Thus we know that $\|\hat{f}\|_q^q \leqslant C\|f\|_{H^1}^q$. On the other hand

$$\|f\|_p \leqslant \|\hat{f}\|_q \leqslant C\|f\|_{H^1}$$

for $\frac{1}{p} + \frac{1}{q} = 1$ and $1 < q < 2$, i.e. $p \in [2, \infty)$.

$(d=1)$ Assume that $f \in \mathscr{C}_c^\infty(\mathbb{R})$. We have

$$f(x) = \int\limits_{-\infty}^{x} f'(t)\mathrm{d}t$$

and therefore

$$f(x)^2 = \int\limits_{-\infty}^{x} 2f(t)f'(t)\mathrm{d}t$$

from which follows

$$|f(x)|^2 = |f(x)^2| = 2\left|\int\limits_{-\infty}^{x} f(t)f'(t)\mathrm{d}t\right| \leqslant 2\|f\|_2\|f'\|_2$$

Thus $\|f\|_\infty^2 \leqslant 2\|f\|_2\|f'\|_2 \leqslant 2\|f\|_{H^1}^2$.
By approximation (as $\mathscr{C}_c^\infty$ is dense) it follows that the inequality holds for all $f \in H^1(\mathbb{R}^d)$.
Consider $f \in H^1(\mathbb{R})$ we find again by approximation via smooth functions that

$$|f(x) - f(y)| = \left|\int\limits_{x}^{y} f'(t)\mathrm{d}t\right| \leqslant \left(\int\limits_{x}^{y} \mathrm{d}t\right)^{1/2} \left(\int\limits_{x}^{y} |f'(t)|^2\mathrm{d}t\right)^{1/2} \leqslant \|f'\|_2\sqrt{|x-y|}$$

Thus f is Hölder continuous and in particular continuous.

q.e.d.

Remark 5.28. If $f \in L^2(\mathbb{R})$, then $f(x)$ does not make sense point-wise. However, the above theorem says that if $f \in H^1$, then there exists a unique representative in $[f]$ which is continuous. In this sense $H^1(\mathbb{R}) \subset \mathbb{R}$. □

Theorem 5.29 (Sobolev Embedding)**.** *Let $(f_n)_n \subset H^1(\mathbb{R}^d)$ be a bounded sequence. Assume that $f_n \rightharpoonup f$ weakly in $H^1(\mathbb{R}^d)$. Then for every bounded set Ω (or more generally $\lambda(\Omega) < \infty$) then*

$$\mathbf{1}_\Omega f_n \xrightarrow[L^p(\mathbb{R}^d)]{n\to\infty} \mathbf{1}_\Omega f$$

where

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

in particular in the last case $L^\infty(\omega) = \mathscr{C}(\Omega)$ with the supremum norm. □

Remark 5.30. Here $f_n \rightharpoonup f$ weakly in H^1 iff for all $g \in H^1$

$$\langle f_n, g\rangle_{H^1} \xrightarrow{n\to\infty} \langle f, g\rangle_{H^1} \tag{$*$}$$

which is equivalent to

$$\begin{cases} f_n \xrightharpoonup{n\to\infty} f & \text{in } L^2 \\ \partial_{x_i} f_n \xrightharpoonup{n\to\infty} \partial_{x_i} f & \text{in } L^2 \end{cases} \tag{$**$}$$

The direction $(**)\Rightarrow(*)$ is trivial. The converse follows since $f_n \rightharpoonup f$ in H^1 implies that $f_n \rightharpoonup f$ in L^2 as the H^1 topology is stronger than the L^2 topology. On the other hand, $\partial_{x_i} f_n$ is bounded in L^2, thus we can descend to a subsequence such that $\partial_{x_i} f \rightharpoonup g_i$ weakly in L^2. The limit $\partial_{x_i} f = g_i$ because for all $\varphi \in H^1$

$$\langle \partial_{x_i} f_n, \varphi\rangle = -\langle f_n, \partial_{x_i}\varphi\rangle \xrightarrow{n\to\infty} -\langle f, \partial_{x_i}\varphi\rangle .$$

Further note that the function $\mathbf{1}_\Omega : f \mapsto \mathbf{1}_\Omega f$ is thus a compact operator $H^1(\mathbb{R}^d) \to L^p(\mathbb{R}^d)$.

□

Proof. We introduce $g_n = e^{t\Delta} f_n$, i.e. $\hat{g}_n(k) = e^{-t4\pi^2|k|^2}\hat{f}_n(k)$.

Then

$$\|g_n - f_n\|_2^2 = \int_{\mathbb{R}^d} |\hat{g}_n - \hat{f}_n|^2 \mathrm{d}k = \int_{\mathbb{R}^d} \left(e^{-t4\pi^2|k|^2} - 1\right)^2 |\hat{f}_n(k)|^2 \mathrm{d}k.$$

Note that

$$1 \geqslant e^{-t4\pi^2|k|^2} \geqslant 1 - t4\pi^2|k|^2$$

thus

$$0 \leqslant 1 - e^{-t4\pi^2|k|^2} \leqslant t4\pi^2|k|^2$$

whence we follow

$$0 \leqslant 1 - e^{-t4\pi^2|k|^2} \leqslant \min\{1, t4\pi^2 k^2\} \leqslant \sqrt{t4\pi^2|k|^2}$$

and therefore

$$\left|1 - e^{-t4\pi^2|k|^2}\right|^2 \leqslant t4\pi^2|k|^2$$

Using this we may estimate

$$\|g_n - f_n\|_2^2 \leqslant \int_{\mathbb{R}^d} t4\pi^2 k^2 |\hat{f}_n(k)|^2 \mathrm{d}k = t \int_{\mathbb{R}^d} |\nabla f_n|^2 \mathrm{d}x \leqslant t\|f\|_{H^1}^2 \leqslant Ct$$

Now

$$\begin{aligned}
\|\mathbf{1}_\Omega f_n - \mathbf{1}_\Omega f\|_2 &= \left\|\mathbf{1}_\Omega f_n - \mathbf{1}_\Omega e^{t\Delta} f_n + \mathbf{1}_\Omega e^{t\Delta}(f_n - f) + \mathbf{1}_\Omega e^{t\Delta} f - \mathbf{1}_\Omega f\right\|_2 \leqslant \\
&\leqslant \|\mathbf{1}_\Omega (f_n - e^{t\Delta} f_n)\|_2 + \|\mathbf{1}_\Omega e^{t\Delta}(f_n - f)\|_2 + \|\mathbf{1}_\Omega (e^{t\Delta} f - f)\|_2 \leqslant \\
&\leqslant \|f_n - e^{t\Delta} f_n\|_2 + \|\mathbf{1}_\Omega e^{t\Delta}(f_n - f)\|_2 + \|e^{t\Delta} f - f\|_2 \leqslant \\
&\leqslant \sqrt{t}(\|f_n\|_{H^1} + \|f\|_{H^1}) + \|\mathbf{1}_\Omega e^{t\Delta}(f_n - f)\|_2
\end{aligned}$$

Using the lemma below we may rewrite the last term as

$$e^{t\Delta}(f_n - f)(x) = \frac{1}{(4\pi t)^{d/2}} \int_{\mathbb{R}^d} e^{-\frac{|x-y|^2}{4t}} (f_n(y) - f(y)) \mathrm{d}y$$

Since $f_n \rightharpoonup f$ weakly in H^1 it follows that $f_n \rightharpoonup f$ in L^2 and thus since for all $x \in \mathbb{R}^d$ $y \mapsto e^{-\frac{|x-y|}{4t}} \in L^2(\mathbb{R}^d)$ it follows that for a.e. $x \in \mathbb{R}^d$

$$e^{t\Delta}(f_n - f)(x) \xrightarrow{n\to\infty} 0.$$

However, we know that

$$\left|e^{t\Delta}(f_n - f)(x)\right| \leqslant \frac{1}{(4\pi t)^{d/2}} \left(\int\limits_{\mathbb{R}^d} e^{-\frac{|x-y|^2}{2t}} \mathrm{d}y \right)^{1/2} \left(\int\limits_{\mathbb{R}^d} |f_n - f|^2 \right)^{1/2} \leqslant C_t$$

Thus we may bound $\mathbf{1}_\Omega e^{t\Delta}(f_n - f) \leqslant \mathbf{1}_\Omega C_t \in L^2(\mathbb{R}^d)$ as $\lambda(\Omega) < \infty$ and therefore by dominated convergence it follows that

$$\mathbf{1}_\Omega e^{t\Delta}(f_n - f) \xrightarrow[L^2]{n\to\infty} 0$$

and therefore we find that

$$\limsup_{n\to\infty} \|\mathbf{1}_\Omega f_n - \mathbf{1}_\Omega f\|_2 \leqslant \sqrt{t}C + 0 \xrightarrow{t\to 0} 0$$

We conclude that $\mathbf{1}_\Omega f_n - \mathbf{1}_\Omega f \to 0$ strongly in $L^2(\mathbb{R}^d)$. Moreover,

$$\|\mathbf{1}_\Omega f_n - \mathbf{1}_\Omega f\|_{p^*} \leqslant \|f_n - f\|_{p^*} \leqslant C\|f_n - f\|_{H^1} \leqslant C$$

by the Sobolev inequality with p^* chosen accordingly.

By interpolation it follows for $p^* < \infty$ now that for all $2 \leqslant p < p^*$

$$\|\mathbf{1}_\Omega f_n - \mathbf{1}_\Omega f\|_p \xrightarrow{n\to\infty} 0.$$

The special case $d = 1, p^* = \infty$ follows from

$$f_n(x) - f_n(0) = \int\limits_0^x f_n'(t)\mathrm{d}t \xrightarrow{n\to\infty} \int\limits_0^x f'(t)\mathrm{d}t = f(x) - f(0)$$

as $f_n' \rightharpoonup f'$ weakly. We will have finished the proof if we can show that $f_n(0) \to f(0)$.

Take $g \in \mathscr{C}_c^\infty(-1,1)$, $\int g = 1$, $g \geqslant$ and $g_n(x) = ng(nx)$. Using the mean value theorem for integrals we know that there exist for all $n \in \mathbb{N}$, $x_n^m \in \left(-\frac{1}{m}, \frac{1}{m}\right) \supset \operatorname{supp} g_m$, such that

$$\int g_m(x) f_n(x)\mathrm{d}x = f_n(x_n^m) \int g_m(x)\mathrm{d}x = f_n(x_n^m)$$

and $x_0 \in \left(-\frac{1}{m}, \frac{1}{m}\right)$ such that

$$\int g_m(x)f(x)\mathrm{d}x = f(x_0^m)\int g_m(x)\mathrm{d}x = f(x_0^m)$$

in particular $f_n(x_n^m) \xrightarrow{n\to\infty} f(x_0^m)$.

As $(f_n)_n$ is weakly convergent it is norm bounded, i.e. there exists $M \in \mathbb{R}$ such that $\|f\|_{H^1}, \|f_n\|_{H^1} \leqslant M$ in particular this family of functions is equicontinuous as for all $n \in \mathbb{N}$

$$|f_n(x) - f_n(y)| \leqslant \|f'\|_2\sqrt{|x-y|} \leqslant M\sqrt{|x-y|}$$

and analogously for f. Thus for any $\varepsilon > 0$ we can find $m \in \mathbb{N}$ large enough such that for all $x, y \in \left(-\frac{1}{m}, \frac{1}{m}\right)$ and $n \in \mathbb{N}$

$$|f_n(x) - f_n(y)| < \frac{\varepsilon}{3}, \quad |f(x) - f(y)| < \frac{\varepsilon}{3}$$

and therefore for n large enough such that $|f_n(x_n^m) - f(x_0^m)| < \frac{\varepsilon}{3}$ we find

$$|f_n(0) - f(0)| \leqslant |f_n(0) - f_n(x_n^m)| + |f_n(x_n^m) - f(x_0^m)| + |f(x_0^m) - f(0)| \leqslant \frac{\varepsilon}{3} + \frac{\varepsilon}{3} + \frac{\varepsilon}{3} < \varepsilon$$

i.e. $f_n(0) \xrightarrow{n\to\infty} f(0)$.

Consider the case Ω is compact. Assume that $\|\mathbf{1}_\Omega(f_n - f)\|_\infty \not\to 0$. Thus there exists a sequence $(x_n)_n \subset \Omega$ such that

$$\|f_n(x_n) - f(x_n)| \geqslant \varepsilon > 0$$

for some $\varepsilon > 0$ and all $n \in \mathbb{N}$. By going to a subsequence if necessary we may assume that $x_n \to x_0$ for some $x_0 \in \Omega$.

Recalling the proof of the Sobolev inequality we note that $|f(x) - f(y)| \leqslant \sqrt{|x-y|}\|f\|_{H^1}$. Thus we have

$$\begin{aligned}\varepsilon \leqslant |f_n(x_n) - f(x_n)| \leqslant |f_n(x_n) - f_n(x_0)| + |f_n(x_0) - f(x_0)| + |f(x_0) - f(x_n)| \leqslant \\ \leqslant \sqrt{|x_n - x_0|}(\|f_n\|_{H^1} + \|f\|_{H^1})|f_n(x_0) - f(x_0)| \xrightarrow{n\to\infty} 0\end{aligned}$$

q.e.d.

Lemma 5.31 (Heat Kernel)**.**

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

□

Remark 5.32. Suppose that $A : D(A) \subset L^2 \to L^2$ with

$$(Au)(x) = \int K(x,y)u(y)\mathrm{d}y$$

the K is called the ***kernel*** of A. In particular consider the operator

$$\widehat{Au}(k) = f(k)\hat{u}(k)$$

and assume that $(Au)(x) = (G * u)(x)$, then

$$\widehat{Au}(k) = \widehat{G * u}(k) = \hat{G}(k)\hat{u}(k)$$

and thus $\hat{G}(k) = f(k)$.
Thus if $\hat{G} = f$, then $Au(x) = G * u$, i.e. $G(x-y)$ is the kernel of A □

Example 5.33. $A = e^{t\Delta}$ for $t > 0$. Then

$$\widehat{Au}(k) = e^{-t4\pi^2k^2}\hat{u}(k) \quad \therefore \quad f(k) = e^{-t4\pi^2k^2}$$

What is G,

$$G(x) = \check{f}(x) = \left(e^{-t4\pi^2k^2}\right)^{\vee}(x)$$

Recalling that

$$\widecheck{e^{-\pi\lambda k^2}} = \frac{1}{\lambda^{d/2}} e^{-\pi\frac{x^2}{\lambda}}$$

it follows that

$$G(x) = \frac{1}{(4\pi t)^{d/2}} e^{-\pi\frac{x^2}{4\pi t}}$$

Consequently
$$\left(e^{t\Delta}u\right)(x) = \frac{1}{(4\pi t)^{d/2}} \int\limits_{\mathbb{R}^d} e^{-\frac{|x-y|^2}{4t}} u(y)\mathrm{d}y.$$

Example 5.34. Consider the operator $A = (-\Delta)^{-1}$, $f(k) = \frac{1}{4\pi^2 k^2}$. The kernel of $(-\Delta)^{-1}$ is
$$G(x) = \widecheck{\frac{1}{4\pi^2|\cdot|^2}}(x)$$
Using the Fourier transform of $|x|^{-\alpha}$ it follows that
$$G(x) = \frac{1}{4\pi^2}\frac{c_{d-2}}{c_2}\frac{1}{|x|^{d-2}}$$
for $d \geqslant 3$.

Theorem 5.35 (Green's Function of the Laplacian)**.**
$$G(x) = \begin{cases} \frac{1}{4\pi^2}\frac{c_{d-2}}{c_2}\frac{1}{|x|^{d-2}}, & \textit{if } d \geqslant 3, \\ -\frac{1}{2\pi}\ln(|x|), & \textit{if } d = 2, \\ -\frac{1}{2}|x|, & \textit{if } d = 1. \end{cases}$$
is the kernel of $(-\Delta)^{-1}$, *i.e.*
$$(-\Delta)^{-1}u(x) = \int\limits_{\mathbb{R}^d} G(x-y)u(y)\mathrm{d}y.$$
□

Theorem 5.36 (Sobolev Inequality/Embedding for $H^s(\mathbb{R}^d)$)**.** *Let* $s \in \mathbb{N}$. *Then*

- $\mathrm{Id} : H^s(\mathbb{R}^d) \to L^p(\mathbb{R}^d)$, $f \mapsto f$ *is a bounded operator for*
$$\begin{cases} 2 \leqslant p \leqslant \frac{2d}{d-2}, & \textit{if } d > 2s, \\ 2 \leqslant p < \infty, & \textit{if } d = 2s \\ 2 \leqslant p \leqslant \infty, & \textit{if } d < s. \end{cases}$$

In the last case $H^s(\mathbb{R}^d) \subset \mathscr{C}(\mathbb{R}^d)$

- *For all bounded sets* Ω, $\mathbf{1}_\Omega : H^s(\mathbb{R}^d) \to L^p(\mathbb{R}^d)$, $f \mapsto \mathbf{1}_\Omega f$ *is a compact operator, where*

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

In particular $H^2(\mathbb{R}^3) \subset \mathscr{C}(\mathbb{R}^3)$ *but* $H^1(\mathbb{R}^3) \not\subset \mathscr{C}(\mathbb{R}^3)$.

□

Proof of $H^2(\mathbb{R}^3) \subset \mathscr{C}(\mathbb{R}^3)$. Take $u \in H^2(\mathbb{R}^3)$. Then $-\Delta u = f \in L^2(\mathbb{R}^3)$. Thus $u = (-\Delta)^{-1} f$.

Step 1 Assume that f has compact support. By the formula for the Green's function of the Laplacian

$$u(x) = (G * f)(x) = \int\limits_{\mathbb{R}^3} \frac{f(y)}{4\pi|x-y|} \mathrm{d}y$$

We have

$$u(x) - u(x') = \int\limits_{\mathbb{R}^3} f(y)\left(\frac{1}{|x-y|} - \frac{1}{|x'-y|}\right)\mathrm{d}y = \int\limits_{\operatorname{supp} f} f(y)\left(\frac{1}{|x-y|} - \frac{1}{|x'-y|}\right)\mathrm{d}y$$

and thus

$$|u(x) - u(x')| = \int\limits_{\operatorname{supp} f} |f(y)|\left|\frac{1}{|x-y|} - \frac{1}{|x'-y|}\right|\mathrm{d}y \leqslant \|f\|_2 \left(\int\limits_{\operatorname{supp} f} \left|\frac{1}{|x-y|} - \frac{1}{|x'-y|}\right|^2 \mathrm{d}y\right)^{1/2}.$$

We have

$$\left|\frac{1}{|x-y|} - \frac{1}{|x'-y|}\right| = \frac{||x-y| - |x'-y||}{|x-y||x'-y|} \leqslant \begin{cases} \frac{|x-x'|}{|x-y||x'-y|} \\ \frac{\max\{|x-y|,|x'-y|\}}{|x-y||x'-y|} \end{cases}$$

and therefore

$$\left|\frac{1}{|x-y|} - \frac{1}{|x'-y|}\right| \leqslant \frac{|x-x'|^\varepsilon \max\{|x-y|,|x'-y|\}^\varepsilon}{|x-y||x'-y|} \leqslant |x-x'|^\varepsilon\left(\frac{1}{|x-y|^{1+\varepsilon}} + \frac{1}{|x'-y|^{1+\varepsilon}}\right)$$

Thus

$$\int\limits_{\operatorname{supp} f} \left|\frac{1}{|x-y|} - \frac{1}{|x'-y|}\right|^2 \mathrm{d}y \leqslant |x-x'|^{2\varepsilon} \int\limits_{\operatorname{supp} f} \left(\frac{1}{|x-y|^{1+\varepsilon}} + \frac{1}{|x'-y|^{1+\varepsilon}}\right)^2 \mathrm{d}y \leqslant$$
$$\leqslant |x-x'|^{2\varepsilon} 2 \int\limits_{\operatorname{supp} f} \left(\frac{1}{|x-y|^{2(1+\varepsilon)}} + \frac{1}{|x'-y|^{2(1+\varepsilon)}}\right) \mathrm{d}y$$

Note that

$$\int\limits_{\operatorname{supp} f} \frac{1}{|x-y|^{2(1+\varepsilon)}} \mathrm{d}y \leqslant C_x < \infty$$

if $2 + 2\varepsilon < d = 3$ (thus this is ok if ε small enough). In conclusion

$$\frac{|u(x) - u(x')|}{|x-x'|^{\varepsilon}} \leqslant C_\Omega$$

if $x, x' \in \Omega$ is bounded, i.e. u is Hölder continuous.

Step 2 Let $f \in L^2(\mathbb{R}^d)$. Take $\chi \in \mathscr{C}_c^\infty$. Then $\chi u \in H^2$ and $\Delta(\chi u) = \Delta\chi u + 2(\nabla\chi) \cdot (\nabla u) + \chi\Delta u = g \in L^2(\mathbb{R}^d)$ and $\operatorname{supp} g \subset \operatorname{supp} \chi$. By Step 1, χu is continuous for all $\chi \in \mathscr{C}_c^\infty$. Thus for any $x \in \mathbb{R}^d$ we can choose χ such that $\chi\big|_U \equiv 1$ for some small neighbourhood of x and therefore u is Hölder continuous at x.

q.e.d.

Theorem 5.37 (Newton)**.** *Let μ be a positive measure on $\mathbb{R}^3$ such that μ is invariant under rotatations, i.e. for all $R \in SO(3)$, $\mu(A) = \mu(RA)$. Then*

$$\int \frac{\mathrm{d}\mu(y)}{|x-y|} = \int \frac{\mathrm{d}\mu(y)}{\max\{|x|, |y|\}}.$$

□

Proof. Because μ is invariant under rotations we may rewrite

$$\int \frac{\mathrm{d}\mu(y)}{|x-y|} = \int \frac{\mathrm{d}\mu(y)}{||x|\omega - y|} \mathrm{d}y$$

for some $\omega \in S^2$. Then

$$\int \frac{\mathrm{d}\mu(y)}{|x-y|} = \frac{1}{|S^2|} \int\limits_{S^2} \int \frac{\mathrm{d}\mu(y)}{||x|\omega - y|} \mathrm{d}y \mathrm{d}S(\omega) \overset{\text{Tonelli}}{=\!=} \frac{1}{|S^2|} \int \int\limits_{S^2} \frac{\mathrm{d}\mu(y)}{||x|\omega - y|} \mathrm{d}S(\omega) \mathrm{d}y$$

W.l.o.g. we may assume that $(|y|, 0, 0) = y \in \mathbb{R}^3$ to calculate

$$\begin{aligned}
\frac{1}{|S^2|} \int\limits_{S^2} \frac{\mathrm{d}\mu(y)}{||x|\omega - y|} \mathrm{d}S(\omega) &= \frac{1}{4\pi} \int_0^{\vartheta} \int_0^{2\pi} \frac{\sin(\vartheta) \mathrm{d}\vartheta \mathrm{d}\varphi}{\sqrt{(|x|\cos(\vartheta) - |y|)^2 + |x|^2(\sin(\vartheta)^2\cos(\varphi)^2 + \sin(\vartheta)^2\sin(\varphi)^2)}} = \\
&= \frac{1}{4\pi} \int_0^{\vartheta} \int_0^{2\pi} \frac{\sin(\vartheta) \mathrm{d}\vartheta \mathrm{d}\varphi}{\sqrt{(|x|\cos(\vartheta) - |y|)^2 + |x|^2\sin(\vartheta)^2}} = \\
&= \frac{1}{2|x|} \int_0^{\vartheta} \frac{\sin(\vartheta) \mathrm{d}\vartheta}{\sqrt{(\cos(\vartheta) - r)^2 + \sin(\vartheta)^2}} \overset{s=\cos(\vartheta)}{=\!=} \\
&= \frac{1}{2|x|} \int_{-1}^{1} \frac{\mathrm{d}s}{\sqrt{(s-r)^2 + 1 - s^2}} = \frac{1}{|x|} \frac{1}{\max\{1, r\}} = \frac{1}{\max\{|x|, |y|\}}.
\end{aligned}$$

q.e.d.

Remark 5.38. 1) For $d \geqslant 3$ we have the generalisation

$$\int \frac{\mathrm{d}\mu(y)}{|x-y|^{d-2}} = \int \frac{\mathrm{d}\mu(y)}{\max\{|x|, |y|\}^{d-2}}$$

however one needs some potential theory to prove this.

2) Note that

$$\iint \frac{\mathrm{d}\mu_1(x)\mathrm{d}\mu_2(y)}{|x-y|} \mathrm{d}x \mathrm{d}y = \frac{\int \mathrm{d}\mu_1 \int \mathrm{d}\mu_2}{|x_1 - x_2|}$$

where x_i is the centre of rotation of the measure μ_i.

□

Chapter 6

Schrödinger Operator $-\Delta + V$

We consider the operator $A = -\Delta + V$ on $L^2(\mathbb{R}^d)$, $V : \mathbb{R}^d \to \mathbb{R}$, $V \in L^1_{\text{loc}}(\mathbb{R}^d)$. A is well-defined on $\mathscr{C}_c^\infty(\mathbb{R}^d)$ at least as a quadratic form

$$\langle u, Au \rangle = \int |\nabla u|^2 + \int V|u|^2$$

When is A bounded from below? In physics this means that the system described by A is ***stable***. $\langle \psi, A\psi \rangle$ gives the (mean) energy of the particle, for $\psi \in L^2(\mathbb{R}^d)$ the wave function of the particle. Further $|\psi(x)|^2$ gives the probability distribution of the position of the particle and $|\hat{\psi}(k)|^2$ the probability distribution of the moment, for $\|\psi\|_2 = 1$.

Example 6.1 (Hydrogen Atom)**.** Let $A = -\Delta - \frac{1}{|x|}$ on $L^2(\mathbb{R}^3)$. Why is

$$\int |\nabla u|^2 - \int \frac{|u|^2}{|x|} \geqslant -C$$

for all u in the domain with $\|u\|_2 = 1$. We can estimate the potential using

$$\frac{1}{|x|} = \frac{1}{|x|}\mathbf{1}_{\{|x| \leqslant R\}} + \frac{1}{|x|}\mathbf{1}_{\{|x| > R\}} \leqslant \frac{1}{|x|}\mathbf{1}_{\{|x| \leqslant R\}} + \frac{1}{R}$$

for all $R > 0$. Thus

$$\int \frac{|u(x)|^2}{|x|}\mathrm{d}x \leqslant \int\limits_{|x| \leqslant R} \frac{|u(x)|^2}{|x|} + \frac{1}{R}.$$

By the Sobolev inequality

$$\int |\nabla u|^2 \geqslant C\Big(\int |u|^6\Big)^{1/3}$$

hence

$$\int_{|x|\leqslant R} \frac{|u(x)|^2}{|x|}\mathrm{d}x \leqslant \left(\int_{|x|\leqslant R} |u(x)|^6\right)^{1/3} \left(\int_{|x|\leqslant R} \frac{1}{|x|^{3/2}}\mathrm{d}x\right)^{2/3} \leqslant CR \int |\nabla u|^2$$

and therefore

$$\langle u, Au\rangle = \int |\nabla u|^2 - \int \frac{|u(x)|^2}{|x|} \geqslant (1 - CR) \int |\nabla u|^2 - \frac{1}{R}.$$

By choosing R small enough we get $\langle u, Au\rangle \geqslant -C$ for all $\|u\|_2 = 1$.

Remark 6.2 (Heisenberg Uncertainty Principle)**.**

$$\int_{\mathbb{R}^3} |\nabla u(x)|^2\mathrm{d}x \int_{\mathbb{R}^3} |x|^2|u(x)|^2\mathrm{d}x \geqslant C_0 > 0$$

for all $u \in H^1(\mathbb{R}^3)$. However, this is not enough to prove the stability of Hydrogen. But using the Sobolev inequality we find for $\|u\|_2 = 1$

$$\int |\nabla u|^2 - \int \frac{|u(x)|^2}{|x|}\mathrm{d}x \geqslant -C$$

Rescaling $u_\ell(x) = \ell^{3/2}u(\ell x)$ such that $\|u_\ell\|_2 = \|u\|_2$ we get

$$\ell \int |\nabla u(x)|^2 - \ell \int \frac{|u(x)|^2}{|x|}\mathrm{d}x \geqslant -C$$

for all $\ell > 0$. Therefore we get the inequality $\ell^2 a - \ell b \geqslant -c$ for all $\ell > 0$ when $a, b, c > 0$, which is equivalent to $2\sqrt{ac} \geqslant b$ or $4ac \geqslant b^2$. Thus for all $\|u\|_2 = 1$

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

This inequality implies the Heisenberg uncertainty principle as

$$\left(\int \frac{|u(x)|^2}{|x|}\mathrm{d}x\right)^2\left(\int |x|^2|u(x)|^2\mathrm{d}x\right) \geqslant \left(\int \left(\frac{|u(x)|^2}{|x|}\right)^{2/3}\left(|x|^2|u(x)|^2\right)^{1/3}\mathrm{d}x\right)^3 =$$
$$= \left(\int |u(x)|^2\mathrm{d}x\right)^3 = 1.$$

□

Returning to the general Schrödinger operator $A = -\Delta + V$ with general V. Considering $d \geqslant 3$ we have

$$\left|\int V|u|^2\right| \leqslant \left(\int |u|^{2p}\right)^{1/p}\left(\int |V|^q\right)^{1/q}$$

with $\frac{1}{p} + \frac{1}{q} = 1$. If we choose $2p = \frac{2d}{d-2}$, i.e. $p = \frac{d}{d-2}$ and $q = \frac{d}{2}$, we get by the Sobolev inequality

$$-\int V|u|^2 \leqslant \left|\int V|u|^2\right| \leqslant C\left(\int |\nabla u|^2\right)\|V\|_{\frac{d}{2}},$$

i.e.

$$\langle u, Au\rangle \geqslant \left(1 - C\|V\|_{d/2}\right)\left(\int |\nabla u|^2\right).$$

If $C\|V\|_{\frac{d}{2}} \leqslant 1$ then $A \geqslant 0$. More generally, for $V \in L^{\frac{d}{2}}(\mathbb{R}^d)$ we can rewrite the potential as

$$V = V\mathbf{1}_{|V|>R} + V\mathbf{1}_{|V|\leqslant R}.$$

Then

$$\left|\int_{\mathbb{R}^3} V|u|^2\right| \leqslant \int_{|V|>R} |V||u|^2 + R\int_{|V|\leqslant R} |u|^2 \leqslant C\left\|V\mathbf{1}_{\{|V|>R\}}\right\|_{\frac{d}{2}}\int |\nabla u|^2 + R$$

and therefore

$$\langle u, Au\rangle \geqslant \left(1 - C\left\|V\mathbf{1}_{\{|x|>R\}}\right\|_{\frac{d}{2}}\right)\int |\nabla u|^2 - R$$

Observing that by dominated convergence

$$\left\|V\mathbf{1}_{\{|x|>R\}}\right\|_{\frac{d}{2}}^{d/2} = \int |V|^{d/2}\mathbf{1}_{\{|x|>R\}} \xrightarrow{R\to\infty} 0$$

we find that by choose R large enough so that $\|V\mathbf{1}_{\{|x|>R\}}\| < C^{-1}$, i.e. so that the factor in front of $\int|\nabla u|^2$ is positive, that $\langle u, Au\rangle \geqslant -R$.

We have thus proven the following theorem in the case of $d \geqslant 3$. Note that the L^∞ part of

V gets estimated away by

$$\left| \int_{\mathbb{R}^3} V|u|^2 \right| \leqslant \|V\|_\infty \int_{\mathbb{R}^3} |u|^2 = \|V\|_\infty$$

and replacing R with $R + \|V\|_\infty$.

Theorem 6.3. *Assume that $V \in L^p(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ where*

$$\begin{cases} p \geqslant \frac{d}{2}, & \text{if } d \geqslant 3 \\ p > 1, & \text{if } d = 2 \\ p \geqslant 1, & \text{if } d = 1 \end{cases}$$

Then $-\Delta + V$ is bounded from below, in fact

$$\langle u, (-\Delta + V)u \rangle \geqslant \frac{1}{2} \int |\nabla u|^2 - C$$

for all $u \in \mathscr{C}_c^\infty(\mathbb{R}^d)$ with $\|u\|_2 = 1$. Consequently $-\Delta + V$ can be extended to a self-adjoint operator by Friedrich's extension theorem, with quadratic form domain $H^1(\mathbb{R}^d)$. □

Lemma 6.4. *If $1 \leqslant p < q \leqslant r \leqslant \infty$ then for all $f \in L^q$, we can write $f = f_1 + f_2$ such that $f_1 \in L^p$ and $f_2 \in L^r$, i.e.*

$$L^q \subset L^p + L^r = \left\{ f_1 + f_2 \,\middle|\, f_1 \in L^p, f_2 \in L^r \right\}$$

□

Remark 6.5. Recall that $-\Delta$ can be extended to a self-adjoint operator $D(-\Delta) = H^2(\mathbb{R}^d)$. The Friedrich's extension of $-\Delta+V$, in general, might have a domain $D(-\Delta+V)$ much bigger than $H^2(\mathbb{R}^d)$. □

Theorem 6.6 (Self-Adjoint Extension of $-\Delta+V$ of $H^2(\mathbb{R}^d)$)**.** *Assume that $V \in L^p+L^\infty$*

with

$$\begin{cases} p \geqslant \frac{d}{2}, & \text{if } d > 4 \\ p > 2, & \text{if } d = 4 \\ p \geqslant 2, & \text{if } d = 1,2,3 \end{cases}$$

Then V is $(-\Delta)$-relatively bounded, where the bound can be chosen as small as necessary, i.e. for all $\varepsilon > 0$

$$\|Vu\|_2 \leqslant \varepsilon\|\nabla u\|_2 + C_\varepsilon\|u\|_2.$$

Consequently, by the Kato-Rellich Theorem $-\Delta + V$ is a self adjoint operator on $D(-\Delta + V) = D(-\Delta) = H^2(\mathbb{R}^d)$ □

Proof.

$(d > 4)$

$$\|Vu\|_2 = \left(\int |V|^2|u|^2\right)^{1/2} \leqslant \left(\int |V|^{2q}\right)^{1/2q} \left(\int |u|^{2p}\right)^{1/2p}$$

where $\frac{1}{p} + \frac{1}{q} = 1$, $2p = \frac{2d}{d-4}$ hence $p = \frac{d}{d-4}$ and $q = \frac{d}{4}$. (Recall that $H^2(\mathbb{R}^d) \subset L^{\frac{2d}{d-4}}(\mathbb{R}^d)$ if $d > 4$.)

Thus $\|Vu\|_2 \leqslant \|V\|_{\frac{d}{2}}\|u\|_{H^2}$. For every $\varepsilon > 0$ if $\|V\|_{\frac{d}{2}}\|u\|_{H^2}$. For every $\varepsilon > 0$ if $\|V\|_{\frac{d}{2}} \leqslant \varepsilon$, then

$$\|Vu\|_2 \leqslant \varepsilon\|u\|_{H^2} \leqslant 2\varepsilon\|\Delta u\|_2 + C_\varepsilon\|u\|_2$$

More generally, if $V \in L^{\frac{d}{2}}$, then we can write $V = V_1 + V_2$ with $V_2 \in L^\infty$, $V_1 \in L^{\frac{d}{2}}$, $\|V_1\|_{\frac{d}{2}} \leqslant \varepsilon$ and

$$\|Vu\|_2 \leqslant \|V_1u\|_2 + \|V_2u\|_2 \leqslant \varepsilon\|u\|_{H^2} + \|V_2\|_\infty\|u\|_2 \leqslant 2\varepsilon\|\Delta u\|_2 + C_\varepsilon\|u\|_2$$

for all $\varepsilon > 0$.

$(d \leqslant 3)$ Using $H^2(\mathbb{R}^d) \subset L^\infty(\mathbb{R}^d)$

$$\|Vu\|_2 \leqslant \|V\|_2\|u\|_\infty \leqslant C\|V\|_2\|u\|_{H^2}$$

If $\|V\|_2 \leqslant \varepsilon$, then we are done. More generally, we proceed as above.

q.e.d.

Theorem 6.7 (Essential Spectrum of $-\Delta + V$ on $H^2(\mathbb{R}^d)$). *Assume that $V \in L^p + L^q$ with*

$$\begin{cases} q, p \geqslant 2, & \text{if } d = 1, 2, 3 \\ q, p > \frac{d}{2}, & \text{if } d \geqslant 4 \end{cases}$$

Then V is $(-\Delta)$-relatively compact and therefore

$$\sigma_{ess}(-\Delta + V) = \sigma_{ess} = [0, \infty).$$

□

Proof. Recall by Theorem 4.21 that the assertion holds if B_1 is B_2-relative compact, i.e. if $B_1(B_2 + i)^{-1}$ is compact. If $B_2 \geqslant 0$ then this is equivalent to $B_1(B_2 + 1)^{-1}$ being compact because

$$B_1(B_2 + 1)^{-1} = \underbrace{B_1(B_2 + i)^{-1}}_{\text{compact}} \underbrace{(B_2 + i)(B_2 + 1)^{-1}}_{\text{bounded}}$$

and the reverse holds.

Why is $V(1 - \Delta)^{-1}$ compact? Take $u_n \rightharpoonup 0$ weakly in L^2, then we have to prove that $V(1-\Delta)^{-1}u_n \to 0$ strongly in L^2. Let $f_n = (1-\Delta)^{-1}u_n$. Since $u_n \rightharpoonup 0$ weakly in L^2, $f_n \rightharpoonup 0$ weakly in H^2 (Exercise!). We want to prove that $Vf_n \to 0$ strongly.

Write $V = V_1 + V_2$, $V_1 = V\mathbf{1}_{\{|x| \leqslant R\}}$ and $V_2 = V\mathbf{1}_{\{|x|>R\}}$. Then

$$\|V_1 f_n\|_2^2 = \int\limits_{|x| \leqslant R} |V_1|^2 |f_n|^2 \xrightarrow{n \to \infty} 0$$

by the compact embedding theorem, since $f_n \mathbf{1}_{\{|x| \leqslant R\}} \to 0$ strongly in L^p with $p < p^*$ in $H^2(\mathbb{R}^d) \subset L^{p^*}(\mathbb{R}^d)$, thus $|f_n|^2 \mathbf{1}_{\{|x| \leqslant R\}} \to 0$ in $L^{p/2}$ and $|V|^2 \in \left(L^{p/2}\right)^*$. From the last fact it follows also that

$$\|V_2 f_n\|_2^2 = \langle \overline{V_2}, f_n \rangle \xrightarrow{n \to \infty} 0.$$

q.e.d.

In particular in $\mathbb{R}^3$ the last theorem tells us that $-\Delta - \frac{1}{|x|^\alpha}$ is self-adjoint on $H^2(\mathbb{R}^d)$ iff

$$\frac{1}{|x|^\alpha} \mathbf{1}_{\{|x| \leqslant 1\}} \in L^2 \iff \int\limits_{|x| \leqslant 1} \frac{1}{|x|^{2\alpha}} \mathrm{d}x < \infty \iff \alpha < \frac{3}{2}$$

and $\sigma_{\text{ess}}(-\Delta - \frac{1}{|x|^\alpha}) = \sigma_{\text{ess}}(-\Delta) = [0, \infty)$.
Thus in physics $\frac{1}{|x|^\alpha}$ with $\alpha < \frac{3}{2}$ is not too singular. A really singular potential would be $\frac{1}{|x|^2}$ in $\mathbb{R}^3$.

Theorem 6.8 (Hardy's Inequality)**.** *For all $u \in H^1(\mathbb{R}^3)$*

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

Here $\frac{1}{4}$ is sharp, i.e. $-\Delta - \frac{c}{|x|^2}$ with $c > \frac{1}{4}$ is not bounded from below. □

Theorem 6.9. *If $V \in L^p + L^q$ with*

$$\begin{cases} \frac{d}{2} \leqslant p < \infty, & \text{if } d \geqslant 4 \\ \frac{d}{2} < p < \infty, & \text{if } d = 1, 2, 3. \end{cases}$$

Then V is $(-\Delta)$-compact, and by Kato-Rellich $-\Delta + V$ is self-adjoint on $H^2(\mathbb{R}^d)$, and by Weyl's theorem (Theorem 4.21)

$$\sigma_{ess}(-\Delta + V) = \sigma_{ess}(-\Delta) = [0, \infty).$$

□

Theorem 6.10 (Friedrich's Extension of Schrödinger Operator)**.** *If $V \in L^p + L^q$ with*

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

Then $-\Delta + V$ is a self-adjoint operator defined by the Friedrich's extension with form domain $H^1(\mathbb{R}^d)$, and

$$\sigma_{ess}(-\Delta + V) = \sigma_{ess}(-\Delta) = [0, \infty).$$

□

Remark 6.11. In the case $d = 3$, we need $V \in L^p$ for $p > \frac{3}{2}$, i.e. for potentials of the form $V(x) = \frac{1}{|x|^\alpha}$ we only require $\alpha < 2$.
Notice the improvement of the conditions on V when $d \leqslant 4$. For example in $d = 3$ $-\Delta + \frac{1}{|x|^s}$ is self-adjoint on $H^2(\mathbb{R}^3)$ if $s < \frac{3}{2}$ but has a Friedrich's extensions when $s < 2$, hence the domain of the Friedrich's extension can be larger than $H^2(\mathbb{R}^3)$. □

Proof. Recall that under the condition $V \in L^p + L^q$, $-\Delta + V$ is bounded from below with

$$\langle u, (-\Delta + V)u \rangle = \int |\nabla u|^2 + \int V|u|^2 \geqslant \frac{1}{2} \int |\nabla u|^2 - C$$

for all $\|u\|_2 = 1$. Then $-\Delta + V$ can be extended using the Friedrich's extension to a self-adjoint operator with quadratic form domain $H^1(\mathbb{R}^d)$. Now we prove that

$$\sigma_{\text{ess}}(-\Delta + V) = \sigma_{\text{ess}}(-\Delta) = [0, \infty).$$

Take $\lambda \in \sigma_{\text{ess}}(-\Delta + V)$. We prove that $\lambda \geqslant 0$. Using Weyl's criterion (Theorem 4.15), there exists a sequence $(u_n)_n$, with $\|u_n\|_2 = 1$, $u_n \rightharpoonup 0$ weakly in L^2, such that $\|(-\Delta + V)u_n - \lambda u_n\|_2 \to 0$.
Then

$$0 = \lim_{n\to\infty} \langle u_n, ((-\Delta + V)u_n - \lambda u_n) \rangle = \lim_{n\to\infty} \left(\int |\nabla u_n|^2 + \int V|u_n|^2 - \lambda \right)$$

If we can prove that $\int V|u_n|^2 \to 0$, then $\lambda \geqslant 0$. Recall that

$$\lambda \xleftarrow{\infty \leftarrow n} \int |\nabla u_n|^2 + \int V|u_n|^2 \geqslant \frac{1}{2} \int |\nabla u_n|^2 - C$$

Thus $\int |\nabla u_n|^2 \leqslant c$ independently of n, i.e. $(u_n)_n$ is bounded in $H^1(\mathbb{R}^d)$. Consequently, we can go to a subsequence such that $u_n \rightharpoonup u$ weakly in $H^1(\mathbb{R}^d)$. Because $u_n \rightharpoonup 0$ in L^2, $u = 0$, i.e. $u_n \rightharpoonup 0$ weakly in H^1.
It is left as an exercise to show that if $V \in L^p + L^q$ as in the assumption and $u_n \rightharpoonup 0$ in H^1, then

$$\int V|u_n|^2 \xrightarrow{n\to\infty} 0.$$

Now take $\lambda \in \sigma_{\text{ess}}(-\Delta) = [0, \infty)$. We have to prove that $\lambda \in \sigma_{\text{ess}}(-\Delta + V)$. By Weyl's criterion there exists a sequence $(u_n)_n$ such that $\|u_n\|_2 = 1$, $u_n \rightharpoonup 0$ in L^2 and

$$\| -\Delta u_n - \lambda u_n\|_2 \xrightarrow{n\to\infty} 0.$$

Now we prove that

$$\|(-\Delta+V)u_n - \lambda u_n\|_2 \xrightarrow{n\to\infty} 0$$

i.e. $\lambda \in \sigma_{\mathrm{ess}}(-\Delta+V)$. This means that we have to prove that $\|Vu_n\|_2 \to 0$.
Let us consider the case $d=3$.

$$\|Vu_n\|_2^2 = \int |V|^2|u_n|^2$$

is difficult to estimate because $V \notin L^2_{\mathrm{loc}}(\mathbb{R}^3)$ (we only know that $V \in L^{3/2}_{\mathrm{loc}}(\mathbb{R}^3)$). Write

$$Vu_n = V(1-\Delta)^{-1}(1-\Delta)u_n = V(1-\Delta)^{-1/2}g_n.$$

Since $\|\Delta u_n - \lambda u_n\|_2 \to 0$, u_n is bounded in $H^2(\mathbb{R}^3)$. This means that

$$\|g_n\|_2^2 = \|(1-\Delta)u_n\|_2^2 = \left\langle u_n, (1-\Delta)^2 u_n\right\rangle \leqslant \|u_n\|_{H^2}^2 \leqslant C$$

Thus we can go to a subsequence and assume that $g_n \rightharpoonup g$ in L^2. Therefore

$$u_n = (1-\Delta)^{-1}g_n \overset{n\to\infty}{\rightharpoonup} (1-\Delta)^{-1}g$$

in L^2, as $(1+\Delta)^{-1}$ is bounded. Thus $(1-\Delta)^{-1}g = 0$, i.e. $g=0$. Now we know that $g_n \rightharpoonup 0$ weakly in L^2, we want to prove $Vu_n = V(1-\Delta)^{-1}g_n \to 0$ strongly in L^2. We are done if we can prove that $V(1-\delta)^{-1}$ is compact in L^2.
By the lemma below $(1-\Delta)^{-1/2}V(1-\Delta)^{-1/2}$ is a Hilbert-Schmidt operator.
Recalling that AB is compact iff BA is, it follows that the compactness of $(1-\Delta)^{-1/2}V(1-\Delta)^{-1/2}$ implies that $V(1-\Delta)^{-1}$ is

q.e.d.

Lemma 6.12. $(1-\Delta)^{-1/2}V(1-\Delta)^{-1/2}$ *is a Hilbert Schmidt operator.* □

Proof. By writing $V = V_+ - V_-$ and considering the two cases separately we may assume that $V \geqslant 0$. We can write

$$(1-\Delta)^{-1/2}V(1-\Delta)^{-1/2} = K^*K$$

with $K = \sqrt{V}(1-\Delta)^{-1/2}$. We know that K^*K and KK^* always have the same non-zero eigenvalues with the same multiplicity, i.e. KK^* is Hilbert Schmidt iff K^*K is. Consider

$KK^* = \sqrt{V}(1-\Delta)^{-1}\sqrt{V}$ (the Birman-Schwinger operator). We can write

$$\Big(\sqrt{V}(1-\Delta)^{-1}\sqrt{V}f\Big)(x) = \sqrt{V(x)}\Big((1-\Delta)^{-1}(\sqrt{V}f)\Big)(x) =$$
$$\sqrt{V(x)}\int G(x,y)(\sqrt{V}f)(y)\mathrm{d}y = \int \sqrt{V(x)}G(x,y)\sqrt{V(y)}f(y)\mathrm{d}y.$$

where $G(x,y)$ is the kernel of $(1-\Delta)^{-1}$. Thus the kernel of KK^* is

$$\sqrt{V(x)}G(x-y)\sqrt{V(y)}$$

Recalling that an operator B is Hilbert Schmidt iff its kernel $b \in L^2$, with $\|B\|_{\mathrm{HS}}^2 = \int\int |b(x,y)|^2 \mathrm{d}x\mathrm{d}y$. Thus KK^* is Hilbert Schmidt iff $\sqrt{V(x)}G(x-y)\sqrt{V(y)} \in L^2$, i.e. we have to show that

$$\iint V(x)|G(x-y)|^2V(y)\mathrm{d}x\mathrm{d}y < \infty.$$

What is the Green's function G of $(1-\Delta)^{-1}$. One can compute it is given by the Yukawa potential $\frac{e^{-|x|}}{|x|}$. However, we do not need to use this as we have already proven that in $\mathbb{R}^3$, the kernel of $(-\Delta)^{-1}$ is $\frac{1}{4\pi|x|}$.

Because $1-\Delta \geqslant -\Delta$ it follows that $(1-\Delta)^{-1} \leqslant (-\Delta)^{-1}$, hence $KK^* \leqslant \sqrt{V}(-\Delta)^{-1}\sqrt{V}$. We conclude that KK^* is Hilbert Schmidt if we can prove that $\sqrt{V}(-\Delta)^{-1}\sqrt{V}$ is Hilbert-Schmidt. By repeating the calculation above we find that

$$\left\|\sqrt{V}(-\Delta)^{-1}\sqrt{V}\right\|_{\mathrm{HS}}^2 = \iint V(x)|G(x-y)|^2V(y)\mathrm{d}x\mathrm{d}y = \frac{1}{16\pi^2}\int\int \frac{V(x)V(y)}{|x-y|^2}\mathrm{d}x\mathrm{d}y \leqslant C\|V\|_p^2$$

by the HLS inequality as

$$\frac{1}{p}+\frac{1}{p}+\frac{2}{3} = 2 \quad \therefore \quad p = \frac{3}{2} = \frac{d}{2},$$

which is the case per the assumption of the theorem above. *q.e.d.*

Why is $-\frac{1}{|x|^s}$ with $s<2$ relevant?. In three dimensions, $s=1$ is the Coulomb potential, in particular

$$-\Delta - \frac{1}{|x|}$$

describes the hydrogen atom. In this case

$$\frac{1}{|x|} = \frac{1}{|x|}\mathbf{1}_{|x|\leqslant 1} + \frac{1}{|x|}\mathbf{1}_{|x|\geqslant 1}$$

where the first summand is L^p for $p<3$ and the second one is in L^q for $q>3$.
By the Kato-Rellich theorem $-\Delta-\frac{1}{|x|}$ is self-adjoint in $H^2(\mathbb{R}^3)$, $\sigma_{\text{ess}}(-\Delta-\frac{1}{|x|})=[0,\infty)$. Actually

$$\sigma(-\Delta-\frac{1}{|x|})=(\mu_n)_n\cup[0,\infty)$$

where the eigenvalues are $-\frac{1}{4n^2}$ with multiplicity n^2. If $s<\frac{3}{2}$, $V=-\frac{1}{|x|^s}\in L^p+L^q$, $p\geqslant 2$ and $-\Delta-\frac{1}{|x|^s}$ is self-adjoint on $H^2(\mathbb{R}^d)$. If $s<2$, $-\Delta-\frac{1}{|x|^s}$ can be extended by Friedrich's theorem.
Why is $s=2$? Because of Hardy's inequality

Theorem 6.13.

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

for all $u\in H^1(\mathbb{R}^3)$ and $\frac{1}{4}$ is the sharp constant. □

Proof.

$$\int\frac{|u|^2}{|x|^2}\mathrm{d}x=\underbrace{\frac{c_1}{c_2}}_{=\pi}\int\frac{\overline{\hat{u}(p)}\hat{u(q)}}{|p-q|}\mathrm{d}p\mathrm{d}q\leqslant\frac{\pi}{2}\int\int\frac{|\hat{u}(p)|^2\frac{|p|^s}{|q|^s}+|\hat{u}(q)|^2\frac{q^s}{|p|^s}}{|p-q|}\mathrm{d}p\mathrm{d}q=$$

$$=\pi\int|\hat{u}(p)|^2|p|^s\int\frac{1}{|q|^s|p-q|}\mathrm{d}q\mathrm{d}p$$

We now compute

$$f(p)=\in\frac{1}{|q|^s}\frac{1}{|q-p|}\mathrm{d}q=\left(\frac{1}{|\cdot|^s}*\frac{1}{|\cdot|}\right)(p)$$

$$\hat{f}(p)=\widehat{\frac{1}{|q|^s}}(p)\widehat{\frac{1}{|q|}}(p)=\frac{c_{3-s}}{\pi c_s}\frac{1}{|p|^{3-s}}\frac{1}{|p|^2}=\frac{1}{|p|^{5-s}}$$

$$f(p)=\frac{c_{3-s}}{\pi c_s}\frac{c_{s-2}}{c_{5-s}}\frac{1}{|p|^{s-2}}$$

This calculation are ok if $5-s<3$, i.e. $s>2$ and $s\in(2,3)$. Thus

$$\int\frac{|u(x)|^2}{|x|^2}\mathrm{d}x\leqslant C\int|\hat{u}(p)|^2|p|^s\frac{1}{|p|^{s-2}}\mathrm{d}p=c\int|\hat{u}(p)|^2|p|^2\mathrm{d}p=c\int|\nabla u|^2\mathrm{d}x$$

Optimising over s we get $c=\frac{1}{4}$. *q.e.d.*

Recalling that for $V\in L^p+L^q$, $1\leqslant p,q<\infty$ if $d=1$ and $\frac{d}{2}<p,q<\infty$ if $d\geqslant 2$ we know that $\sigma_{\text{ess}}(-\Delta + V) = [0, \infty)$.

We are interested in the negative eigenvalues described by the min-max values

$$\mu_n = \mu_n(-\Delta + V) = \inf_{\substack{M \subset H^2(\mathbb{R}^d) \\ \dim M = n}} \max_{\substack{u \in M \\ \|u\|_2 = 1}} \langle u, (-\Delta + V)u \rangle$$

with $\mu_n \uparrow \mu_\infty = 0$. If $\mu_n < 0$, then μ_n is an eigenvalue (the corresponding eigenfunction is called a ***bound state***).

We are interested in the existence of negative eigenvalues: Recall that if $d \geqslant 3$, if $V \in L^{d/2}$ and $\|V\|_{d/2}$ small, then $-\Delta + V \geqslant 0$ by the Sobolev inequality, i.e. for all $u \in H^1(\mathbb{R}^d)$

$$\int |\nabla u|^2 + \int V|u|^2 \geqslant 0$$

and thus there are no negative eigenvalues, hence $\sigma(-\Delta + V) = \sigma_{\text{ess}}(-\Delta + V) = [0, \infty)$.

Theorem 6.14. *Suppose that $d = 1, 2$. If $V \in \mathscr{C}_c^\infty(\mathbb{R}^d)$, $V \leqslant 0$, $V \not\equiv 0$. Then $-\Delta + V$ has at least one negative eigenvalue.* □

Proof. Assume that $-\mu$ is an eigenvalue, $\mu > 0$ and u is an eigenfuction, i.e.

$$(-\Delta + V)u = -\mu \quad \therefore \quad (-\Delta + \mu)u = -Vu = |V|u \quad \therefore \quad u = (-\Delta + \mu)^{-1}|V|u$$

which can be rewritten as

$$\varphi = \sqrt{|V|}u = \sqrt{|V|}(-\Delta + \mu)^{-1}\sqrt{|V|}\sqrt{|V|}u = \sqrt{|V|}(-\Delta + \mu)^{-1}\sqrt{|V|}\varphi$$

therefore we define the Birman-Schwinger operator

$$K_\mu = \sqrt{|V|}(-\Delta + \mu)^{-1}\sqrt{|V|}$$

for $\mu > 0$. The above equation means that $\varphi = \sqrt{|V|}u$ would be an eigenfunction of K_μ with eigenvalue 1.

Now let us prove that there exists some $\mu > 0$ such that K_μ has eigenvalue 1. Once we have proven its existence then we can conclude that there exists $\varphi \neq 0$, $\varphi \in L^2$ with

$$\varphi = K_\mu \varphi = \sqrt{|V|}(-\Delta + \mu)^{-1}\sqrt{|V|}\varphi$$

and define

$$u := (-\Delta + \mu)^{-1}\sqrt{|V|}\varphi \in H^2(\mathbb{R}^d)$$

as $\sqrt{|V|}\varphi \in L^2$. Now we prove that $(-\Delta + V)u = -\mu u$. Indeed

$$\begin{aligned}\sqrt{|V|}\varphi = \sqrt{|V|}\sqrt{|V|}(-\Delta + \mu)^{-1}\sqrt{|V|}\varphi &= \sqrt{|V|}u \\ u = (-\Delta + \mu)^{-1}\sqrt{|V|}\varphi &= (-\Delta + \mu)^{-1}|V|u \\ \therefore \quad (-\Delta + \mu)u = |V|u = -Vu & \end{aligned}$$

To finish, we need to prove the existence of $\mu > 0$ such that K_μ has eigenvalue 1.

Recall that K_μ is a Hilbert-Schmidt operator with kernel

$$K_\mu(x, y) = \sqrt{|V(x)|}G_\mu(x - y)\sqrt{|V(y)|}$$

Here $G_\mu(x - y)$ is the kernel of $(-\Delta + \mu)^{-1}$ and $\hat{G}_\mu(k) = (4\pi^2|k|^2 + \mu)^{-1}$.

In the case $d = 1, 2$ and $V \in \mathscr{C}_c^\infty$ then

$$\begin{aligned}\int\int |K_\mu(x, y)|^2 \mathrm{d}x\mathrm{d}y = \int |V(x)||G_\mu(x - y)|^2|V(y)|\mathrm{d}x\mathrm{d}y \leqslant \|V\|_\infty\|V\|_1\|G_\mu\|_2^2 = \\ = \|V_\infty\|\|V\|_1\|\hat{G}_\mu(k)\|_2^2 \leqslant C_\mu < \infty,\end{aligned}$$

i.e. K_μ is Hilbert-Schmidt (actually this holds also for $d = 3$).

We also know that $K_\mu \geqslant 0$, we can write K_μ using the spectral decomposition and in particular, $\|K_\mu\|$ is an eigenvalue of K_μ. Thus it suffices to prove that there exists a $\mu > 0$ such that $\|K_\mu\| = 1$.

We have

$$\begin{aligned}\|K_\mu\| = \sup_{\|\eta\|_2=1} \langle \eta, K_\mu\eta\rangle = \sup_{\|\eta\|_2=1} \int\int \overline{\eta(x)}\sqrt{|V(x)|}G_\mu(x - y)\eta(y)\sqrt{|V(y)|}\mathrm{d}x\mathrm{d}y = \\ = \sup_{\|\eta\|_2=1} \int_{\mathbb{R}^d} \frac{|\widehat{\eta\sqrt{|V|}}(k)|^2}{4\pi^2k^2 + \mu}\mathrm{d}k\end{aligned}$$

If $\mu \to 0$, then $\|K_\mu\| \to \infty$. Indeed take $\eta_0 \in \mathscr{C}_c^\infty$, $\eta \geqslant 0$ and $\int \eta_0\sqrt{|V|} > 0$ then

$$\lim_{\mu\to 0} \|K_\mu\| \geqslant \lim_{\mu\to 0} \int \frac{\left|\widehat{\eta_0\sqrt{|V|}}(k)\right|^2}{4\pi^2k^2 + \mu}\mathrm{d}k \xlongequal[\text{conv}]{\text{mon}} \int \frac{\left|\widehat{\eta_0\sqrt{|V|}}(k)\right|^2}{4\pi^2k^2}\mathrm{d}k = \infty$$

Here the assumption $d=1,2$ is needed as in higher dimensions $\frac{1}{|k|^2}$ is integrable at 0 but not in $d=1,2$.
If $\mu\to\infty$,

$$K_\mu=\sqrt{|V|}(-\Delta+\mu)^{-1}\sqrt{|V|}\leqslant\sqrt{|V|}\mu^{-1}\sqrt{|V|}\leqslant\|V\|_\infty\mu^{-1}$$

hence $\|K_m u\|\leqslant\|V\|_\infty\mu^{-1}\xrightarrow{\mu\to\infty}0$.
We now want to prove that $\mu\mapsto\|K_\mu\|$ is continuous on $(0,\infty)$ from which the existence of the sought-after μ follows by the intermediate value theorem.
Take $\mu_1,\mu_2>0$, $\mu_2\to\mu_1$. Then

$$\begin{aligned}|\|K_{\mu_1}\|-\|K_{\mu_2}\||\leqslant\|K_{\mu_1}-K_{\mu_2}\|&=\left\|\sqrt{|V|}\big((-\Delta+\mu_1)^{-1}-(-\Delta+\mu_2)^{-1}\big)\sqrt{|V|}\right\|=\\&=\left\|\sqrt{|V|}(-\Delta+\mu_1)^{-1})(\mu_2-\mu_1)(-\Delta+\mu_2)^{-1}\sqrt{|V|}\right\|\leqslant\\&\leqslant|\mu_1-\mu_2|\left\|\sqrt{|V|}\right\|\|(-\Delta+\mu_1)^{-1}\|\|(-\Delta+\mu_2)^{-1}\|\left\|\sqrt{|V|}\right\|\leqslant\\&\leqslant\|V\|_\infty\frac{|\mu_2-\mu_1|}{\mu_2\mu_1}\xrightarrow{\mu_2\to\mu_1}0\end{aligned}$$

where $\|\cdot\|$ denotes the operator-norm unless otherwise indicated. *q.e.d.*

Theorem 6.15 (Existence of Infinitely Many Negative Eigenvalues for Singular Potentials)**.** *Let $V\in L^p+L^q$, with*

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

(i.e. such that $\sigma_{ess}(-\Delta+V)=[0,\infty)$) Assume further that $V(x)\leqslant-\frac{c_0}{|x|^s}$, when $|x|$ is large enough where $c_0>0$, and $0<s<2$ are given constants. Then $-\Delta+V$ has infinitely many negative eigenvalues. □

Proof. We will use the min-max principle, i.e.

$$\mu_n:=\mu_n(-\Delta+V)=\inf_{\substack{M\subset H^2(\mathbb{R}^d)\\ \dim M=n}}\max_{\substack{u\in M\\ \|u\|_2=1}}\langle u,(-\Delta+V)u\rangle$$

We know that $\mu_n\uparrow\mu_\infty=0$ and if $\mu_n<0$, then μ_n is an eigenvalue. It suffices to show that $\mu_n<0$ for all $n\in\mathbb{N}$. Let us choose M: for a fixed $n\in\mathbb{N}$, we can choose $(u_i)_{i=1}^n$ such that $u_i\in\mathscr{C}_c^\infty(\mathbb{R}^d)$, $\|u_i\|_2=1$, $\operatorname{supp}u_i$ are disjoint and $\inf_{x\in\bigcup_i\operatorname{supp}u_i}|x|\geqslant 1$.

Take a parameter $\ell > 0$ and define $u_i^{(\ell)}(x) = \ell^{d/2} u_i(\ell x)$ for all $i \in \{1, \ldots, n\}$. Then $\|u_i^{(\ell)}\|_2 = \|u_i\|_2 = 1$. Thus $\left(u_i^{(\ell)}\right)_{i=1}^n$ is an ONF of L^2, indeed $\left(u_i^{(\ell)}\right)$ have disjoint supports. Moreover,

$$\inf_{x \in \bigcup_i \operatorname{supp} u_i^{(\ell)}} |x| \geqslant \frac{1}{\ell}.$$

Now consider

$$\left\langle u_i^{(\ell)}, (-\Delta + V) u_i^{(\ell)} \right\rangle = \int |\nabla u_i^{(\ell)}|^2 + \int V |u_i^{(\ell)}|^2 = \int |\nabla u_i^{(\ell)}|^2 + \int V(x) \mathbf{1}_{\{|x| \geqslant \frac{1}{\ell}\}} |u_i^{(\ell)}(x)|^2 \mathrm{d}x$$

If ℓ is small enough

$$\begin{aligned} \left\langle u_i^{(\ell)}, (-\Delta + V) u_i^{(\ell)} \right\rangle &\leqslant \int |\nabla u_i^{(\ell)}|^2 - \int \frac{c_0}{|x|^s} \mathbf{1}_{\{|x| \geqslant \frac{1}{\ell}\}} |u_i^{(\ell)}(x)|^2 \mathrm{d}x = \\ &= \ell^2 \int |\nabla u_i|^2 - \ell^s \int \frac{c_0}{|x|^s} |u_i(x)|^2 \mathrm{d}x < 0 \end{aligned}$$

if ℓ small enough, because $s < 2$.
Chose $M = \operatorname{span}\left(u_i^{(\ell)}\right)_{i=1}^n$, $\dim M = n$. So

$$\mu_n \leqslant \sup_{\substack{u \in M \\ \|u\|_2 = 1}} \langle u, (-\Delta + V) u \rangle$$

Since $u \in M$, we can write as

$$u = \sum_{i=1}^n \vartheta_i u_i^{(\ell)}$$

for $\vartheta_i \in \mathbb{C}$ and $\|u\|_2^2 = \sum_{i=1}^n |\vartheta_i|^2 = 1$. Now

$$\begin{aligned} \langle u, (-\Delta + V) u \rangle &= \int |\nabla u|^2 + \int V |u|^2 = \int \left| \nabla \sum_{i=1}^n \vartheta_i u_i^{(\ell)} \right|^2 \int V |\sum_{i=1}^n \vartheta_i u_i^{(\ell)}|^2 = \\ &= \sum_{i,j} \overline{\vartheta}_i \vartheta_j \left(\int \overline{\nabla u_i^{(\ell)}} \cdot \nabla u_j^{(\ell)} + \int V |u_i^{(\ell)}| u_j^{(\ell)} \right) = \\ &= \sum_i |\vartheta_i|^2 \underbrace{\left(\int |\nabla u_i^{(\ell)}|^2 + \int V |u_i^{(\ell)}|^2 \right)}_{<0} < 0 \end{aligned}$$

q.e.d.

Theorem 6.16 (Trapping Potentials)**.** *Assume that* $V \in L^p_{loc}(\mathbb{R}^d)$*,* $p > \frac{d}{2}$*, and* $V \uparrow \infty$ *as* $x \uparrow |\infty|$*, i.e.*

$$\lim_{R\to\infty} \operatorname*{ess\,inf}_{|x|\geqslant R} V(x) = +\infty$$

Then $-\Delta + V$ *is a self-adjoint operator by Friedrich's extension and it has a compact resolvent, i.e.* $(-\Delta + V + C)^{-1}$ *is a compact operator for* C *large enough. In particular there exists an ONB for* $L^2(\mathbb{R}^d)$ *consisting of eigenfunctions of* $-\Delta + V$*, i.e.* $(-\Delta + V)u_n = \lambda_n u_n$ *for all* $n \in \mathbb{N}$ *where* $(u_n)_n$ *is an ONB and* $\lambda_n \xrightarrow{n\to\infty} 0$*.* □

Such potentials are of interest as they represent trapping potentials (almost) confining particle in some small physical region. In particular an important example is $V = |x|^2$ with $-\Delta + |x|^2$ representing the quantum harmonic oscillator.

Proof. $V \in L^p_{\text{loc}}(\mathbb{R}^d)$ and $V \uparrow \infty$ implies that $-\Delta + V$ is bounded from below. Now we have to prove that $-\Delta + V$ has eigenvalues $(\lambda_n)_n$ with $\lambda_n \uparrow +\infty$. By the min-max principle, this means that the min-max values $\mu_n \uparrow +\infty$ as $n \to \infty$. Assume by contradiction that $\mu_n \to \mu_\infty < \infty$. Then $\mu_\infty = \inf \sigma_{\text{ess}}(-\Delta + V)$.
By Weyl theory there exists a sequence of unit vectors (φ_n) that converges weakly to 0 in L^2 and

$$\|(-\Delta + V)\varphi_n - \mu_\infty \varphi_n\|_2 \xrightarrow{n\to\infty} 0$$

or equivalently

$$\int |\nabla \varphi_n|^2 + \int V|\varphi_n|^2 - \mu_\infty \xrightarrow{n\to 0} \infty.$$

For the first step, $V \in L^p_{\text{loc}}$ can be written as

$$V = V_1 + V_2$$

with $V = V_1 + V_2$, $V_1 \in L^p(\mathbb{R}^d)$, $V_2 \geqslant 0$, $V_2 \uparrow \infty$ as $|x| \to \infty$. By the Sobolev inequality

$$\int |\nabla \varphi_n|^2 + V_1|\varphi_n|^2 \geqslant \frac{1}{2}\int |\nabla \varphi_n|^2 - C$$

Thus

$$\frac{1}{2}\int |\nabla \varphi_n|^2 + \int V_2|\varphi_n|^2 \leqslant C$$

i.e. φ_n is bounded in H^1 and therefore there exists an H^1 weakly convergent subsequence. Further $\int V_2|\varphi_n|^2 \leqslant C$. As $\varphi_n \rightharpoonup 0$ in L^2 and φ_n bounded in H^1, $\varphi_n \rightharpoonup 0$ weakly in H^1. By

the Sobolev embedding $\mathbf{1}_{\{|x|\leqslant R\}}\varphi_n \to 0$ strongly in L^2.
On the other hand

$$C \geqslant \int V_2|\varphi_n|^2 \geqslant \int\limits_{|x|\geqslant R} V_2|\varphi_n|^2 \geqslant \left(\inf_{|x|\geqslant R} V_2\right) \int\limits_{|x|\geqslant R} |\varphi_n|^2$$

thus

$$\int\limits_{|x|\geqslant R} |\varphi_n|^2 \leqslant C\left(\inf_{|x|\geqslant R} V_2\right)^{-1} \xrightarrow{R\to\infty} 0$$

independently of n. Now we have

$$\int\limits_{\mathbb{R}^d} |\varphi_n|^2 = \int\limits_{|x|\leqslant R} |\varphi_n|^2 + \int\limits_{|x|>R} |\varphi_n|^2 \leqslant \int\limits_{|x|\leqslant R} |\varphi_n|^2 + C\left(\inf_{|x|\geqslant R} V_2\right)^{-1}$$

thus

$$\limsup_{n\to\infty} \int\limits_{\mathbb{R}^d} |\varphi_n|^2 \leqslant 0 + C\left(\inf_{|x|\geqslant R} V_2\right)^{-1} \xrightarrow{R\to\infty} 0$$

Therefore $\varphi_n \xrightarrow{n\to\infty} 0$ strongly in L^2. This contradicts $\|\varphi_n\|_2 = 1$. *q.e.d.*

Chapter 7

Semi-Classical Estimates

Remark 7.1 (Rigorous Results)**.** If V is nice enough, then $-\Delta+V$ has a finite number of eigenvalues.
Recall that for $e>0$, $V\leqslant 0$

$$(-\Delta+V)u=-eu \iff \varphi=K_e\varphi,\ K_e=\sqrt{|V|}(-\Delta+e)^{-1}\sqrt{|V|}$$

□

Remark 7.2 (Birmann-Schwinger Principle)**.**

- $-\Delta+V$ has an eigenvalue $-e$ iff K_e has an eigenvalue 1.
- If we call $N_{<-e}(-\Delta+V)$ the number of eigenvalues smaller than $-e$, then $N_{<-e}$ equals the number of eigenvalues of K_e which strictly greater 1.

□

Theorem 7.3 (Birmann-Schwinger Bound)**.** *Assume that* $0\geqslant V\in L^{d/2}(\mathbb{R}^d)$ *and* $d\geqslant 3$. *Then*

$$\textit{number of negative eigenvalues of } (-\Delta+V)\leqslant C\|V\|_{d/2}^2$$

with C *being a constant independent of* V. □

Proof. Let us assume that $d=3$. Then $V\in L^{3/2}$ and $K_e=\sqrt{|V|}(-\Delta+e)^{-1}\sqrt{|V|}$ is a

Hilbert-Schmidt operator with kernel

$$\begin{aligned}
K_e(x,y) &= \sqrt{|V(x)|}G_e(x-y)\sqrt{|V(y)|},\\
\|K_e\|_{\mathrm{HS}}^2 &= \mathrm{Tr}(K_eK_e) = \iint |V(x)|G_e(x-y)^2|V(y)|\mathrm{d}x\mathrm{d}y,\\
\hat{G}_e(k) &= \frac{1}{|2\pi k|^2+e},\\
G_e(x) &= \frac{e^{-\sqrt{e}|x|}}{4\pi|x|}.
\end{aligned}$$

Thus we find that

$$\|K_e\|^2 \leqslant \frac{1}{16\pi^2}\iint \frac{|V(x)V(y)|}{|x-y|^2}e^{-\sqrt{e}|x-y|}\mathrm{d}x\mathrm{d}y \leqslant \frac{1}{16\pi^2}\iint \frac{|V(x)V(y)|}{|x-y|^2}\mathrm{d}x\mathrm{d}y \leqslant C\|V\|_{3/2}^2$$

where the Hardy-Littlewood-Sobolev inequality was used in the last inequality.
From the second Birmann-Schwinger principle we therefore get

$$\begin{aligned}
N_{<-e} &= \text{number of eigenvalues of } (-\Delta+V) \text{ which are } < -e =\\
&= \text{number of eigenvalues of } K_e \text{ which are } > 1 =\\
&= \text{number of eigenvalues of } K_e^2 \text{ which are } > 1 \leqslant\\
&\leqslant \sum \text{ all eigenvalues of } K_e^2 = \|K_e\|_{\mathrm{HS}}^2 \leqslant C\|V\|_{3/2}^2
\end{aligned}$$

q.e.d.

Remark 7.4. The Birmann-Schwinger bound

$$N_{<0}(-\Delta+V) \leqslant C\|V\|_{3/2}^2$$

is not good semi-classically! The semi-classical approximation yields

$$N_{<0}(-\Delta+\lambda V) = \mathcal{O}(\lambda^{3/2})$$

in $\mathbb{R}^3$ as $\lambda \to \infty$. The Birman-Schwinger bound only gives us

$$N_{<0}(-\Delta + \lambda V) \leqslant C\lambda^2.$$

$\square$

Theorem 7.5 (Lieb-Thirring Inequality)**.** *For all $d \geqslant 1$ and $V = V_+ - V_-$ with $V_+ \in L^1_{loc}(\mathbb{R}^d)$, $V_- \in L^{1+\frac{d}{2}}(\mathbb{R}^d)$, then*

$$\mathrm{Tr}(-\Delta + V_-)_- \leqslant C \int\limits_{\mathbb{R}^d} V_-^{1+\frac{d}{2}}.$$

$\square$

Proof. Without loss of generality let us assume that $V \leqslant 0$ (why?). Let us consider $d = 3$.

$$\mathrm{Tr}(-\Delta + V)_- = \sum_{\lambda_i < 0} |\lambda_i(-\Delta + V)| = \sum_{\lambda_i<0} \int\limits_0^\infty \mathbf{1}_{\{|\lambda_i|>e\}} \mathrm{d}e = \int\limits_0^\infty \sum_{\lambda_i<0} \mathbf{1}_{\{\lambda_i<e\}} \mathrm{d}e =$$
$$= \int\limits_0^\infty N_{<-e}(-\Delta + V)\mathrm{d}e$$

Then from the Birgmann-Schwinger principle, we know that

$$N_{<-e}(-\Delta + V) \leqslant \|K_e\|^2 = \iint |V(x)||G_e(x-y)|^2|V(y)|\mathrm{d}x\mathrm{d}y \leqslant$$
$$\leqslant \iint \frac{|V(x)|^2 + |V(y)|^2}{2} |G_e(x-y)|^2 \mathrm{d}x\mathrm{d}y = \|V\|_2^2 \|G_e\|_2^2$$

Further

$$\|G_e\|_2^2 = \left\|\hat{G}_e\right\|_2^2 = \int\limits_{\mathbb{R}^d} \frac{1}{(|2\pi k|^2 + e)^2} \mathrm{d}k \overset{k=\sqrt{e}\ell}{=\!=} \int\limits_{\mathbb{R}^d} \frac{e^{d/2}\mathrm{d}\ell}{e^2(|2\pi\ell|^2+1)^2} = e^{\frac{d}{2}-1}\mathrm{const}$$

with the constant being finite for $d \leqslant 3$. Thus $N_{<-e}(-\Delta + V) \leqslant Ce^{\frac{d}{2}-2} \int V_-(x)^2 \mathrm{d}x$ and therefore

$$N_{<-e}(-\Delta + V) = N_{<-\frac{e}{2}}(-\Delta + V + \frac{e}{2}) \leqslant C\Big(\frac{e}{2}\Big)^{\frac{d}{2}-2} \int [V(x) + \frac{e}{2}]_-^2 \mathrm{d}x$$

Now

$$\begin{aligned}\operatorname{Tr}(-\Delta+V)_- &= \int_0^\infty N_{<-e}(-\Delta+V)\mathrm{d}e \leqslant C\int_{\mathbb{R}^d}\int_0^\infty \left(\frac{e}{2}\right)^{\frac{d}{2}-2}\left[V(x)+\frac{e}{2}\right]_-^2 \mathrm{d}e\mathrm{d}x = \\ &= C\int_{\mathbb{R}^d} |V_-(x)|^{1+\frac{d}{2}}\mathrm{d}x\end{aligned}$$

where the substitution $e = 2V(x)t$ was used in the last equality.

When $d \geqslant 4$, the proof has to be changed. *q.e.d.*

Remark 7.6. 1) Kato-Rellich: For a symmmetric operator B and a self-adjoint operator A, if B is A-bounded, with relative bound $a < 1$, i.e.

$$\|Bu\| \leqslant a\|Au\| + C\|u\|$$

for all $u \in D(A) \subset D(B)$. Then $A + B$ is self-adjoint with $D(A + B) = D(A)$.

2) If B is A-compact, i.e. $B(A + i)^{-1}$ if is compact, then

- B is A-bounded with relative bound $\varepsilon > 0$ for ε sufficiently small, in particular $A + B$ is self-adjoint with $D(A + B) = D(A)$.
- $\sigma_{\text{ess}}(A + B) = \sigma_{\text{ess}}(A)$.

3) Friedrich's Extension: If K is symmetric, $K \geqslant -C$ then there exists a self-adjoint extension (but we do not know the domain).

□

Example 7.7 (Schrödinger Operators)**.** $-\Delta + V$, $D(-\Delta) = H^2(\mathbb{R}^d)$, $A = -\Delta$, $B = V$.

1) If $V \in L^p + L^q$ with

$$\begin{cases} 2 \leqslant p, q \leqslant \infty, & \text{if } d = 1, 2, 3 \\ \frac{d}{2} < p, q \leqslant \infty, & \text{if } d \geqslant 4 \end{cases}$$

Then V is $(-\Delta)$-bounded with relative bounded $\varepsilon > 0$ for all sufficiently small $\varepsilon > 0$. Consequently, $-\Delta + V$ is self-adjoint in H^2.

2) If $V \in L^p + L^q$ with

$$\begin{cases} 2 \leqslant p, q < \infty, & \text{if } d = 1, 2, 3 \\ \frac{d}{2} < p, q < \infty, & \text{if } d \geqslant 4 \end{cases}$$

Then V is $(-\Delta)$-compact, consequently

$$\sigma_{\text{ess}}(-\Delta + V) = \sigma_{\text{ess}}(-\Delta) = [0, \infty)$$

Here $V \in L^\infty$ is not allowed! Because if $V = 1$,

$$\sigma_{\text{ess}}(-\Delta + 1) = \sigma_{\text{ess}}(-\Delta) + 1 = [1, \infty).$$

3) Quadratic Form Approach: If $V \in L^p + L^q$ with

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

Then $-\Delta + V \geqslant -C$ hence there exits a self-adjoint extension of $-\Delta + V$. We do not know the domain, but we know that the quadratic form domain is H^2.

If $V \in L^p + L^q$ with

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

then $\sigma_{\text{ess}}(-\Delta + V) = \sigma_{\text{ess}}(-\Delta) = [0, \infty)$. But we do not know if V $(-\Delta)$-compact!

4) $\sqrt{-\Delta} - \frac{a}{|x|}$ is self-adjoint on $H^1(\mathbb{R}^3)$ for $0 < a < \frac{1}{2}$.

We have to prove that $-\frac{a}{|x|}$ is $\sqrt{-\Delta}$-bounded with relative bound < 1.

??????????????

Theorem 7.8 (Kinetic Version of the Lieb-Thirring Inequality)**.** *Let γ be a finite-rank* *projection, i.e.*

$$\gamma = \sum_{i=1}^{N} |u_i\rangle \langle u_i|$$

for an ONF $(u_i)_{i=1}^N$ *in* $L^2(\mathbb{R}^d)$ *with kernel*

$$\gamma(x,y) = \sum_{i=1}^{N} u_i(x)\overline{u_i(y)}$$

We may define the density of γ *to be*

$$\rho_\gamma(x) = \gamma(x,x) = \sum_{i=1}^{N} |u_i(x)|^2.$$

Then we have the inequality

$$\sum_{i=1}^{N} \int_{\mathbb{R}^d} |\nabla u_i|^2 \geqslant \kappa \int_{\mathbb{R}^d} \rho_\gamma(x)^{1+\frac{2}{d}} \mathrm{d}x$$

with a universal constant $\kappa = \kappa(d) > 0$*. Consequently, we obtain the Lieb-Thirring inequality for the sum of negative eigenvalues*

$$\mathrm{Tr}[-\Delta + V]_- \leqslant C \int_{\mathbb{R}^d} V_-^{1+\frac{d}{2}}$$

for a universal constant $C = C(d) > 0$*.* □

Proof.

Step 1 Why does the kinetic inequality imply the Lieb-Thirring inequality? Assume that $-\Delta + V$ has negative eigenvalues $-\mu_i$ and eigenfunctions u_i with $\mu_i > 0$ and

$$(-\Delta + V)u_i = -\mu_i u_i$$

Take $N \in \mathbb{N}$. Define $\gamma = \sum_{i=1}^N |u_i\rangle \langle u_i|$. Then

$$\sum_{i=1}^N -\mu_i = \sum_{i=1}^N \langle u_i, (-\Delta + V)u_i\rangle = \sum_{i=1}^N \left(\int |\nabla u_i|^2 + \int V|u_i|^2 \right) = \sum_{i=1}^N \int |\nabla u_i|^2 + \int V \rho_\gamma \geqslant$$

$$\geqslant \kappa \int \rho_\gamma^{1+\frac{2}{d}} - \int V_- \rho_\gamma \geqslant \int \left(\kappa \rho_\gamma^{1+\frac{2}{d}} - \frac{\rho_\gamma^{1+\frac{2}{d}}}{1+\frac{2}{d}} - \frac{V_-^{1+\frac{d}{2}}}{1+\frac{d}{2}} \right) \geqslant -\frac{1}{1+\frac{d}{2}} \int V_-^{1+\frac{d}{2}}$$

where $\kappa > \frac{1}{1+\frac{2}{d}}$ for $d \geqslant 1$ is used in the last inequality which is proven below.

Thus we find

$$\sum_{i=1}^N \mu_i \leqslant \frac{1}{1+\frac{d}{2}} \int V_-^{1+\frac{d}{2}}$$

taking N to ∞ yields then the conclusion.

Step 2 Proof of the Kinetic inequality.

Originally, Lieb and Thirring proved in 1975 their inequality via the Kinetic inequality and a duality argument (i.e. optimising V). Here we present a new proof of the kinetic inequality by Rumin 2011 (Solovej's Version)

$$\int\limits_{\mathbb{R}^d} |\nabla u_i|^2 = \int\limits_{\mathbb{R}^d} |2\pi k|^2 |\hat{u}_i(k)|^2 \mathrm{d}k = \int\limits_{\mathbb{R}^d} \int\limits_0^\infty \mathbf{1}_{\{|2\pi k|^2 > e\}} |\hat{u}_i(k)|^2 \mathrm{d}e \mathrm{d}k$$

Define

$$\hat{u}_i^+(k) := \hat{u}_i(k) \mathbf{1}_{\{|2\pi k|^2 > e\}}$$
$$\hat{u}_i^-(k) := \hat{u}_i(k) \mathbf{1}_{\{|2\pi k|^2 \leqslant e\}}$$

in particular $u_i = u_i^+ + u_i^-$ (where $u_i^\pm := \check{\hat{u}}_i^\pm$). Thus

$$\sum_{i=1}^N \int |\nabla u_i|^2 = \sum_{i=1}^N \int\limits_{\mathbb{R}^d} \int\limits_0^\infty |\hat{u}_i^+(k)|^2 \mathrm{d}e \mathrm{d}k = \sum_{i=1}^N \int\limits_0^\infty \int\limits_{\mathbb{R}^d} |u_i^+(x)|^2 \mathrm{d}k \mathrm{d}e =$$

$$= \sum_{i=1}^N \int\limits_0^\infty \int\limits_{\mathbb{R}^d} |u_i(x) - u_i^-(x)|^2 \mathrm{d}k \mathrm{d}e$$

Using the reverse triangle inequality we find

$$\left(\sum_{i=1}^{N}|u_i(x)-u_i^-(x)|^2\right)^{1/2}\geqslant\left|\left(\sum_{i=1}^{N}|u_i(x)|^2\right)^{1/2}-\left(\sum_{i=1}^{N}|u_i^-(x)|^2\right)^{1/2}\right|$$

from which we get

$$\sum_{i=1}^{N}\int|\nabla u_i|^2\geqslant\int\limits_{\mathbb{R}^d}\int\limits_0^{\infty}\left|\sqrt{\sum_{i=1}^{N}|u_i(x)|^2}-\sqrt{\sum_{i=1}^{N}|u_i^-(x)|^2}\right|^2$$

Here

$$\sum_{i=1}^{N}|u_i(x)|^2=\rho_\gamma(x)$$

and

$$\sum_{i=1}^{N}|u_i^-(x)|^2=\sum_{i=1}^{N}\left|\int\limits_{\mathbb{R}^d}\hat{u}_i^-(k)e^{2\pi ikx}\mathrm{d}k\right|^2=\sum_{i=1}^{N}\left|\int\limits_{\mathbb{R}^d}\hat{u}_i(k)\mathbf{1}_{|2\pi k|^2\leqslant e}e^{2\pi ikx}\mathrm{d}k\right|^2\leqslant$$
$$\leqslant\int\limits_{\mathbb{R}^d}\left|\mathbf{1}_{|2\pi k|^2\leqslant e}e^{2\pi ikx}\right|^2\mathrm{d}k=\int\limits_{\mathbb{R}^d}\mathbf{1}_{|k|\leqslant\frac{\sqrt{e}}{2\pi}}\mathrm{d}k=|B_1|\left(\frac{\sqrt{e}}{2\pi}\right)^d$$

where the Bessel inequality was used in the last inequality.

Noting that for $0\leqslant b\leqslant b'$, $a\geqslant 0$

$$|a-b|\geqslant[a-b]_+\geqslant[a-b']_+$$

Thus we conclude

$$\sum_{i=1}^{N}\int|\nabla u_i|^2\geqslant\int\limits_{\mathbb{R}^d}\int\limits_0^{\infty}\left[\sqrt{\rho_\gamma(x)}-\sqrt{|B_1|}\left(\frac{\sqrt{e}}{2\pi}\right)^{d/2}\right]_+^2\mathrm{d}e\mathrm{d}x=\kappa\int\limits_{\mathbb{R}^d}\rho_\gamma(x)^{1+\frac{2}{d}}$$

as

$$\int\limits_0^{\infty}\left[a-e^{\frac{d}{4}}\right]_+^2\mathrm{d}e=\int\limits_0^{a^{4/d}}(a-e^{d/4})^2\mathrm{d}e=ca^{2+\frac{4}{d}}$$

with

$$\kappa(d)=\frac{4d^2\pi}{8+6d+d^2}\Gamma\left(1+\frac{d}{2}\right)^{2/d}$$

which satisfies

$$\kappa(d) > \frac{1}{1+\frac{2}{d}}$$

for $d \geqslant 1$.

q.e.d.

Theorem 7.9 (CLR Bound)**.** *If $V_- \in L^{\frac{d}{2}}(\mathbb{R}^d)$, $d \geqslant 3$ then*

$$N(-\Delta + V) \leqslant C \int_{\mathbb{R}^d} V_-^{\frac{d}{2}}$$

where $N(-\Delta + V)$ denotes the number of negative eigenvalues. □

Remark 7.10. 1) The Lieb-Thirring inequality is true for all $d \geqslant 1$, but CLR is true only for $d \geqslant 3$. The reason for this is that for $d = 1, 2$ and $V \in \mathscr{C}_c^\infty$, $V \leqslant 0$, $V \not\equiv 0$ then $-\Delta + V$ has at least one negative eigenvector.

2) The CLR bound is stronger than the LT bound (when $d \geqslant 3$). For example we can prove LT by using CLR as follows

$$\left|\sum \text{negative eigenvalues}\right| = \int_0^\infty N_{<-e}(-\Delta + V)\mathrm{d}e = \int_0^\infty N_{<-\frac{e}{2}}(-\Delta + V + \frac{e}{2})\mathrm{d}e \leqslant$$

$$\leqslant C \int_0^\infty \int_{\mathbb{R}^d} \left[V + \frac{e}{2}\right]_-^{\frac{d}{2}} \mathrm{d}x\mathrm{d}e = C \int_{\mathbb{R}^d} V_-^{1+\frac{d}{2}}\mathrm{d}x$$

□

Proof. We shall prove the CLR bound via the Rumin method. Assume $-\Delta + V$ has $\geqslant N$ negative eigenvalues, i.e. $\dim(P(-\Delta + V < 0)) \geqslant N$, i.e. the space spanned by negative eigenvalue eigenfunctions. Thus $\dim(\sqrt{-\Delta}P(-\Delta + V < 0)) \geqslant N$ as $\sqrt{-\Delta}$ has a trivial kernel. Thus we can choose $(\varphi_i)_{i=1}^N$ in $P(-\Delta + V < 0)$ such that $\left(\sqrt{-\Delta}\varphi_i\right)_{i=1}^N$ is an ONF on L^2 i.e. $\left\langle\sqrt{-\Delta}\varphi_i, \sqrt{-\Delta}\varphi_j\right\rangle = \delta_{ij}$.

Using the same notation as in the proof of the LT bound we have

$$N=\sum_{i=1}^N\|\sqrt{-\Delta}\varphi_i\|^2=\sum_{i=1}^N\int_{\mathbb{R}^d}|\nabla\varphi_i|^2\mathrm{d}x=\sum_{i=1}^N\int_{\mathbb{R}^d}\int_0^\infty|\varphi_i^+|^2\mathrm{d}e\mathrm{d}x=\sum_{i=1}^N\int_{\mathbb{R}^d}\int_0^\infty|\varphi_i(x)-\varphi_i^-(x)|^2\mathrm{d}e\mathrm{d}x\geqslant$$

$$\geqslant\int_{\mathbb{R}^d}\int_0^\infty\left[\sqrt{\sum_{i=1}^N|\varphi_i(x)|^2}-\sqrt{\sum_{i=1}^N|\varphi_i^-(x)|^2}\right]_+^2\mathrm{d}e\mathrm{d}x$$

Note that

$$\begin{aligned}\sum_{i=1}^N|\varphi_i^-(x)|^2&=\sum_{i=1}^N\left|\int\hat{\varphi}_i^-(x)\mathbf{1}_{\{|2\pi k|^2\leqslant e\}}e^{2\pi ikx}\mathrm{d}x\right|^2=\\&=\sum_{i=1}^N\left|\int|2\pi k|\hat{\varphi}_i^-(x)\frac{\mathbf{1}_{\{|2\pi k|^2\leqslant e\}}}{|2\pi k|}e^{2\pi ikx}\mathrm{d}x\right|^2\overset{\text{Bessel}}{\leqslant}\\&\leqslant\int\frac{\mathbf{1}_{\{|2\pi k|^2\leqslant e\}}}{|2\pi k|^2}\mathrm{d}k=(2\pi)^{-d}\int\frac{\mathbf{1}_{\{|k|^2\leqslant e\}}}{|k|^2}\mathrm{d}k=\frac{2\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)(2\pi)^d}\int_0^\infty\frac{\mathbf{1}_{\{r^2<e\}}}{r^2}r^{d-1}dr=\\&=\frac{2\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)(2\pi)^d}\int_0^{\sqrt{e}}r^{d-3}\mathrm{d}r=\frac{2\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)(2\pi)^d(d-2)}e^{\frac{d-2}{2}}\end{aligned}$$

Thus

$$N=\sum_{i=1}^N\int|\nabla\varphi_i|^2\geqslant\int_{\mathbb{R}^d}\int_0^\infty\left[\sqrt{\rho(x)}-ce^{\frac{d-2}{4}}\right]_+^2\mathrm{d}e\mathrm{d}x=K\int\rho(x)^{\frac{d}{d-2}}$$

where

$$K(d)=\frac{(d-2)^2}{d(d+2)}\left(\frac{\Gamma\left(\frac{d}{2}\right)(d-2)}{2^{1-d}\pi^{-\frac{d}{2}}}\right)^{\frac{2}{d-2}}$$

which satisfies $K(d)>20$ for $d\geqslant 3$.

Therefore we conclude that

$$\begin{aligned}0\geqslant\sum_{i=1}^N\langle u_i,(-\Delta+V)u_i\rangle&=N+\int V\rho\geqslant\frac{N}{2}+\frac{K}{2}\int\rho^{\frac{d}{d-2}}-\int V_-\rho\geqslant\\&\geqslant\frac{N}{2}+\frac{K}{2}\int\rho^{\frac{d}{d-2}}-\frac{d-2}{d}\int\rho^{\frac{d}{d-2}}-\frac{2}{d}\int V_-^{\frac{d}{2}}\geqslant\frac{N}{2}-\frac{2}{d}\int V_-^{\frac{d}{2}}\end{aligned}$$

where Young's inequality $ab\leqslant\frac{a^p}{p}+\frac{b^q}{q}$, for $p^{-1}+q^{-1}=1$, was used in the penultimate inequality and used that $\frac{K(d)}{2} - \frac{d-2}{d} > 0$. Hence

$$N \leqslant \frac{4}{d} \int V_-^{\frac{d}{2}}.$$

q.e.d.

Remark 7.11 (Semi-Classical Approximation)**.** In quantum mechanics a particle is described by $\psi \in L^2(\mathbb{R}^d)$ with $|\psi(x)|^2$ being the probability density of the position and $|\hat{\psi}(k)|^2$ the probability density of the momentum. In classical mechanics on the other hand a particle is described by a point $(x, k) \in \mathbb{R}^d \times \mathbb{R}^d$.
For a semiclassical approximation we are interested in the non-positive eigenvalues of a Schrödinger operator $-\Delta + V$ for which

$$\operatorname{Tr}[-\Delta + V]_- \approx \iint \left[|2\pi k|^2 + V(x)\right]_- \mathrm{d}k\mathrm{d}x = L_{\mathrm{cl}} \int\limits_{\mathbb{R}^d} V_-(x)^{1+\frac{d}{2}} \mathrm{d}x$$

Here $a_\pm = \max\{\pm a, 0\}$. Changing variables to $|2\pi k|^2 = V_- \ell^2$ which is equivalent to

$$k = \frac{\sqrt{V_-}}{2\pi} \ell, \quad \mathrm{d}k = \frac{V_-^{\frac{d}{2}}}{(2\pi)^d} d\ell$$

we get

$$\int \left[|2\pi k|^2 + V(x)\right]_- \mathrm{d}k = \int \left[V_- |\ell|^2 + V\right] \frac{V_-^{\frac{d}{2}}}{(2\pi)^d} \mathrm{d}\ell = V_-(x)^{\frac{d}{2}+1} \int \frac{[\ell^2 + 1]_-}{(2\pi)^d} \mathrm{d}\ell$$

here we therefore have

$$L_{\mathrm{cl}} = \int \frac{[\ell^2 + 1]_-}{(2\pi)^d} \mathrm{d}\ell = \frac{1}{(2\pi)^d} \frac{2|S^{d-1}|}{d(d+2)}$$

called the semi-classical constant.

$\square$

Theorem 7.12 (Lieb-Thirring Inequality)**.** *If $V_- \in L^{1+\frac{d}{2}}(\mathbb{R}^d)$, then*

$$\operatorname{Tr}[-\Delta + V]_- \leqslant C \int V_-(x)^{1+\frac{d}{2}} \mathrm{d}x$$

where C is independent of V. □

Theorem 7.13 (Weyl Assymptotics). *If $V_- \in L^{1+\frac{d}{2}}(\mathbb{R}^d)$, then*

$$\lim_{\lambda\to\infty} \frac{1}{\lambda^{1+\frac{d}{2}}} \operatorname{Tr}[-\Delta + \lambda V]_- = L_{cl} \int_{\mathbb{R}^d} V_-^{1+\frac{d}{2}}$$

i.e.

$$\operatorname{Tr}(-\Delta + \lambda V)_- = L_{cl} \int (\lambda V_-)^{1+\frac{d}{2}} + o\Big(\lambda^{1+\frac{d}{2}}\Big).$$

Here

$$\operatorname{Tr}(-\Delta + \lambda V)_- = \lambda \operatorname{Tr}\left[\frac{1}{\lambda}(-\Delta) + V\right]_-$$

Therefore, Weyl's theorem is equivalent to

$$\operatorname{Tr}\big[\hbar^2(-\Delta) + V\big]_- = \hbar^{-d} L_{cl} \int_{\mathbb{R}^d} V_-(x)^{1+\frac{d}{2}} \mathrm{d}x + o(\hbar^{-d})$$

when $\hbar \downarrow 0$. Here $\hbar$ is interpreted as the reduced Plank's constant. □

Definition 7.14 (Coherent States (Schrödinger 1926)). Take $G \in \mathscr{C}_c^\infty(\mathbb{R}^d)$ with $G(x) = G(-x)$ and $\|G\|_2 = 1$. For every $(k, y) \in \mathbb{R}^d \times \mathbb{R}^d$, we defined

$$F_{k,y}(x) = e^{2\pi i k\cdot x} G(x - y)$$

Also we denote projection

$$\pi_{k,y} := |F_{k,y}\rangle \langle F_{k,y}| \,.$$

□

Lemma 7.15 (Coherent States Identities). *For every $(k, y) \in \mathbb{R}^d \times \mathbb{R}^d$, $F_{k,y} \in L^2(\mathbb{R}^d)$*

and $\|F_{k,y}\|_2 = 1$. *Moreover, we have for all* $\psi \in L^2(\mathbb{R}^d)$

$$\int\limits_{\mathbb{R}^d} |\langle F_{k,y}, \psi\rangle|^2 \mathrm{d}k = (|G|^2 * |\psi|^2)(y)$$

$$\int\limits_{\mathbb{R}^d} |\langle F_{k,y}, \psi\rangle|^2 \mathrm{d}y = (|\hat{G}|^2 * |\hat{\psi}|^2)(k)$$

in particular

$$\int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} |\langle F_{k,y}, \psi\rangle|^2 \mathrm{d}k\mathrm{d}y = \|\psi\|_2^2$$

which can be suggestively written as

$$\int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} \pi_{k,y} \mathrm{d}k\mathrm{d}y = \mathbf{1}$$

□

Proof. Let $\psi \in L^2$, then

$$\int\limits_{\mathbb{R}^d} |\langle F_{k,y}, \psi\rangle|^2 \mathrm{d}k = \int\limits_{\mathbb{R}^d}\left|\int\limits_{\mathbb{R}^d} \overline{e^{2\pi i k\cdot x} G(x-y)}\psi(x)\mathrm{d}x\right|^2 \mathrm{d}k = \int\limits_{\mathbb{R}^d}\left|\widehat{G(\cdot - y)\psi}(\cdot)(k)\right|^2 \mathrm{d}k =$$
$$= \int\limits_{\mathbb{R}^d} |G(x-y)\psi(x)|^2 \mathrm{d}x = |G|^2 * |\psi|^2(y)$$

The second identity is left to the exercises and the last equation follows from the first with Fubini as

$$\int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} |\langle F_{k,y}, \psi\rangle|^2 \mathrm{d}k\mathrm{d}y = \int\limits_{\mathbb{R}^d} |G|^2 * |\psi|^2(y)\mathrm{d}y = \int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} |G(x-y)|^2|\psi(x)|^2 \mathrm{d}x\mathrm{d}y =$$
$$= \int\limits_{\mathbb{R}^d} |\psi(x)|^2 \int\limits_{\mathbb{R}^d} |G(x-y)|^2 \mathrm{d}y\mathrm{d}x = \int\limits_{\mathbb{R}^d} |\psi(x)|^2 \mathrm{d}x = \|\psi\|_2^2$$

q.e.d.

Lemma 7.16. *For every $\psi \in H^1(\mathbb{R}^d)$,*

$$\int\limits_{\mathbb{R}^d} |\nabla\psi|^2 = \int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} |2\pi k|^2 |\left\langle F_{k,y}, \psi\right\rangle|^2 \mathrm{d}k\mathrm{d}y - \|\nabla G\|_2^2 \|\psi\|_2^2$$

and

$$\int\limits_{\mathbb{R}^d} (V * |G|^2)|\psi|^2 = \int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} V(y) |\left\langle F_{k,y}, \psi\right\rangle|^2 \mathrm{d}k\mathrm{d}y$$

□

Proof. From the previous lemma we know that

$$\int\limits_{\mathbb{R}^d} |\left\langle F_{k,y}, \psi\right\rangle|^2 \mathrm{d}y = (|\hat{G}|^2 * |\hat{\psi}|^2)(k)$$

therefore

$$\begin{aligned}\int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} |2\pi k|^2 |\left\langle F_{k,y}, \psi\right\rangle| \mathrm{d}k\mathrm{d}y &= \int\limits_{\mathbb{R}^d} |2\pi k|^2 \Big(|\hat{G}|^2 * |\hat{\psi}|^2\Big)(k)\mathrm{d}k = \int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} |2\pi k|^2 |\hat{G}(k-q)|^2 |\hat{\psi}(q)|^2 \mathrm{d}q\mathrm{d}k = \\ &= \int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} |2\pi(k-q+q)|^2 |\hat{G}(k-q)|^2 |\hat{\psi}(q)|^2 \mathrm{d}q\mathrm{d}k = \\ &= \int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} \big(|2\pi(k-q)|^2 + (2\pi)^2 2(k-q)\cdot q + |2\pi q|^2\big) |\hat{G}(k-q)|^2 |\hat{\psi}(q)|^2 \mathrm{d}q\mathrm{d}k\end{aligned}$$

Concerning the first term

$$\begin{aligned}\int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} |2\pi(k-q)|^2 |\hat{G}(k-q)|^2 |\hat{\psi}(q)|^2 \mathrm{d}q\mathrm{d}k &= \int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} |2\pi\ell|^2 |\hat{G}(\ell)|^2 |\hat{\psi}(q)|^2 \mathrm{d}q\mathrm{d}\ell = \\ &= \int\limits_{\mathbb{R}^d} |2\pi\ell|^2 |\hat{G}(\ell)|^2 \mathrm{d}\ell \int\limits_{\mathbb{R}^d} |\hat{\psi}(q)|^2 \mathrm{d}q = \|\nabla G\|_2^2 \|\psi\|_2^2\end{aligned}$$

Similarly

$$\int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} |2\pi q|^2 |\hat{G}(k-q)|^2 |\hat{\psi}(q)|^2 \mathrm{d}q\mathrm{d}k = \|\nabla\psi\|_2^2 \|G\|_2^2 = \|\nabla\psi\|_2^2$$

and for the second term

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}(2\pi)^2 2(k-q)\cdot q|\hat{G}(k-q)|^2|\hat{\psi}(q)|^2\mathrm{d}q\mathrm{d}k = \underbrace{\left(\int_{\mathbb{R}^d}\ell|\hat{G}(\ell)|^2\mathrm{d}l\right)}_{=0}\cdot\left(\int_{\mathbb{R}^d}q|\hat{\psi}(q)|^2\mathrm{d}q\right) = 0$$

as $|\hat{G}(-\ell)| = |\hat{G}(\ell)|$ as follows from the symmetry of G.

For the second identity we use

$$\int_{\mathbb{R}^d} |\langle F_{k,y},\psi\rangle|^2\mathrm{d}k = (|G|^2 * |\psi|^2)(y)$$

from which follows

$$\begin{aligned}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} V(y)|\langle F_{k,y},\psi\rangle|^2\mathrm{d}k\mathrm{d}y &= \int_{\mathbb{R}^d} V(y)(|G|^2 * |\psi|^2)(y)\mathrm{d}y = \\ &= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} V(y)\underbrace{|G(y-z)|^2}_{=|G(z-y)|^2}|\psi(z)|^2\mathrm{d}y\mathrm{d}z = \\ &= \int (V * |G|^2)(z)|\psi(z)|^2\mathrm{d}z\end{aligned}$$

q.e.d.

Proof of Theorem 7.13. Let us consider the case $d \geqslant 3$ such that we can use the CLR bound.

Step 1 Assume that $V \in \mathscr{C}_c^\infty(\mathbb{R}^d)$. Take $(u_i)_{i=1}^N$ to be a finite ONF in $L^2(\mathbb{R}^d)$ such that $u_i \in H^1(\mathbb{R}^d)$. We want to prove that

$$\sum_{i=1}^N \langle u_i, (-\Delta + V)u_i\rangle \geqslant -L_{\mathrm{cl}}\int_{\mathbb{R}^d} V_-^{1+\frac{d}{2}} + \text{error}$$

We have

$$\sum_{i=1}^N \left\langle u_i, (-\Delta + V * \left| G \right|^2)u_i\right\rangle = \sum_{i=1}^\infty \iint \big(|2\pi k|^2 + V(y)\big)|\langle F_{k,y}, u_i\rangle|^2\mathrm{d}k\mathrm{d}y - N\|\nabla G\|_2^2$$

The key observation is to note that for all $(k,y) \in \mathbb{R}^d \times \mathbb{R}^d$

$$0 \leqslant \sum_{i=1}^{N} |\langle F_{k,y}, u_i\rangle|^2 \leqslant \|F_{k,y}\|_2^2 = 1$$

which leads to

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \big(|2\pi k|^2 + V(y)\big) \sum_{i=1}^{N} |\langle F_{k,y}, u_i\rangle| \mathrm{d}k\mathrm{d}y \geqslant -\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \big[|2\pi k|^2 + V(y)\big]_- \mathrm{d}k\mathrm{d}y = -L_{\mathrm{cl}} \int V_-^{1+\frac{d}{2}}$$

Step 2 Assume that $-\Delta + V$ has N negative eigenvalues with eigenfunctions u_i. When $d \geqslant 3$ and V is nice enough we have the CLR bound

$$N \leqslant C \int_{\mathbb{R}^d} V^{\frac{d}{2}}.$$

Take $0 < \eta < 1$ and write

$$\sum_{i=1}^{N} \langle u_i, (-\Delta + V) u_i\rangle = \sum_{i=1}^{N} \big\langle u_i, \big((1-\eta)(-\Delta) + V * |G|^2\big) u_i\big\rangle + \sum_{i=1}^{N} \big\langle u_i, \big(\eta(-\Delta) + (V - V * |G|^2)\big) u_i\big\rangle$$

We can estimate the two terms separately. From Step 1 we have

$$\begin{aligned}\sum_{i=1}^{N} \big\langle u_i, \big((1-\eta)(-\Delta) + V * |G|^2\big) u_i\big\rangle &= (1-\eta) \sum_{i=1}^{N} \left\langle u_i, \left((-\Delta) + \frac{V}{1-\eta} * |G|^2\right) u_i\right\rangle \geqslant \\ &\geqslant (1-\eta)\left(-L_{\mathrm{cl}} \int_{\mathbb{R}^d} \left(\frac{V_-}{1-\eta}\right)^{1+\frac{d}{2}} - N\|\nabla G\|_2^2\right).\end{aligned}$$

For the second term we use the Lieb-Thirring inequality

$$\begin{aligned}\sum_{i=1}^{N} \big\langle u_i, \big(\eta(-\Delta) + (V - V * |G|^2)\big) u_i\big\rangle &= \eta \sum_{i=1}^{N} \left\langle u_i, \left(-\Delta + \frac{V - V * |G|^2}{\eta}\right) u_i\right\rangle \geqslant \\ &\geqslant -\eta \operatorname{Tr}\left[-\Delta + \frac{V - V * |G|^2}{\eta}\right]_- \geqslant \\ &\geqslant -C\eta \int_{\mathbb{R}^d} \left|\frac{V - V * |G|^2}{\eta}\right|^{1+\frac{d}{2}}\end{aligned}$$

Thus we have

$$
\begin{aligned}
-\operatorname{Tr}[-\Delta+V]_- = \sum_{i=1}^{N} \langle u_i, (-\Delta+V)u_i\rangle \geqslant \\
\geqslant -\frac{L_{\mathrm{cl}}}{(1-\eta)^{\frac{d}{2}}}\int V_-^{1+\frac{d}{2}} - C\int V_-^{\frac{d}{2}}\|\nabla G\|_2^2 - \frac{C}{\eta^{\frac{d}{2}}}\int \left|V - V*|G|^2\right|^{1+\frac{d}{2}}
\end{aligned}
$$

for all $0<\eta<1$.

Replacing V by λV and dividing by $\lambda^{1+\frac{d}{2}}$ we get

$$
-\frac{1}{\lambda^{1+\frac{d}{2}}}\operatorname{Tr}[-\Delta+V]_- \geqslant -\frac{L_{\mathrm{cl}}}{(1-\eta)^{\frac{d}{2}}}\int V_-^{1+\frac{d}{2}} - \frac{C}{\lambda}\int V_-^{\frac{d}{2}}\|\nabla G\|_2^2 - \frac{C}{\eta^{\frac{d}{2}}}\int \left|V - V*|G|^2\right|^{1+\frac{d}{2}}
$$

We gain the lower bound

$$
\liminf_{\lambda\to\infty} -\frac{1}{\lambda^{1+\frac{d}{2}}}\operatorname{Tr}[-\Delta+V]_- \geqslant -\frac{L_{\mathrm{cl}}}{(1-\eta)^{\frac{d}{2}}}\int V_-^{1+\frac{d}{2}} - \frac{C}{\eta^{\frac{d}{2}}}\int \left|V - V*|G|^2\right|^{1+\frac{d}{2}}
$$

for all $0<\eta<1$ and all G satisfying the assumption for the coherent state.

Next, we can choose $G_s(x) = \frac{1}{\sqrt{s^d}}G_0\left(\frac{x}{s}\right)$ where G_0 is some fixed, nice function and take $s\to 0$.

We know that $\lim_{s\to 0}(V - V*|G_s|^2)$ in $L^{1+\frac{d}{2}}$ strongly if $V^{1+\frac{d}{2}}$. This means that

This means that

$$
\liminf_{\lambda\to\infty} -\frac{1}{\lambda^{1+\frac{d}{2}}}\operatorname{Tr}[-\Delta+V]_- \geqslant -\frac{L_{\mathrm{cl}}}{(1-\eta)^{\frac{d}{2}}}\int V_-^{1+\frac{d}{2}}
$$

taking $\eta\to 0$ this gives us the lower bound

$$
\liminf_{\lambda\to\infty} -\frac{1}{\lambda^{1+\frac{d}{2}}}\operatorname{Tr}[-\Delta+V]_- \geqslant -L_{\mathrm{cl}}\int V_-^{1+\frac{d}{2}}.
$$

Step 3 For a general potential V, $V_-\in L^{1+\frac{d}{2}}$ we note that $-\Delta+V\geqslant -\Delta-V_-$ as a quadratic form thus

$$
-\operatorname{Tr}[-\Delta+V]_- \geqslant -\operatorname{Tr}[-\Delta-V_-]_-.
$$

This follows from the general fact that if $A\geqslant B$ as quadratic forms then $\mu_i(A)\geqslant\mu_i(B)$ for all $i\in\mathbb{N}$, where μ_i is the i^{th} min-max-value (by the min-max principle).

For the lower bound, we can therefore assume that $V\leqslant 0$ and $V\in L^{1+\frac{d}{2}}$. Since $V\in L^{1+\frac{d}{2}}$, we can choose $V_n \in \mathscr{C}_c^\infty(\mathbb{R}^d)$ and $V_n \to V$ strongly in $L^{1+\frac{d}{2}}$. We can write

$$\begin{aligned}\liminf_{\lambda\to\infty} \frac{1}{\lambda^{1+\frac{d}{2}}} \operatorname{Tr}[-\Delta+V]_- &= \liminf_{\lambda\to\infty}\left(\frac{1}{\lambda^{1+\frac{d}{2}}}\operatorname{Tr}[(1-\eta)(-\Delta)+\lambda V_n]_- + \frac{1}{\lambda^{1+\frac{d}{2}}}\operatorname{Tr}[\eta(-\Delta)+\lambda(V_n-V)]_-\right) \geqslant \\ &\geqslant \liminf_{\lambda\to\infty}(1-\eta)\left(-\frac{\operatorname{Tr}\left[-\Delta+\frac{\lambda V}{(1-\eta)}\right]_-}{\lambda^{1+\frac{d}{2}}}\right) - \eta\liminf_{\lambda\to\infty}\frac{\operatorname{Tr}[-\Delta+\frac{\lambda}{\eta}(V_n-V)]_-}{\lambda^{1+\frac{d}{2}}} \geqslant \\ &\geqslant (1-\eta)L_{\mathrm{cl}}\int V_n^{1+\frac{d}{2}} - C\frac{1}{\eta^{\frac{d}{2}}}\int |V_n-V|^{1+\frac{d}{2}}.\end{aligned}$$

Taking $n\to\infty$ the second term vanishes and first term gives us

$$\liminf_{\lambda\to\infty}\frac{1}{\lambda^{1+\frac{d}{2}}}\operatorname{Tr}[-\Delta+V]_- \geqslant (1-\eta)L_{\mathrm{cl}}\int V^{1+\frac{d}{2}}$$

for all $0<\eta<1$. Finally take η to 0.

For the upper bound the idea is to find u_i such that

$$\sum_{i=1}^N |\langle F_{k,y}, u_i\rangle|^2 \simeq \begin{cases} 1, & \text{if } |2\pi k|^2 + V(y) < 0 \\ 0, & \text{if } |2\pi k|^2+V(y)\geqslant 0\end{cases}$$

For this we need the Lemma below.

We have to prove that

$$\limsup_{\lambda\to\infty} -\frac{1}{\lambda^{1+\frac{d}{2}}}\operatorname{Tr}[-\Delta+V]_- \leqslant -\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\left[|2\pi k|^2+V(y)\right]_- \mathrm{d}k\, dy$$

Step 1 Define the operator $\gamma: L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)$

$$\gamma = \iint_{\mathcal{M}} |F_{k,y}\rangle\langle F_{k,y}|\,\mathrm{d}k\mathrm{d}y$$

where

$$\mathcal{M} := \left\{(k,y)\,\middle|\,|2\pi k|^2+V(y)<0\right\}$$

In fact

$$\langle f,\gamma f\rangle = \iint_{\mathcal{M}} |\langle F_{k,y}, f\rangle|^2\mathrm{d}k\mathrm{d}y$$

for all $f\in L^2(\mathbb{R}^d)$. We claim $0\leqslant\gamma\leqslant 1$ and that γ is trace class.

The first claim is equivalent to

$$\forall f \in L^2(\mathbb{R}^d) : 0 \leqslant \langle f, \gamma f\rangle \leqslant \|f\|_2^2 \iff \forall f \in L^2(\mathbb{R}^d) : 0 \leqslant \iint\limits_M |\langle F_{k,y}, f\rangle|^2 \mathrm{d}k\mathrm{d}y \leqslant \|f\|_2^2$$

The first inequality is trivially true and the second follows from the fact that

$$\int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} |\langle F_{k,y}, f\rangle|^2 \mathrm{d}k\ dy = \|f\|_2^2.$$

Concerning the second claim we have

$$\begin{aligned}\operatorname{Tr}\gamma &= \operatorname{Tr}\left[\iint\limits_M |F_{k,y}\rangle\langle F_{k,y}|\,\mathrm{d}k\mathrm{d}y\right] = \iint\limits_M \operatorname{Tr}[|F_{k,y}\rangle\langle F_{k,y}|]\mathrm{d}k\mathrm{d}y = \iint\limits_M 1\mathrm{d}k\mathrm{d}y = \\ &= \int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} \mathbf{1}_{\{|2\pi k|^2+V(y)<0\}}\mathrm{d}k\mathrm{d}y = C\int\limits_{\mathbb{R}^d} V_-^{\frac{d}{2}} < \infty\end{aligned}$$

Step 2 Assume that $V \in \mathscr{C}_c^\infty(\mathbb{R}^d)$. Because γ is trace class, $0 \leqslant \gamma \leqslant 1$ we can write

$$\gamma = \sum_{i=1}^N v_i\,|u_i\rangle\langle u_i|$$

for some ONB $(u_i)_{i\in\mathbb{N}}$ and $0 \leqslant v_i \leqslant 1$. Then by the lemma below for $A = -\Delta + V$

$$\begin{aligned}-\operatorname{Tr}[-\Delta+V]_- &= \sum_{\mu_i<0}\mu_i(A) \leqslant \sum_{i=1}^\infty v_i\,\langle u_i, Au_i\rangle = \operatorname{Tr}[A\gamma] = \operatorname{Tr}\left[A\iint\limits_{\mathcal{M}} |F_{k,y}\rangle\langle F_{k,y}|\,\mathrm{d}k\mathrm{d}y\right] = \\ &= \iint\limits_{\mathcal{M}} \operatorname{Tr}[A\,|F_{k,y}\rangle\langle F_{k,y}|]\mathrm{d}k\mathrm{d}y = \iint\limits_{\mathcal{M}} \langle F_{k,y}, AF_{k,y}\rangle\,\mathrm{d}k\mathrm{d}y\end{aligned}$$

Now we calculate

$$\langle F_{k,y}, AF_{k,y}\rangle = \langle F_{k,y}, (-\Delta_x + V)F_{k,y}\rangle = \int\limits_{\mathbb{R}^d}\big(|\nabla_x F_{k,y}(x)|^2 + V(x)|F_{k,y}(x)|^2\big)\mathrm{d}x.$$

Noting that

$$\begin{aligned}|\nabla_x F_{k,y}(x)|^2 &= \left|2\pi i k e^{2\pi i k} G(x-y) + e^{2\pi i k}\nabla_x G(x-y)\right|^2 = |2\pi i k G(x-y) + \nabla_x G(x-y)|^2 = \\ &= |2\pi k|^2 |G(x-y)|^2 + |\nabla_x G(x-y)|^2 + 2\underbrace{\Re\Big(\overline{2\pi i k G(x-y)}\nabla_x G(x-y)\Big)}_{\substack{=0 \\ \text{as } G \text{ is chosen to be real}}}\end{aligned}$$

Thus

$$\begin{aligned}\langle F_{k,y}, AF_{k,y}\rangle &= \int\limits_{\mathbb{R}^d} \big(|2\pi k|^2 |G(x-y)|^2 + |\nabla_x G(x-y)|^2 + V(x)|(x-y)|^2\big)\mathrm{d}x = \\ &= |2\pi k|^2 + \|\nabla G\|_2^2 + (V * |G|^2)(y).\end{aligned}$$

and therefore

$$\begin{aligned}-\operatorname{Tr}[-\Delta+V]_- &\leqslant \iint\limits_{\mathcal{M}} \big(|2\pi k|^2 + \|\nabla G\|_2^2 + (V*|G|^2)(y)\big)\mathrm{d}k\mathrm{d}y = \\ &= \iint\limits_{\mathcal{M}} \big(|2\pi k|^2 + V(y)\big)\mathrm{d}k\mathrm{d}y + \iint\limits_{\mathcal{M}} \big(\|\nabla G\|_2^2 + (V*|G|^2)(y) - V(y)\big)\mathrm{d}k\mathrm{d}y\end{aligned}$$

Because $\mathcal{M} := \{|2\pi k|^2 + V(y) < 0\}$

$$\iint\limits_{\mathcal{M}} \big(|2\pi k|^2 + V(y)\big)\mathrm{d}k\mathrm{d}y = -\int\limits_{\mathbb{R}^d}\int\limits_{\mathbb{R}^d} \big[|2\pi k|^2 + V(y)\big]_- \mathrm{d}k\mathrm{d}y = -L_{\mathrm{cl}} \int\limits_{\mathbb{R}^d} V_-^{1+\frac{d}{2}}.$$

Moreover,

$$\begin{aligned}\iint\limits_{\mathcal{M}} \big(\|\nabla G\|_2^2 + (V*|G|^2)(y) - V(y)\big)\mathrm{d}k\mathrm{d}y &\leqslant \big(\|\nabla G\|_2^2 + \|V*|G|^2) - V\|_\infty\big) \iint\limits_{\mathcal{M}} \mathrm{d}k\mathrm{d}y = \\ &= C\big(\|\nabla G\|_2^2 + \|V*|G|^2) - V\|_\infty\big) \int\limits_{\mathbb{R}^d} V_-^{\frac{d}{2}}.\end{aligned}$$

In conclusion

$$-\operatorname{Tr}[-\Delta+V]_- \leqslant -L_{\mathrm{cl}} \int V_-^{1+\frac{d}{2}} + C\big(\|\nabla G\|_2^2 + \|V*|G|^2) - V\|_\infty\big) \int\limits_{\mathbb{R}^d} V_-^{\frac{d}{2}}.$$

Replacing V by λV we obtain

$$-\frac{1}{\lambda^{1+\frac{d}{2}}}\operatorname{Tr}[-\Delta+\lambda V]_- \leqslant -L_{\mathrm{cl}}\int V_-^{1+\frac{d}{2}} + C\left(\frac{\|\nabla G\|_2^2}{\lambda} + \|V * |G|^2) - V\|_\infty\right)\int_{\mathbb{R}^d} V_-^{\frac{d}{2}}$$

taking the limit we get

$$\limsup_{\lambda\to\infty} -\frac{1}{\lambda^{1+\frac{d}{2}}}\operatorname{Tr}[-\Delta+\lambda V]_- \leqslant -L_{\mathrm{cl}}\int V_-^{1+\frac{d}{2}} + C\|V * |G|^2) - V\|_\infty \int_{\mathbb{R}^d} V_-^{\frac{d}{2}}$$

Now we have to optimise over G: Because $V \in \mathscr{C}_c^\infty$, if we choose

$$G_s(x)^2 = \frac{1}{s^d} G_0\left(\frac{x}{s}\right)^2$$

with $G_0 \in \mathscr{C}_c^\infty$, $\|G_0\|_2 = 1$ then

$$\left\|V * |G_s|^2 - V\right\|_\infty \xrightarrow{s\to 0} 0$$

Thus

$$\limsup_{\lambda\to\infty} -\frac{1}{\lambda^{1+\frac{d}{2}}}\operatorname{Tr}[-\Delta+\lambda V]_- \leqslant -L_{\mathrm{cl}}\int V_-^{1+\frac{d}{2}}$$

Step 3 Assume that $V_- \in L^{1+\frac{d}{2}}(\mathbb{R}^d)$. Then we can find $(V_n)_n \subset \mathscr{C}_c^\infty$ with $[V_n]_- \to V_-$ in $L^{1+\frac{d}{2}}(\mathbb{R}^d)$.

We can try to use the procedure as for the lower bound i.e.

$$-\Delta + \lambda V = (1-\eta)(-\Delta) + \lambda V_n + \eta(-\Delta) + \lambda(V - V_n)$$

thus

$$-\operatorname{Tr}[-\Delta+V]_- \geqslant \underbrace{-\operatorname{Tr}[(1-\eta)(-\Delta)+\lambda V_n]_-}_{\text{semiclassical } V_n\in\mathscr{C}_c^\infty} - \underbrace{\operatorname{Tr}[\eta(-\Delta)+\lambda(V-V_n)]_-}_{\geqslant C_n}$$

however this is only heuristic argument and does not actually work. The proof is left as an exercise

q.e.d.

Lemma 7.17 (Min-Max principle for Sums of Eigenvalues)**.** *Assume that A is a symmetric operator, bounded from below. Let $\mu_i(A)$ be the i^{th} min-max value of A. Then*

(1)

$$\sum_{i=1}^{N} \mu_i(A) = \inf\left\{\sum_{i=1}^{N} \langle u_i, Au_i\rangle \;\middle|\; (u_i)_{i=1}^{N} \text{ ONF}\right\}$$

(2)

$$\sum_{\mu_i<0} \mu_i(A) = \inf\left\{\sum_{i=1}^{\infty} v_i \langle u_i, Au_i\rangle \;\middle|\; (u_i)_{i=1}^{N} \text{ ONF and } 0 \leqslant v_i \leqslant 1\right\}$$

□

Proof. (1) The proof is given in Exercise 3.3.

(2) Assume that $\mu_i(A) < 0$ for $i \leqslant N$. Then by (1) for all $\varepsilon > 0$ there exists an ONF $(u_i)_{i=1}^{N}$ such that

$$\sum_{i=1}^{N} \mu_i(A) \geqslant \sum_{i=1}^{N} \langle u_i, Au_i\rangle \geqslant \inf\left\{\sum_{i=1}^{\infty} v_i \langle u_i, Au_i\rangle \;\middle|\; (u_i)_{i=1}^{N} \text{ ONF and } 0 \leqslant v_i \leqslant 1\right\} - \varepsilon$$

Take $N \uparrow \infty$ (or $N \uparrow M$ if A has M negative min-max values). Thus

$$\sum_{\mu_i<0} \mu_i(A) \geqslant \inf\left\{\sum_{i=1}^{\infty} v_i \langle u_i, Au_i\rangle \;\middle|\; (u_i)_{i=1}^{N} \text{ ONF and } 0 \leqslant v_i \leqslant 1\right\} - \varepsilon$$

and take $\varepsilon \to 0$.

For the converse inequality take an arbitrary $(u_i)_{i\in\mathbb{N}}$, $0 \leqslant v_i \leqslant 1$. We prove that

$$\sum_{i=1}^{\infty} v_i \langle u_i, Au_i\rangle \geqslant \sum_{\mu_i<0} \mu_i(A)$$

W.l.o.g. we may assume that $\langle u_i, Au_i\rangle$ (otherwise just choose the corresponding $v_i = 0$). In this case

$$\sum_{i=1}^{N} v_i \underbrace{\langle u_i, Au_i\rangle}_{<0} \geqslant \sum_{i=1}^{N} \langle u_i, Au_i\rangle \geqslant \sum_{i=1}^{N} \mu_i(A) \geqslant \sum_{\mu_i<0} \mu_i(A)$$

where we used (1) in the penultimate inequality. Taking $N \uparrow \infty$ we find that

$$\sum_{i=1}^{\infty} v_i \langle u_i, Au_i \rangle \geqslant \sum_{\mu_i < 0} \mu_i(A).$$

q.e.d.

Remark 7.18 (Lieb-Thirring Conjecture)**.** If $V_- \in L^{1+\frac{d}{2}}(\mathbb{R}^d)$, then

$$-\operatorname{Tr}[-\Delta + V]_- \geqslant -\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \left[|2\pi k|^2 + V(y)\right]_- \mathrm{d}k\mathrm{d}y = -L_{\mathrm{cl}} \int_{\mathbb{R}^d} V_-^{1+\frac{d}{2}}$$

for all $d \geqslant 3$.

The Weyl theorem only tells us that

$$-\frac{1}{\lambda^{1+\frac{d}{2}}} \operatorname{Tr}[-\Delta + \lambda V]_- \xrightarrow{\lambda \to \infty} L_{\mathrm{cl}} \int V_-^{1+\frac{d}{2}}$$

i.e. that the conjecture holds asymptotically.

Furthermore for the constant L in the Lieb-Thirring inequality

$$-\operatorname{Tr}[-\Delta + V]_- \geqslant -L \int_{\mathbb{R}^d} V_-^{1+\frac{d}{2}}$$

it is easy to see that if $L > 0$ then

$$\boxed{L \geqslant L_{\mathrm{cl}}}$$

however no sharp bound has been found yet.

There is also a dual kinetic version of the conjecture: If $(u_i)_{i=1}^N$ is an ONF in $L^2(\mathbb{R}^d)$ then

$$\sum_{i=1}^{N} \int_{\mathbb{R}^d} |\nabla u_i|^2 \geqslant K_{\mathrm{cl}} \int_{\mathbb{R}^d} \rho(x)^{1+\frac{2}{d}} \mathrm{d}x$$

where $\rho(x) = \sum_{i=1}^N |u_i(x)|^2$ and

$$K_{\mathrm{cl}} = \frac{d}{d+2}\left(\frac{d+2}{2} L_{\mathrm{cl}}\right)^{-\frac{2}{d}} = \frac{d}{d+2} \frac{4\pi^2}{|B_1|^{\frac{2}{d}}}$$

where B_1 is the unit ball in $\mathbb{R}^d$, in particular in $d = 3$

$$K_{\text{cl}} = \frac{3}{5}\left(6\pi^2\right)^{2/3}$$

and

$$L_{\text{cl}} = \frac{1}{15\pi^2}.$$

Assuming that the LT kinetic conjecture is correct. Define $A = -\Delta$ on $\mathscr{C}_c^\infty(\Omega)$ where Ω is an open and bounded domain in $\mathbb{R}^d$. Since $A \geqslant 0$ it follows that A can be extended to a self-adjoint operator by the Friedrich's method. The resulting operator is called the Dirichlet Laplacian $-\Delta_D$.

We shall show that

$$\text{LT conjecture} \implies \sum_{i=1}^{N} \mu_i(-\Delta_D) \geqslant \frac{K_{\text{cl}}}{|\Omega|^{\frac{2}{d}}} N^{1+\frac{2}{d}}$$

where the latter inequality is called the Berezin-Li-Yau inequality.

Proof. Take u_i to be a normalised eigenfunction of $-\Delta_d$.

$$\sum_{i=1}^{N} \mu_i(-\Delta_D) = \sum_{i=1}^{N} \int_\Omega |\nabla u_i|^2 \mathrm{d}x \geqslant K_{\text{cl}} \int_\Omega \rho(x)^{1+\frac{2}{d}}$$

Further we can use the Hölder inequality

$$N = \sum_{i=1}^{N} \int |u_i(x)|^2 = \int \rho \leqslant \left(\int \rho^{1+\frac{2}{d}}\right)^{\frac{d}{d+2}} \Bigg(\underbrace{\int_\Omega 1}_{=|\Omega|}\Bigg)^{\frac{2}{d+2}}$$

hence

$$K_{\text{cl}} \int_\Omega \rho^{1+\frac{2}{d}} \geqslant \frac{K_{\text{cl}}}{|\Omega|} N^{1+\frac{2}{d}}.$$

$\square$

There is a further important conjecture the Pólya conjecture (1961)

$$\mu_N(-\Delta_D) \geqslant \frac{K_{\text{cl}}}{|\Omega|^{\frac{2}{d}}} \frac{d+2}{d} N^{\frac{2}{d}}$$

for all $N \geqslant 1$. This conjecture also implies BLY inequality

Proof.

$$\sum_{i=1}^{N} \mu_i \geqslant \frac{K_{\mathrm{cl}}}{|\Omega|^{\frac{2}{d}}} \frac{d+2}{d} \sum_{i=1}^{N} i^{\frac{2}{d}}$$

with

$$\frac{d+2}{d} \sum_{i=1}^{N} i^{\frac{2}{d}} = N^{1+\frac{2}{d}} \frac{d+2}{d} \frac{1}{N} \sum_{i=1}^{N} \left(\frac{i}{N}\right)^{\frac{2}{d}} = N^{1+\frac{2}{d}} \underbrace{\frac{d+2}{d} \int_0^1 t^{\frac{2}{d}} \mathrm{d}t}_{n=1} = N^{1+\frac{2}{d}}$$

□

□

Definition 7.19.

$$H^1(\Omega) = \left\{ f \in L^2(\Omega) \,\middle|\, \forall i \in \{1, \ldots, d\} : \partial_i f \in L^2(\Omega) \right\}$$
$$\|f\|^2_{H^1(\Omega)} = \|f\|^2_{L^2(\Omega)} + \|\nabla f\|^2_{L^2(\Omega)}$$

We can show that

$$\begin{aligned} \overline{\mathscr{C}^\infty(\overline{\Omega})}^{H^1(\Omega)} &= H^1(\Omega) \\ \overline{\mathscr{C}^\infty(\overline{\Omega})}^{H^1(\Omega)} &= H^1_0(\Omega) \neq H^1(\Omega) \end{aligned}$$

where formally one may say that $H^1_0(\Omega)$ contains $f \in H^1(\Omega)$ if $f = 0$ on $\partial\Omega$.

□

Lemma 7.20. *If* $u \in H^1(\Omega)$ *and* $\operatorname{supp} u \subset\subset \Omega$*, then* $u \in H^1_0(\Omega)$. □

Proof. Because $\operatorname{supp} u \subset\subset \Omega$ there exists a $\varepsilon > 0$ such that

$$\operatorname{supp} u + B_\varepsilon(0) \subset \Omega.$$

Choose $g \in \mathscr{C}_c^\infty(\mathbb{R}^d)$, $\operatorname{supp} g \subset B_1(0)$, $\int g = 1$. Define

$$g_n(x) = n^d g(nx),\ g_n \in \mathscr{C}_c^\infty,\ \operatorname{supp} g_n \subset B_{\frac{1}{n}}(0),\ \int g_n = 1$$

Denote

$$\tilde{u} = \begin{cases} u(x), & \text{if } x \in \Omega \\ 0, & \text{if } x \notin \Omega \end{cases}$$

Consider $\varphi_n = (\tilde{u} * g_n)$. We can show that $\varphi_n \in \mathscr{C}_c^\infty(\mathbb{R}^d)$, $\operatorname{supp} \varphi_n \subset\subset \Omega$ and $\varphi_n \to u$ in $H^1(\Omega)$. *q.e.d.*

Remark 7.21 (On $H_0^1(\Omega)$)**.** 1) We can prove that if $u \in H^1(\Omega)$, $u \in \mathscr{C}(\overline{\Omega})$, $u\big|_{\partial\Omega} = 0$. Then $u \in H_0^1(\Omega)$.

2) For the converse: if $\partial\Omega \in \mathscr{C}^1$ (i.e. it is a (once) differentiable manifold) then: If $u \in H^1(\Omega)$, $u \in \mathscr{C}(\overline{\Omega})$ and $u \in H_0^1(\Omega)$ and $u \in H_0^1(\Omega)$ then $u\big|_{\partial\Omega} = 0$.

3) To understand $H_0^1(\Omega)$ better, you need to develop the idea of the "trace of u on $\partial\Omega$" (the bounded map $H^1(\Omega) \ni u \mapsto u\big|_{\partial\Omega} \in L^2(\partial\Omega)$) and extension of $u \in H_0^1(\Omega)$ iff $\tilde{u} \in H^1(\mathbb{R}^d)$.

□

Definition 7.22 (Dirichlet Laplacian)**.** Ω is open, bounded set in $\mathbb{R}^d$. Consider $A = -\Delta$ on $D(A) = \mathscr{C}_c^\infty(\Omega)$, $\mathscr{H} = L^2(\Omega)$. Denote by $-\Delta_D$ the Friedrich's extension of A over $\mathscr{H}$. We know that the quadratic form

$$q_A(u) = \int_\Omega |\nabla u|^2 \geqslant 0$$

with quadratic form domain $H_0^1(\Omega)$. □

Theorem 7.23 (Berezin-Li-Yau Inequality)**.** *Take μ_i be the i^{th} eigenvalue of $-\Delta_D$ with*

$\mu_i \leqslant \mu_{i+1}$ *for all* $i \in \mathbb{N}$. *Then*

$$\sum_{i=1}^{N} \mu_i \geqslant K_{cl} N^{1+\frac{2}{d}}.$$

□

Proof. Consider μ_i as the min-max values. We know that

$$\sum_{i=1}^{N} \mu_i = \inf \left\{ \sum_{i=1}^{N} \langle u_i, A u_i \rangle \,\middle|\, (u_i)_{i=1}^{N} \text{ ONF} \right\}.$$

This means that we need to prove that for all ONF's $(u_i)_{i=1}^{N}$,

$$\sum_{i=1}^{N} \langle u_i, A u_i \rangle \geqslant K_{\mathrm{cl}} N^{1+\frac{2}{d}} \iff \sum_{i=1}^{N} \int_{\Omega} |\nabla u_i|^2 \geqslant K_{\mathrm{cl}} N^{1+\frac{2}{d}}, \quad u_i \in D(A) = \mathscr{C}_c^{\infty}(\Omega).$$

We have

$$\sum_{i=1}^{N} \int_{\Omega} |\nabla u_i|^2 = \sum_{i=1}^{N} \int_{\mathbb{R}^d} |\nabla u_i|^2 = \sum_{i=1}^{N} \int_{\mathbb{R}^d} |2\pi k|^2 |\hat{u}_i|^2 = \int_{\mathbb{R}^d} |2\pi k|^2 f(k) \mathrm{d}k$$

where $f(k) = \sum_{i=1}^{N} |\hat{u}_i(k)|^2$. Note that

$$0 \leqslant f = \sum_{i=1}^{N} \left| \int_{\Omega} u_i(x) e^{-2\pi i k \cdot x} \mathrm{d}x \right| \leqslant \int_{\Omega} \left| e^{-2\pi i k \cdot x} \right|^2 \mathrm{d}x = |\Omega|.$$

and

$$\int_{\mathbb{R}^d} f(k) dk = \sum_{i=1}^{N} \int_{\mathbb{R}^d} |\hat{u}_i(k)|^2 \mathrm{d}k = \sum_{i=1}^{N} \int_{\mathbb{R}^d} |u_i(x)|^2 \mathrm{d}x = N$$

We claim that

$$\inf \left\{ \int_{\mathbb{R}^d} |2\pi k|^2 f(k) \mathrm{d}k \,\middle|\, 0 \leqslant f \leqslant |\Omega|, \int f = N \right\}$$

is attained by

$$\tilde{f}(k) = \begin{cases} |\Omega|, & \text{if } |k| \leqslant |k_0| \\ 0, & \text{if } |k| \geqslant k_0. \end{cases}$$

where k_0 is determined by

$$N = \int \tilde{f} = \int\limits_{|k|\leqslant k_0} |\Omega| \mathrm{d}k = |\Omega||B_1|k_0^d \quad \therefore \quad k_0 = \left(\frac{N}{|\Omega||B_1|}\right)^{\frac{1}{d}}$$

Thus

$$\int\limits_{\mathbb{R}^d} |2\pi k|^2 f(k) \mathrm{d}k \geqslant \int\limits_{|k|\leqslant k_0} |2\pi k|^2 |\Omega| \mathrm{d}k = |\Omega| \left(\int\limits_0^{k_0} (2\pi r)^2 r^{d-1} \mathrm{d}r \right) |S^{d-1}| = |\Omega||S^{d-1}|(2\pi)^2 \frac{k_0^{d+2}}{d+2} =$$

$$= \frac{|\Omega||B_1|d}{d+2}(2\pi)^2 k_0^{d+2} = \frac{|\Omega||B_1|d}{d+2}(2\pi)^2 \left(\frac{N}{|\Omega||B_1|}\right)^{\frac{d+2}{d}} = \underbrace{\frac{d}{d+2}\frac{4\pi^2}{|B_1|^{\frac{2}{d}}}}_{=K_{\mathrm{cl}}} \frac{1}{|\Omega|^{\frac{2}{d}}} N^{1+\frac{2}{d}}$$

q.e.d.

A natural question to ask now is whether

$$\frac{\sum_{i=1}^N \mu_i}{N^{1+\frac{2}{d}}} \xrightarrow{N\to\infty} \frac{K_d}{|\Omega|^{\frac{2}{d}}} ?$$

The answer is yes if $\partial\Omega$ is sufficiently "nice". However, it is not true general.

Theorem 7.24. *We assume that Ω is open, bounded in $\mathbb{R}^d$, $|\partial\Omega| < \infty$ where*

$$|\partial\Omega| := \limsup_{r\downarrow 0} \frac{\lambda^d\big(\{x \in \Omega \,\big|\, \mathrm{dist}(x, \partial\Omega) < r\}\big)}{r}$$

which is called the Minkowski content of $\partial\Omega$. Then

$$\frac{\sum_{i=1}^N \mu_i}{N^{1+\frac{2}{d}}} \xrightarrow{N\to\infty} \frac{K_d}{|\Omega|^{\frac{2}{d}}}$$

□

Proof. We need to prove the upper bound

$$\frac{\sum_{i=1}^N \mu_i}{N^{1+\frac{2}{d}}} \leqslant \frac{K_d}{|\Omega|^{\frac{2}{d}}} + o(1)_{N\to\infty}$$

By the min-max principle, we know

$$\sum_{i=1}^{N} \mu_i = \inf\left\{ \sum_{i=1}^{N} \langle u_i, Au_i \rangle \,\middle|\, (u_i)_{i=1}^{N} \text{ ONF} \right\} =$$
$$= \inf\left\{ \sum_{i=1}^{\infty} v_i \langle u_i, Au_i \rangle \,\middle|\, (u_i)_{i=1}^{N} \text{ ONF}, 0 \leqslant v_i \leqslant 1, \sum_{i=1}^{\infty} v_i \geqslant N \right\}$$

(similar to lemma concerning the sum of the negative eigenvalues).

Define

$$K = \int\limits_{\mathbb{R}^d} \int\limits_{\mathbb{R}^d} M(k,y) \left| f_{k,y} \right\rangle \left\langle f_{k,y} \right| \; dk\mathrm{d}y$$

where

$$f_{k,y} = e^{2\pi i k\cdot x} G(x-y)$$

is a coherent state and $0 \leqslant M \leqslant 1$, $M(k,y) = 0$ if $y \notin \Omega_r$ for some $\Omega_r \subset\subset \Omega$.

Then we can show that $0 \leqslant K \leqslant 1$ and

$$\operatorname{Tr} K = \operatorname{Tr}\left[\iint M(k,y) \left| f_{k,y} \right\rangle \left\langle f_{k,y} \right| \mathrm{d}k\mathrm{d}y \right] = \iint M(k,y) \mathrm{d}k\mathrm{d}y < \infty$$

We will choose $M(k,y)$ such that this is finite. Then we can write

$$K = \sum_{i=1}^{\infty} v_i \left| u_i \right\rangle \left\langle u_i \right|, \; u_i \text{ ONF}, u_i \in H^1(\Omega_r), 0 \leqslant v_i \leqslant 1.$$

Here $\operatorname{supp} u_i \subset \Omega_r$ because $M(k,y) = 0$ if $y \notin \Omega_r$ thus $u_i \in H_0^1(\Omega)$ by the lemma we discussed. Thus by the variational principle, if we know

$$\sum_{i=1}^{N} v_i = \operatorname{Tr} K \geqslant N$$

then

$$\sum_{i=1}^{N} \mu_i = \sum_{i=1}^{\infty} v_i \langle u_i, Au_i \rangle = \operatorname{Tr}(AK) =$$
$$= \operatorname{Tr}\left[-\Delta \iint M(k,y) \left| f_{k,y} \right\rangle \left\langle f_{k,y} \right| \mathrm{d}k\mathrm{d}y \right] =$$
$$= \iint M(k,y) |2\pi k|^2 \mathrm{d}k\mathrm{d}y + \operatorname{Tr}[K] \|\nabla G\|^2$$

Choose M such that $0 \leqslant M \leqslant 1$. Then

$$\iint M(k,y)\mathrm{d}k\mathrm{d}y = N + \varepsilon, \varepsilon > 0$$

fixed. Explicitly we can choose

$$M(k,y) = \mathbf{1}_{\{|k|\leqslant k_0\}}\mathbf{1}_{\Omega_r}$$

with $k_0 = \left(\frac{N+\varepsilon}{|B_1||\Omega_r|}\right)^{\frac{1}{d}}$.
Concluding as

$$\sum_{i=1}^{N} \mu_i \leqslant \frac{K_{\mathrm{cl}}}{|\Omega_r|^{\frac{2}{d}}}(N+\varepsilon)^{1+\frac{2}{d}} + (N+\varepsilon)\|\nabla G\|_2^2$$

then

$$\limsup_{N\to\infty} \frac{\sum_{i=1}^{N}\mu_i}{N^{1+\frac{2}{d}}} \leqslant \frac{K_{\mathrm{cl}}}{|\Omega_r|^{\frac{2}{d}}}$$

for all $\Omega_r \subset\subset \Omega$. Choose $\Omega_r := \left\{x \in \Omega \,\middle|\, \mathrm{dist}(x, \partial\Omega) \geqslant r\right\}$ for which

$$|\Omega_r| \geqslant |\Omega| - 2r|\partial\Omega|$$

if $r > 0$ small enough. In particular it follows that

$$\lim_{r\downarrow 0} |\Omega_r| = |\Omega|.$$

q.e.d.

We just prove that if $|\partial\Omega| < \infty$ then

$$\sum_{i=1}^{N} \mu_i = K_{\mathrm{cl}} N^{1+\frac{2}{d}} + o\left(N^{1+\frac{2}{d}}\right)_{N\to\infty}$$

the dual version of this inequality is

Theorem 7.25. *When $\Lambda \to \infty$, then*

$$\sum_{i=1}^{N} [\mu_i - \Lambda]_- = L_{cl} \Lambda^{1+\frac{d}{2}} + o\Big(\Lambda^{1+\frac{d}{2}}\Big)$$

. □

Remark 7.26. Formally if you consider a potential

$$V = \begin{cases} -1, & \text{if } x \in \Omega \\ \infty, & \text{if } x \notin \Omega \end{cases}$$

Then

$$\sum_{i=1}^{\infty} [\mu_i - \Lambda]_- \simeq \mathrm{Tr}[-\Delta + \Lambda V]_- \simeq L_{\mathrm{cl}} \int_{\mathbb{R}^d} [\Lambda V]_-^{1+\frac{d}{2}} = L_{\mathrm{cl}} |\Omega| \Lambda^{1+\frac{d}{2}}.$$

□

A consequence of the above theorem is ***Weyl's Law***: If we denote by $N(\Lambda)$ the number of eigenvalues $\mu_i \leqslant \Lambda$, then

$$N(\Lambda) = \frac{|\Omega||B_1|}{(2\pi)^d} \Lambda^{\frac{d}{2}} + o\Big(\Lambda^{\frac{d}{2}}\Big)_{\Lambda \to \infty}$$

To deduce it from the asymptotics of $\sum [\mu_i - \Lambda]_-$ we need the Tauberian lemma.

Lemma 7.27 (Tauberian)**.** *Given any increasing sequence $(\mu_i)_i$ with $\mu_i \geqslant 0$, then the following are equivalent*

1) $\sum_{i=1}^{\infty} [\mu_i - \Lambda]_- = A\Lambda^{a+1} + o(\Lambda^{a+1})$.

2) $|\{\mu_i \leqslant \Lambda\}| = \sum_{i=1}^{\infty} [\mu_i - \Lambda]_-^0 = (a+1)A\Lambda^a + o(\Lambda^a)$.

□

Chapter 8

Many-Body Schrödinger Operator

The one-body Schrödinger operator is $-\Delta + V(x)$ on $L^2(\mathbb{R}^d)$.
For an N-body system the Hamiltonian is give by

$$H_N = \sum_{i=1}^{N}(-\Delta_{x_i} + V(x_i)) + \sum_{1\leqslant i<j\leqslant n} \omega(x_i - x_j)$$

with $x_i \in \mathbb{R}^d$. Here we always assume $V : \mathbb{R}^d \to \mathbb{R}$ is an external operator and $\omega : \mathbb{R}^d \to \mathbb{R}$, $\omega(-x) = \omega(x)$ is an interaction potential.
Depending the type of particles considered there are several combinations of N-body Hilbert spaces

1) N different particles, i.e. no symmetry, $\mathscr{H} = \bigotimes_{i=1}^{N} L^2(\mathbb{R}^d) = L^2(\mathbb{R}^{dN})$.

2) N identical ***Bosons***, i.e. the wave function has to be totally symmetric, $\mathscr{H} = L^2_s(\mathbb{R}^{dN})$, where for all $\psi \in L^2_s(\mathbb{R}^{dN})$ and all $\sigma \in \mathfrak{S}(n)$

$$\psi(x_1, \ldots, x_N) = \psi(x_{\sigma(1)}, \ldots, x_{\sigma(n)}).$$

3) N identical ***Fermions***, i.e. the wave function has to be totally antisymmetric, $\mathscr{H} = L^2_a(\mathbb{R}^{dN})$, where for all $\psi \in L^2_a(\mathbb{R}^{dN})$ and all $\sigma \in \mathfrak{S}(n)$

$$\psi(x_1, \ldots, x_N) = \operatorname{sgn}(\sigma)\psi(x_{\sigma(1)}, \ldots, x_{\sigma(n)}).$$

which is equivalent to requiring that for all $i, j \in \{1, \ldots, N\}$

$$\psi(\ldots, x_i, \ldots, x_j, \ldots) = -\psi(\ldots, x_j, \ldots, x_i, \ldots).$$

4) Any combination of the above where the corresponding Hilbert space is constructed by taking the tensor product of the corresponding Hilbert spaces for each particle species and number.

Example 8.1 (Atomic Hamiltonian)**.**

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

with $x_i \in \mathbb{R}^3$ which describes an atom with N electrons of charge -1 and one nucleus of charge Z.

The natural questions to ask is whether H_N is bounded from below, what $\sigma(H_N)$ looks like and whether there are any asymptotics for $N \to \infty$.

Theorem 8.2 (Kato)**.** *Assuming that $V, \omega \in L^p(\mathbb{R}^d) + L^q(\mathbb{R}^d)$ with*

$$\begin{cases} 2 \leqslant p, q < \infty, & \text{if } d \leqslant 3 \\ \frac{d}{2} < p, q < \infty, & \text{if } d \geqslant 4 \end{cases}$$

Then H_N is self-adjoint operator on $H^2(\mathbb{R}^{dN})$ and it is bound from below. □

Example 8.3. If $V, \omega \sim \frac{1}{|x|}$ in $\mathbb{R}^3$ then these potentials satisfy the condition as

$$\frac{1}{|x|} = \frac{1}{|x|} \mathbf{1}_{\{|x| \leqslant 1\}} + \frac{1}{|x|} \mathbf{1}_{\{|x| > 1\}} \in L^2(\mathbb{R}^3) + L^4(\mathbb{R}^3).$$

Proof. We use Theorem 2.12. Define

$$H_0 = \sum_{i=1}^{N} -\Delta_{x_i} = -\Delta_{\mathbb{R}^{dN}}$$

i.e. H_0 is self-adjoint in $H^2(\mathbb{R}^{dN})$ and

$$H_N = H_0 + \sum_{i=1}^{N} V(x_i) + \sum_{i<j}^{N} \omega(x_i - x_j)$$

We prove that $V(x_i)$ and $\omega(x_i - x_j)$ are H_0-bounded with the relative bound as small as we want.

Consider $V(x_1)$. We need to prove

$$\int\limits_{\mathbb{R}^{dN}} |V(x_1)\psi(x_1,\ldots,x_N)|^2 \mathrm{d}x_1\cdots\mathrm{d}x_N \leqslant \varepsilon \int\limits_{\mathbb{R}^{dN}} |\nabla_{x_1}\psi(x_1,\ldots,x_N)|^2 + C_\varepsilon \|\psi\|_2^2$$

which follows from the inequality

$$\int\limits_{\mathbb{R}^d} |V(x)f(x)|^2 \leqslant \varepsilon \int\limits_{\mathbb{R}^d} |\nabla f(x)|^2 + C_\varepsilon \int\limits_{\mathbb{R}^d} |f|^2$$

proven in Theorem 6.6 and by Fubini's theorem

$$\int\limits_{\mathbb{R}^{dN}} |V(x_1)\psi|^2 = \int\limits_{\mathbb{R}^{d(N-1)}} \left(\int\limits_{\mathbb{R}^d} |V(x_1)\psi(x_1,\ldots,x_N)|^2 \mathrm{d}x_1 \right) \mathrm{d}x_2\cdots\mathrm{d}x_N \leqslant$$
$$\leqslant \int\limits_{\mathbb{R}^{d(N-1)}} \left(\varepsilon \int\limits_{\mathbb{R}^d} |\nabla x_1 \psi|^2 \mathrm{d}x_1 + C_\varepsilon \int\limits_{\mathbb{R}^d} |\psi|^2 \mathrm{d}x_1 \right) \mathrm{d}x_2\cdots\mathrm{d}x_N.$$

Now consider $\omega(x_1 - x_2)$. We have

$$\int\limits_{\mathbb{R}^{dN}} |\omega(x_1 - x_2)\psi(x_1,\ldots,x_N)|^2 \mathrm{d}x_1\cdots\mathrm{d}x_N = \int\limits_{\mathbb{R}^{d(N-1)}} \left(\int\limits_{\mathbb{R}^d} |\omega(x_1-x_2)\psi(x_1,\cdots,x_N)|^2 \right) \mathrm{d}x_2\cdots\mathrm{d}x_N$$

Considering $d \geqslant 4$ we get via Hölder's inequality

$$\int\limits_{\mathbb{R}^d} |\omega(x_1-x_2)|^2 |\psi(x_1,\cdots,x_N)|^2 \mathrm{d}x_1 \leqslant \left(\int\limits_{\mathbb{R}^d} |\omega(x_1-x_2)|^p \right)^{\frac{2}{p}} \left(\int\limits_{\mathbb{R}^d} |\psi(x_1,\ldots,x_N)|^r \mathrm{d}x_1 \right)^{\frac{2}{r}}$$

where $\frac{2}{p} + \frac{2}{r} = 1$. Thus

$$\left(\int_{\mathbb{R}^d} |\omega(x_1 - x_2)|^p \mathrm{d}x_1\right)^{\frac{2}{p}} = \|\omega\|_p^2$$

$$\left(\int_{\mathbb{R}^d} |\psi(x_1, \ldots, x_N)|^r \mathrm{d}x_1\right)^{\frac{2}{r}} \leqslant \int_{\mathbb{R}^d} \big(|\nabla\psi|^2 + |\psi|^2\big)\mathrm{d}x_1.$$

The conclusion follows by minimising the proof for the external potential. *q.e.d.*

Remark 8.4.

- In general $\sigma_{\mathrm{ess}}(H_N) \neq \sigma_{\mathrm{ess}}(H_0) = [0, \infty)$.
- Even when $V(x_i)$ is H_0-compact, but $\omega(x_i - x_j)$ is not H_0-compact.

□

Theorem 8.5 (HVZ - Huntiker, Van Winter, Zhislin)**.** *Denote by*

$$E_N = \inf \sigma(H_N) = \inf_{\|\psi\|_2 = 1} = \langle \psi, H_N \psi \rangle$$

where

$$H_N = \sum_{i=1}^{N} (-\Delta_X + V(x_i)) + \sum_{i<j}^{N} \omega(x_i - x_j)$$

with $V, \omega \in L^p + L^q(\mathbb{R}^d)$ where

$$\begin{cases} 2 \leqslant p, q < \infty, & \text{if } d \leqslant 3 \\ \frac{d}{2} < p, q < \infty, & \text{if } d \geqslant 4 \end{cases}$$

Then for $\omega \geqslant 0$,

$$\sigma_{ess}(H_N) = [E_{N-1}, \infty)$$

□

Remark 8.6. The physical motivation behind this theorem is as follows: Assume that you have an N-particle with energy E_N. Then it is natural to assume that it requires energy to extract one of this particles from the bound state hence the energy of the new state has to satisfy $E_{N-1} \geqslant E_N$. □

Proof. The main tool we shall use is Weyl theorem Theorem 4.15.

Step 1) $[E_{N-1}, \infty) \subset \sigma_{\text{ess}}(H_N)$

Take $\lambda \geqslant 0$. We have to prove that $E_{N-1} + \lambda \in \sigma_{\text{ess}}(H_N)$.

We use Weyl's lemma for the essential spectrum, i.e. we find a sequence $\left(\psi_N^{(k)}\right)_{k\in\mathbb{N}}$ such that $\|\psi_N^{(k)}\|_2 = 1$, $\psi_N^{(k)} \xrightarrow{k\to\infty} 0$ and

$$\left\|(H_N - E_{N-1} - \lambda)\psi_N^{(k)}\right\|_2 \xrightarrow{k\to\infty} 0.$$

- Because $E_{N-1} = \inf(\sigma(H_{N-1})) \in \sigma(H_{N-1})$, by Weyl's lemma for $\sigma(H_{N-1})$, there exists a sequence $\left(\psi_{N-1}^{(k)}\right)_k \subset L^2(\mathbb{R}^{d(N-1)})$ such that $\|\psi_{N-1}\|_2 = 1$ and

$$\left\|(H_{N-1} - E_{N-1})\psi_{N-1}^{(k)}\right\|_2 \xrightarrow{k\to\infty} 0.$$

- Because $\lambda \geqslant 0$, $\lambda \in \sigma_{\text{ess}}(-\Delta_{\mathbb{R}^d})$. Thus there exists a sequence $\left(u^{(k)}\right)_{k\in\mathbb{N}} \subset L^2(\mathbb{R}^d)$ such that $\|u^{(k)}\| = 1$, $u^{(k)} \xrightarrow{k\to\infty} 0$ and

$$\|(-\Delta - \lambda)u^{(k)}\|_2 \xrightarrow{k\to\infty} 0.$$

- Consider $\psi_N^{(k)} = \psi_{N-1}^{(k)} \otimes u^{(k)}$, i.e. $\psi_N^{(k)}(x_1, \dots, x_N) = \psi_{N-1}^{(k)}(x_1, \dots, x_{N-1})u^{(k)}(x_N)$. We want to show that
  - $\|\psi_N^{(k)}\|_2 = 1$, which is trivially true,
  - $\psi_N^{(k)} \xrightarrow{k\to\infty} 0$, which is left as a homework exercise,
  - $\left\|(H_N - E_{N-1} - \lambda)\psi_N^{(k)}\right\|_2 \xrightarrow{k\to\infty} 0$.

  We have
$$H_N = H_{N-1} + \left(-\Delta_{X_N} + V(X_N) + \sum_{i=1}^{N-1} \omega(x_i - x_N)\right)$$
  thus

$$(H_N - E_{N-1} - \lambda)\psi_N^{(k)} = (H_{N-1} + E_{N-1})\psi_N^{(k)} + (-\Delta_{x_N} - \lambda)\psi_N^{(k)} + \\ + \left(V(x_N) + \sum_{i=1}^{N-1} \omega(x_i - x_{N-1})\right)\psi_N^{(k)}.$$

By our choice of $\psi_{N-1}^{(k)}$ and $u^{(k)}$, it is straightforward to check that

$$\left\|(H_{N-1}-E_{N-1})\psi_N^{(k)}\right\|_2 = \left\|(H_{N-1}-E_{N-1})\psi_{N-1}^{(k)}\right\|_2 \|u^{(k)}\|_2 \xrightarrow{k\to\infty} 0$$
$$\left\|(-\Delta_{x_N}-\lambda)\psi_N^{(k)}\right\|_2 = \left\|(-\Delta_{x_N}-\lambda)u^{(k)}\right\|_2 \|\psi_{N-1}^{(k)}\|_2 \xrightarrow{k\to\infty} 0.$$

It remains to check that

$$\left\|\left(V(x_N)+\sum_{i=1}^{N-1}\omega(x_i-x_N)\right)\psi_N^{(k)}\right\|_2 \xrightarrow{k\to\infty} 0 \tag{$*$}$$

To prove $(*)$, for simplicity, we first choose $\psi_{N-1}^{(k)}$ and $u^{(k)}$ slightly better.

- By a density argument, we may assume that $\psi_{N-1}^{(k)} \in \mathscr{C}_c^\infty\left(\mathbb{R}^{d(N-1)}\right)$, and $u^{(k)} \in \mathscr{C}_c^\infty\left(\mathbb{R}^d\right)$.
- Moreover, we can assume that there exists a sequence $\mathbb{R}_+ \ni R_k \to \infty$ such that

$$\begin{cases} \operatorname{supp}\psi_{N-1}^{(k)} \subset B_{R_k}(0) \subset \mathbb{R}^{d(N-1)} \\ \operatorname{supp} u^{(k)} \subset B_{2R_k}(0)^C \subset \mathbb{R}^d \end{cases}$$

(the second inclusion can be done because $-\Delta-\lambda$ is translation invariant).

Now we prove $(*)$

$$\begin{aligned}\left\|V(x_N)\psi_N^{(k)}\right\|_2 &= \left\|V(x_N)u^{(k)}(x_N)\right\|_2 \left\|\psi_{N-1}^{(k)}\right\|_2 = \\ &= \Big\| \underbrace{V(x_N)\mathbf{1}_{\{|x_N|\geqslant 2R_k\}}}_{\substack{\xrightarrow{k\to\infty} 0 \\ \text{in } L^p+L^q\text{, and } u^{(k)} \text{ bounded in } H^2(\mathbb{R}^d)}} u^{(k)}(x_N)\Big\|_2 \xrightarrow{k\to\infty} 0\end{aligned}$$

and

$$\begin{aligned}\left\|\omega(x_1-x_N)\psi_N^{(k)}\right\| &= \left\|\omega(x_1-x_N)\mathbf{1}_{\{|x_1|\leqslant R_k\}}\mathbf{1}_{\{|x_N|\geqslant 2R_k\}}\psi_{N-1}^{(k)}(x_1,\dots,x_{N-1})u^{(k)}(x_N)\right\|_2 = \\ &= \Big\|\underbrace{\omega(x_1-x_N)\mathbf{1}_{\{|x_1-x_N|\leqslant R_k\}}}_{\substack{\omega(x)\mathbf{1}_{\{|x|\geqslant R_k\}}\xrightarrow{k\to\infty} 0 \\ \text{in } L^p+L^q}}\psi_{N-1}^{(k)}(x_1,\dots,x_{N-1})u^{(k)}(x_N)\Big\|_2 \xrightarrow{k\to\infty} 0\end{aligned}$$

Step 2 $\sigma_{\text{ess}}(H_N) \subset [E_{N-1},\infty)$, we need to use $\omega \geqslant 0$ and a localisation technique which is proven in the lemma below.

Take $\lambda \in \sigma_{\text{ess}}(H_N)$. We have to prove that $\lambda \geqslant E_{N-1}$. By Weyl's lemma there exists a sequence of unit vectors $\left(\psi_N^{(k)}\right)_k \subset \mathbb{R}^{dN}$ such that $\psi_N^{(k)} \rightharpoonup 0$ and $\|(H_N - \lambda)\psi_N^{(k)}\|_2 \to 0$. We know that $\psi_N^{(k)}$ is bounded in $H^2(\mathbb{R}^d)$, thus $\psi_N^{(k)} \rightharpoonup 0$ in $H^2(\mathbb{R}^{dN})$. By Sobolev embedding for all $R > 0$

$$\psi_N^{(k)} \mathbf{1}_{B_R(0)} \xrightarrow[L^2(\mathbb{R}^{dN})]{k\to\infty} 0$$

Now we use the IMS localisation as follows

- We choose 2 function $\chi, \eta : \mathbb{R}^d \to \mathbb{R}$ satisfying $\chi \in \mathscr{C}_c^\infty(\mathbb{R}^d)$, $\chi, \eta \geqslant 0$, $\chi^2 + \eta^2 = 1$ and require

  $$\operatorname{supp} \chi \subset \{|x| \leqslant 2\}, \ \operatorname{supp} \eta \subset \{|x| \geqslant R\}$$

  and $|\nabla \chi|, |\nabla \eta| \leqslant \frac{C}{R}$.

- On $\mathbb{R}^{dN}$ take

  $$1 = \prod_{i=1}^{N} \big(\chi(x_i)^2 + \eta(x_i)^2\big) = \chi(x_1)^2 \chi(x_2)^2 \cdots \chi(x_N)^2 + \eta(x_1)^2 \chi(x_2)^2 \cdots \chi(x_N)^2 + \cdots =$$
  $$= \varphi_0^2 + \sum_{j=1}^{K} \varphi_j^2$$

  where $K = 2^N - 1$ and $\varphi_0, \varphi_j \in \mathscr{C}^\infty(\mathbb{R}^{dN})$ and

  $$\operatorname{supp} \varphi_0 \big\{(x_1, \ldots, x_N) \,\big|\, \forall i \in \{1, \ldots, N\} : |x_i| \leqslant 2R\big\} \subset B_{C_N R}(0) \subset \mathbb{R}^{dN}$$

  and for every $j \in \{1, \ldots, K\}$ there exists a $j' \in \{1, \ldots, N\}$ such that

  $$\operatorname{supp} \varphi_j \subset \big\{(x_1, \ldots, x_N) \,\big|\, |x_{j'}| \geqslant R\big\}$$

  Moreover $|\nabla \varphi_0|, |\nabla \varphi_j| \leqslant \frac{C}{R}$. Now we apply the IMS formula for φ_j

  $$(-\Delta)_{\mathbb{R}^{dN}} = \sum_{j=0}^{K} \varphi_j (-\Delta_{\mathbb{R}^{dN}}) \varphi_j - \sum_{j=0}^{K} |\nabla \varphi_j|^2$$

  therefore

  $$H_N = \sum_{j=0}^{K} \varphi_j H_N \varphi_j - \sum_{j=1}^{K} |\nabla \varphi_j|^2$$

hence

$$\left\langle \psi_N^{(k)}, H_N \psi_N^{(k)} \right\rangle = \sum_{j=0}^{N} \left\langle \psi_N^{(k)}, \varphi_j H_N \varphi_j \psi_N^{(k)} \right\rangle - \left\langle \psi_N^{(k)}, \sum_{j=0}^{K} |\nabla \varphi_j|^2 \psi_N^{(k)} \right\rangle.$$

We know that

$$\left\langle \psi_N^{(k)}, H_N \psi_N^{(k)} \right\rangle \xrightarrow{k\to\infty} \lambda$$

Now we want to estimate the right hand side of the expansion. Because $|\nabla \varphi_j| \leqslant \frac{C}{R}$,

$$\left\langle \psi_N^{(k)}, \sum |\nabla \varphi_j|^2 \psi_N^{(k)} \right\rangle \leqslant \frac{C}{R^2}$$

with the constant C depending on N, d but independent of R.

Consider $j = 0$

$$\left\langle \psi_N^{(k)}, \varphi_0 H_N \varphi_0 \psi_N^{(k)} \right\rangle = \langle \varphi_0 \psi_N^{(k)}, \underbrace{H_N}_{\geqslant E_N = \inf \sigma(H_N)} \varphi_0 \psi_N^{(k)} \rangle \geqslant E_N \|\varphi_0 \psi_N^{(k)}\|_2^2 \xrightarrow{k\to\infty} 0.$$

Consider $j \in \{1, \dots, K\}$. Then there exists a $j' \in \{1, \dots, N\}$ such that

$$\operatorname{supp} \varphi_j \subset \left\{ (x_1, \dots, x_N) \,\middle|\, |x_{j'}| \geqslant R \right\}.$$

Let us assume that $j' = N$ for simplicity of notation (which we can do by relabelling if necessary).

We have

$$\begin{aligned}
\left\langle \psi_N^{(k)}, \varphi_j H_N \varphi_j \psi_N^{(k)} \right\rangle &= \left\langle \varphi_j \psi_N^{(k)}, \left(H_{N-1} + (-\Delta_{x_N}) + V(x_N) + \sum_{j=1}^{N-1} \omega(x_i - x_N) \right) \varphi_j \psi_N^{(k)} \right\rangle \geqslant \\
&\geqslant \left\langle \varphi_j \psi_N^{(k)}, (E_{N-1} + V(x_N)) \varphi_j \psi_N^{(k)} \right\rangle = \\
&= E_{N-1} \|\varphi_j \psi_N^{(k)}\|_2^2 + \int V(x_N) |\varphi_j|^2 |\psi_N^{(k)}|^2 \geqslant \\
&\geqslant E_{N-1} \|\varphi_j \psi_N^{(k)}\|_2^2 - \underbrace{\int |V(x)| \mathbf{1}_{\{|x_N| \geqslant R\}} |\psi_N^{(k)}|^2}_{=: \varepsilon_R \geqslant 0}
\end{aligned}$$

Concluding we find

$$\lambda = \lim_{k\to\infty} \left\langle \psi_N^{(k)}, H_N \psi_N^{(k)} \right\rangle \geqslant -\frac{C}{R^2} + E_{N-1} \underbrace{\lim_{k\to\infty} \left(\sum_{j=1}^{K} \|\varphi_j \psi_N^{(k)}\|_2^2 \right)}_{=1} - \varepsilon_R \xrightarrow{R\to\infty} E_{N-1}$$

as $\varepsilon_R \xrightarrow{R\to\infty} 0$ and

$$1 = \int |\psi_N^{(k)}|^2 = \sum_{j=0}^{K} \int |\varphi_j|^2 |\psi_N^{(k)}|^2 = \sum_{j=1}^{K} \int |\varphi_j|^2 |\psi_N^{(k)}|^2 + o(1)_{k\to\infty}$$

Thus $\lambda \geqslant E_{N-1}$ as we wanted.

q.e.d.

Lemma 8.7 (IMS - Localisatio, Ismagilov, Morgan, Morgan- Simon, I.M. Sigal)**.** *Assume that* $\{\varphi_j\}_{j=1}^k \subset \mathscr{C}^2\big(\mathbb{R}^d\big)$*, satisfy* $\varphi_j \geqslant 0$ *and* $\sum_{j=1}^k \varphi_j^2 = 1$*, then*

$$-\Delta_{\mathbb{R}^d} = \sum_{j=1}^{k} \varphi_j (-\Delta) \varphi_j - \sum_{j=1}^{k} |\nabla \varphi_j|^2$$

as operators on $L^2(\mathbb{R}^d)$*.* □

Proof. We prove that if $\varphi \geqslant 0$, $\varphi \in \mathscr{C}^2$, then

$$\frac{\varphi^2(-\Delta) + (-\Delta)\varphi^2}{2} = \varphi(-\Delta)\varphi - |\nabla\varphi|^2$$

as quadratic forms on $\mathscr{C}_c^\infty(\mathbb{R}^d)$. Let $f \in \mathscr{C}_c^\infty(\mathbb{R}^d)$ then

$$\begin{aligned}
\left\langle f, \frac{\varphi^2(-\Delta) + (-\Delta)\varphi^2}{2} f \right\rangle &= \Re \int_{\mathbb{R}^d} \bar{f} \varphi^2 (-\Delta f) = \Re \int_{\mathbb{R}^d} \nabla\big(\bar{f}\varphi^2\big) \nabla \varphi = \\
&= \Re \int_{\mathbb{R}^d} \big((\nabla \bar{f})\varphi^2 + \bar{f}\big(\nabla \varphi^2\big)\big) \nabla f = \int |\nabla f|^2 \varphi^2 + 2\,\Re \int \bar{f} \varphi \nabla \varphi \nabla f \\
\big\langle f, \big(\varphi(-\Delta)\varphi - |\nabla\varphi|^2\big) f \big\rangle &= \int \bar{f}\bar{\varphi}(-\Delta)\varphi f - \int |\nabla\varphi|^2 |f|^2 = \int |\nabla(\varphi f)|^2 - \int |\nabla \varphi|^2 |f|^2 = \\
&= \int |\varphi|^2 |\nabla f|^2 + 2\,\Re \int \overline{(\nabla\varphi) f} \varphi \nabla f.
\end{aligned}$$

Applying this to $\varphi = \varphi_j$ and summing over j yields the result. *q.e.d.*

Remark 8.8. The Kato Theorem (which tells us that H_N is self-adjoint in H^2 and bounded from below) and the HVZ thoerem hold in all 3 cases

- $L^2(\mathbb{R}^{dN})$ with no symmetry
- $L^2_a(\mathbb{R}^{dN})$ anti-symmetric/fermionic case
- $L^2_s(\mathbb{R}^{dN})$ symmetric/bosonic case.

□

Remark 8.9. If $V, \omega \in L^p + L^q$, $\omega \geqslant 0$ and if $E_N < E_{N-1}$ then E_N is an eigenvalue of H_N. The quantity $E_{N-1} - E_N$ is called the ionisation energy. Thus we are led to the ***Ionisation problem***: When is $E_N < E_{N-1}$? How many electrons can a nucleus bind? □

The Atomic Hydrogen Hamiltonian is given by

$$H_N = \sum_{i=1}^{N} \left(-\Delta_{x_i} - \frac{Z}{|x|} \right) + \sum_{1 \leqslant i < j \leqslant N} \frac{1}{|x_i - x_j|}$$

with $x_j \in \mathbb{R}^3$ on either $L^2\big(\mathbb{R}^{3N}\big), L^2_s\big(\mathbb{R}^{3N}\big)$ or $L^2_a\big(\mathbb{R}^{3N}\big)$.
By the Theorem 8.5 $\sigma(H_N) = [E_{N-1}, \infty)$, $E_N = \inf \sigma(H_N)$.

Corollary 8.10. *If $E_N < E_{N-1}$, Then E_N is an isolated eigenvalue of H_N.* □

The Question to ask now is when does $E_N < E_{N-1}$ occur?

Remark 8.11. 1) $E_N \leqslant E_{N-1}$ always holds.

2) If $E_N < E_{N-1}$ then E_N is an eigenvalue of H_N. If E_N is an eigenvalue then $E_N < E_{N-1}$.

□

Theorem 8.12 (Zhislin)**.** *Let $Z > 0$ (not necessarily an integer) and $N \in \mathbb{N}$. If $N < Z + 1$, then $E_N < E_{N-1}$ and H_N has therefore a ground state.* $\square$

Proof. We shall proceed by induction. If $N = 1$, the $H_N = -\Delta - \frac{Z}{|x|}$ in $L^2(\mathbb{R}^3)$. This is the hydrogen atom,

$$\inf \sigma\left(-\Delta - \frac{Z}{|x|}\right) = -\frac{Z^2}{4}.$$

Thus $E_1 = \frac{Z^2}{4} < E_0 = 0$.

Assume that we have $E_{N-1} < E_{N-2}$ and $N < Z + 1$. Then we have to prove $E_N < E_{N-1}$. Because $E_{N-1} < E_{N-2}$ we know that H_{N-1} has a ground state Ψ_{N-1}, i.e. $H_{N-1}\Psi_{N-1} = E_{N-1}\Psi_{N-1}$.

We want to construct a wave function Ψ_N such that

$$\langle \Psi_N, H_N \Psi_N \rangle < E_{N-1}$$

Consider a state $\Psi_N = \Psi_{N-1} \otimes u$, $u \in L^2(\mathbb{R}^3)$ with $\|u\|_2 = 1$ and

$$\Psi_N(x_1, \ldots, x_N) = \Psi_{N-1}(x_1, \ldots, x_{N-1})u(x_N)$$

For this state

$$\begin{aligned}\langle \Psi_N, H_N \Psi_N \rangle &= \left\langle \Psi_N, \left(H_{N-1} - \Delta_{x_N} - \frac{Z}{|x_N|} + \sum_{i=1}^{N-1} \frac{1}{|x_i - x_N|}\right)\Psi_N \right\rangle = \\ &= E_{N-1} + \int\limits_{\mathbb{R}^3} |\nabla u|^2 - \int\limits_{\mathbb{R}^3} \frac{Z}{|x|}|u(x)|^2 + \sum_{i=1}^{N-1} \int\limits_{\mathbb{R}^{3N}} \frac{|\Psi_{N-1}(x_1, \ldots, x_{N-1})u(x_N)|^2}{|x_i - x_N|} \mathrm{d}x_1 \cdots \mathrm{d}x_N\end{aligned}$$

We shall use Newton's Theorem Theorem 5.37 to calculate this. Assuming that u is radially symmetric and thus by Newton's theorem

$$\int\limits_{\mathbb{R}^3} \frac{|u(x_N)|^2}{|y - x_N|} \mathrm{d}x_N = \int\limits_{\mathbb{R}^3} \frac{|u(x_N)|^2}{\max\{|y|, |x_N|\}} \mathrm{d}x_N \leqslant \int\limits_{\mathbb{R}^3} \frac{|u(x_N)|^2}{|x_N|} \mathrm{d}x_N$$

and therefore

$$\sum_{i=1}^{N-1} \int \frac{|\varphi_{N-1}(x_1, \dots, x_N)|^2 |u(x_N)|^2}{|x_i - x_N|} \leqslant \sum_{i=1}^{N-1} \int |\varphi_{N-1}(x_1, \dots, x_N)|^2 \frac{|u(x_N)|^2}{|x_N|} =$$
$$= (N-1) \int \frac{|u(x)|^2}{|x|} \mathrm{d}x$$

Concluding we get

$$E_N \leqslant \langle \Psi_N, H_N \Psi_N \rangle \leqslant E_{N-1} + \int\limits_{\mathbb{R}^3} |\nabla u|^2 + (N-1-Z) \int\limits_{\mathbb{R}^3} \frac{|u(x)|^2}{|x|} \mathrm{d}x$$

By our assumption $N - 1 - Z < 0$. Choosing $\varphi \in \mathscr{C}_c^\infty(\mathbb{R}^3)$, φ radial and $\int |\varphi|^2 = 1$, further define $u_\ell(x) = \ell^{\frac{3}{2}} \varphi(\ell x)$ for which $u_\ell \in \mathscr{C}_c^\infty$ and $\int |u_\ell|^2 = 1$. Furthermore we have

$$\int |\nabla u_\ell|^2 = \ell^2 \int |\nabla \varphi|^2$$
$$\int \frac{|u_\ell(x)|^2}{|x|} \mathrm{d}x = \ell \int \frac{|\varphi(x)|^2}{|x|} \mathrm{d}x$$

Thus

$$E_n \leqslant E_{N-1} + \ell^2 \int |\nabla \varphi|^2 + \underbrace{(N-1-Z)}_{<0} \ell \int \frac{|\varphi(x)|^2}{|x|} \mathrm{d}x$$

for all $\ell > 0$. By taking $\ell > 0$ small enough we conclude that

$$E_N < E_{N-1}.$$

q.e.d.

Remark 8.13 (Ionisation Conjecture)**.** If $N > Z + 2$, then $E_N = E_{N-1}$ and H_N has no ground state.
Physically one may interpret this as there not existing anions of charge -3 or higher. □

Example 8.14. In particular H and H^- exist, but H^{2-} does not, but we do not know anything for other atoms.

Theorem 8.15 (Lieb)**.** *If $N \geqslant 2Z+1$ then $E_N = E_{N-1}$ and H_N has no ground state.* □

Proof. Let us assume that H_N has a ground state

$$H_N\Psi_N = E_N\Psi_N$$

multiplying this with $|x_N|\overline{\Psi_N}$ and integrating we get

$$\begin{aligned}0 &= \langle |x_N|\Psi_N, (H_N - E_N)\Psi_N\rangle = \\ &= \left\langle |x_N|\Psi_N, \left(H_{N-1} - E_N - \Delta_{x_N} - \frac{Z}{|x_N|} + \sum_{i=1}^{N-1}\frac{1}{|x_i - x_N|}\right)\Psi_N\right\rangle\end{aligned}$$

1) $\langle |x_N|\Psi_N, (H_{N-1} - E_N)\Psi_N\rangle \geqslant \langle |x_N|\Psi_N, (E_{N-1} - E_n)\Psi_N\rangle \geqslant 0.$

2) $\langle |x_N|\Psi_N, -\Delta_{x_N}\Psi_N\rangle \geqslant 0$ (proved later using Hardy's inequality).

3) $\left\langle |x_N|, -\frac{Z}{|x_N|\Psi_N}\right\rangle = -Z$

4)
$$\left\langle |x_N|\Psi_N, \sum_{i=1}^{N-1}\frac{1}{|x_i - x_N|}\Psi_N\right\rangle = \sum_{i=1}^{N-1}\int |\Psi_N|\frac{|x_N|}{|x_i - x_N|}$$

Thus
$$0 \geqslant -Z + \sum_{i=1}^{N-1}\int |\Psi_N|\frac{|x_N|}{|x_i - x_N|} \iff Z \geqslant \sum_{i=1}^{N-1}\int |\Psi_N|\frac{|x_N|}{|x_i - x_N|}$$

Similarly we get for all $j \in \{1, \ldots, N\}$

$$| \geqslant \sum_{i \neq j}\int |\Psi_N|^2\frac{|x_i|}{|x_i - x_j|}$$

Summing all of these inequalities we get

$$NZ \geqslant \sum_{\substack{i,j=1\\ i\neq j}}^{N}\int |\Psi_N|^2\frac{|x_i|}{|x_i - x_j|} = \frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\int |\Psi_N|^2\underbrace{\frac{|x_i| + |x_j|}{|x_i - x_j|}}_{\geqslant 1} \geqslant \frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N} 1 = \frac{1}{2}(N-1)N$$

thus $Z > \frac{N-1}{2}$, i.e. $N < 2Z+1$. ↯ *q.e.d.*

It is known that if $N > Z + cZ^{1-\varepsilon}$, $\varepsilon > 0$ small enough, then H_N has no minimiser. It is an open question whether $N > Z + C$ (with C independent of Z) implies that H_N has no ground state.
It is further conjectured that $N \mapsto E_N$ is a convex function, i.e.

$$E_{N-1} - E_{N-2} < E_N - E_{N-1} \iff E_{N-1} - E_N < E_{N-2} - E_{N-1}$$

In particular if H_N has a bound state (ground state + isolated eigenvalues) then H_{N-1} has a bound state (open!).
Now we turn to the question of $E_{N,Z}$ looks like for $Z \to \infty$, $N \sim O(Z)$.
We will restrict ourselves to the anti-symmetric case.

Remark 8.16. Recall that for a symmetric function for all $i, j \in \{1, \dots, N\}$

$$\Psi_N(x_1, \dots, x_i, \dots, x_j, \dots, x_N) = \Psi_N(x_1, \dots, x_j, \dots, x_i, \dots, x_N)$$

For example this is the case for some $u \in L^2\big(\mathbb{R}^d\big)$

$$\Psi_N(x_1, \dots, x_N) = u(x_1) \cdots u(x_N) = u^{\otimes n}(x_1, \dots, x_N)$$

which is called a Hartree state and is used to describe Bosons.
Antisymmetric functions on the other hand describe fermions and satisfy for all $i, j \in \{1, \dots, n), i \neq j$

$$\Psi_N(x_1, \dots, x_i, \dots, x_j, \dots, x_N) = -\Psi_N(x_1, \dots, x_j, \dots, x_i, \dots, x_N)$$

For example in the case $N = 2$

$$\Psi_2(x_1, x_2) = \mathrm{const}(u(x_1)v(x_2) - v(x_1)u(x_2))$$

For the general we can construct such a state via the so-called ***Slater determinant***, used in Hartree-Fock theory. □

Definition 8.17 (Slater Determinant)**.** For $N \in \mathbb{N}$, and $(u_i)_{i=1}^N$ an ONF in $L^2(\mathbb{R}^d)$

$$\Psi_N := u_1 \wedge u_2 \wedge \cdots \wedge u_N = \frac{1}{\sqrt{N!}} \det[u_i(x_j)]_{1 \leqslant i,j \leqslant N} = \frac{1}{\sqrt{N!}} \sum_{\sigma \in \mathfrak{S}_n} \operatorname{sgn}(\sigma) u_1(x_{\sigma(1)}) \cdots u_n(x_{\sigma(n)}).$$

□

Remark 8.18 (Question)**.** Why is antisymmetry crucial? Because it implies the Pauli exclusion principle

"2 particles ***cannot*** occupy the same quantum state."

□

Definition 8.19 (One-Body Density Matrix)**.** Given an antisymmetric N-body-wave function Ψ_N, we define its one body density matrix to be the operator

$$\gamma^{(1)}_{\Psi_N} : L^2(\mathbb{R}^d) \longrightarrow L^2(\mathbb{R}^d)$$

with kernel

$$\gamma^{(1)}_{\Psi_N}(x,y) = N \int \Psi_N(x, x_2, \ldots, x_N) \overline{\Psi_N(y, x_2, \ldots, x_N)} \mathrm{d}x_2 \cdots \mathrm{d}x_N$$

It satisfies $\gamma^{(1)}_{\Psi_N} \geqslant 0$ and $\operatorname{Tr} \gamma^{(1)}_{\Psi_N} = N$. □

Definition 8.20. For $\Psi_N \in L^2_a(\mathbb{R}^{dN})$ the corresponding density matrix is defined as $|\Psi_N\rangle\langle\Psi_N|$. This is a projection operator on $L^2_a(\mathbb{R}^{dN})$ with kernel

$$(|\Psi_N\rangle\langle\Psi_N|)(x_1, \ldots, x_N, y_1, \ldots, y_N) = \Psi_N(x_1, \ldots, x_N)\overline{\Psi_N(y_1, \ldots, y_N)}$$

and therefore

$$\gamma^{(1)}_{\Psi_N} = N \operatorname{Tr}_{x_2, \ldots, x_N} |\Psi_N\rangle\langle\Psi_N|$$

where we have taken the partial trace w.r.t. $x_2, \ldots, x_N$, which equivalent to the marginal probability w.r.t. x_1. □

Example 8.21. If $\Psi_N = u_1 \wedge u_2 \wedge \cdots \wedge u_N$ then

$$\gamma^{(1)} = \sum_{i=1}^{N} |u_i\rangle \langle u_i|$$

Definition 8.22 (One-Body Density Matrix)**.** For $\Psi_N \in L_a^2(\mathbb{R}^{dN})$ we define $\gamma_{\Psi_N}^{(1)} : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ by

$$\gamma_{\Psi_N}^{(1)}(x,y) := N \int \Psi_N(x, x_2, \ldots, x_N)\overline{\Psi_N(y, x_2, \ldots, x_N)}\mathrm{d}x_2 \cdots \mathrm{d}x_N$$

Thus $\gamma_{\Psi_N}^{(1)} \geqslant 0$, trace class, $\operatorname{Tr}\gamma_N^{(1)} = N$. We can also define the one body density

$$\rho_{\psi_N}(x) = \gamma_{\Psi_N}^{(1)}(x,x) = N \int |\Psi_N(x, x_2, \ldots, x_N)|^2 \mathrm{d}x_2 \cdots \mathrm{d}x_N$$

This satisfies $\rho_{\Psi_N} \geqslant 0$, $\int \rho_{\Psi_N}(x)\mathrm{d}x = N$. □

Lemma 8.23. *If h is a self-adjoint operator on $L^2(\mathbb{R}^d)$, then*

$$H_N := \sum_{i=1}^{N} h_{x_i}$$

is a self-adjoint operator on $L_a^2(\mathbb{R}^{dN})$ with domain $\Lambda^N D(h)$. Moreover,

$$\langle \Psi_N, H_N \Psi_n \rangle = \operatorname{Tr}\left(h\gamma_{\Psi_N}^{(1)}\right)$$

□

Example 8.24.

$$\left\langle \Psi_N, \sum_{i=1}^{N} (-\Delta_{x_i})\Psi_N \right\rangle = \operatorname{Tr}\left(-\Delta\gamma_N^{(1)}\right)$$

$$\left\langle \Psi_N, \sum_{i=1}^{N} V(x_i)\Psi_N \right\rangle = \operatorname{Tr}\left(V\gamma_{\Psi_N}^{(1)}\right) = \int V(x)\rho_{\Psi_N}(x)\mathrm{d}x$$

The last equality on the second line can be verified by using the spectral decomposition of the density matrix

$$\gamma^{(1)}_{\Psi_N} \sum_{i=1}^{N} |u_i\rangle\langle u_i| \quad \therefore \quad \rho_{\Psi_N}(x) = \sum_{\lambda_i} |u_i(x)|^2.$$

Theorem 8.25 (Pauli Exclusion Principle)**.** *If Ψ_N is a wave function in $L^2_a\big(\mathbb{R}^{dN}\big)$, then*

$$0 \leqslant \gamma^{(1)}_{\Psi_N} \leqslant 1$$

□

Remark 8.26. If $\Psi_N \in L^2\big(\mathbb{R}^{dN}\big)$ or $L^2_s\big(\mathbb{R}^{dN}\big)$ then we only know that

$$0 \leqslant \gamma^{(1)}_{\Psi_N} \leqslant N = \operatorname{Tr}\gamma^{(1)}_{\Psi_N}$$

In fact, if $\Psi_N = u^{\otimes N}$, then $\gamma^{(1)}_{\Psi_N} = N\,|u\rangle\langle u|$. □

Corollary 8.27 (Ground State Energy of Non-Interacting Fermi Gas)**.** *Consider $H_N = \sum_{i=1}^N h_{x_i}$ on $L^2_a\big(\mathbb{R}^{dN}\big)$ with h self adjoint, bounded from below on $L^2\big(\mathbb{R}^d\big)$. Then*

$$\inf\sigma(H_N) = \sum_{i=1}^{N} \mu_i(h)$$

where μ_n is the n^{th} min-max value of h. □

Proof. Take $\Psi_N \in L^2_a\big(\mathbb{R}^{dN}\big)$, $\|\Psi_N\|_2 = 1$. Then $\langle \Psi_N, H_N\Psi_N\rangle = \operatorname{Tr}\Big(h\gamma^{(1)}_{\Psi_N}\Big)$. Because $\gamma^{(1)}_{\Psi_N}$ is trace class, $0 \leqslant \gamma^{(1)}_{\Psi_N} \leqslant 1$, $\operatorname{Tr}\gamma^{(1)}_{\Psi_N} = N$,

$$\gamma^{(1)}_{\Psi_N} = \sum_{i=1}^{\infty} \lambda_i\,|u_i\rangle\langle u_i|\,,$$

$0 \leqslant \lambda_i \leqslant 1$, $\sum \lambda_i = N$. Thus

$$\begin{aligned}\langle \Psi_N, H_N \Psi_N \rangle &= \sum_{i=1}^{\infty} \lambda_i \langle u_i, h u_i \rangle \geqslant \\ &\geqslant \inf \left\{ \sum_{i=1}^{\infty} \eta_i \langle v_i, h v_i \rangle \,\middle|\, 0 \leqslant \eta_i \leqslant 1, \sum \eta_i = N, (v_i)_i \text{ ONF} \right\} = \\ &= \sum_{i=1}^{N} \mu_i(h)\end{aligned}$$

thus $\inf \sigma(H_N) \geqslant \sum_{i=1}^N \mu_i(h)$.
Concerning the upper bound, we use the Slater determinant. Using

$$\sum_{i=1}^{N} \mu_i(h) = \inf \left\{ \sum_{i=1}^{N} \langle v_i, h v_i \rangle \,\middle|\, (v_i)_{i=1}^N \text{ ONF} \right\}$$

Thus for all $\varepsilon > 0$, there exists an ONF $(v_i)_{i=1}^N$ such that

$$\sum_{i=1}^{N} \langle v_i, h v_i \rangle \leqslant \sum_{i=1}^{N} \mu_i(h) + \varepsilon$$

Now we choose

$$\Psi_N = v_1 \wedge v_2 \wedge \cdots \wedge v_N = \frac{1}{\sqrt{N!}} \det[v_i(x_j)]_{1 \leqslant i,j \leqslant N} = \frac{1}{\sqrt{N!}} \sum_{\sigma \in \mathfrak{S}_n} \operatorname{sgn}(\sigma) v_1(x_{\sigma(1)}) \cdots v_n(x_{\sigma(n)}).$$

Then $\gamma_{\Psi_N}^{(1)} = \sum_{i=1}^N |v_i\rangle \langle v_i|$ and therefore

$$\langle \Psi_N, H_N \Psi_N \rangle = \operatorname{Tr}\Big(h \gamma_{\Psi_N}^{(1)}\Big) = \sum_{i=1}^{N} \langle v_i, h v_i \rangle \leqslant \sum_{i=1}^{N} \mu_i(h) + \varepsilon$$

thus $\inf \sigma(H_N) \leqslant \sum_{i=1}^N \mu_i(h) + \varepsilon$. Taking $\varepsilon \to 0$ finishes the proof. *q.e.d.*

Corollary 8.28 (Kinetic Energy Estimate)**.** *If Ψ_N is a wave function in $L_a^2\big(\mathbb{R}^{dN}\big)$, then*

$$\left\langle \Psi_N, \sum_{i=1}^{N} \Psi_N \right\rangle = \operatorname{Tr}\Big(-\Delta \gamma_{\Psi_N}^{(1)}\Big) \geqslant K \int_{\mathbb{R}^d} \rho_{\Psi_N}(x)^{1+\frac{2}{d}} \mathrm{d}x$$

□

Proof. Follows from the Pauli exclusion principle and the Lieb-Thirring inequality. *q.e.d.*

Remark 8.29. Lieb-Thirring conjectured that $K = K_{\mathrm{cl}} = \frac{d}{d+2}\frac{4\pi^2}{|B_1|^{\frac{2}{d}}}$. □

Lemma 8.30 (Tensor Product of Hilbert Spaces)**.** *Let Ω_1, Ω_2 be two measure spaces. Then $L^2(\Omega_1 \times \Omega_2) \simeq L^2(\Omega_1) \otimes L^2(\Omega_2)$ where*

$$L^2(\Omega_1) \otimes L^2(\Omega_2) := \overline{\operatorname{span}\left\{u \otimes v \,\middle|\, u \in L^2(\Omega_1), v \in L^2(\Omega_2)\right\}}$$

and

$$(u \otimes v)(x, y) = u(x)v(y)$$

Moreover, if $(u_i)_{i\in\mathbb{N}}$ is ONB for $L^2(\Omega_1)$ and $(v_i)_{i\in\mathbb{N}}$ for $L^2(\Omega_2)$. Then

$$(u_i \otimes v_j)_{i,j\in\mathbb{N}}$$

is an ONB for $L^2(\Omega_1 \times \Omega_2)$. □

Proof. We need only to check that $(u_i \otimes v_j)_{i,j\in\mathbb{N}}$ is an ONB for $L^2(\Omega_1 \times \Omega_2)$.

- $(u_i \otimes v_j)_{i,j\in\mathbb{N}}$ is an ONF in $L^2(\Omega_1 \times \Omega_2)$ as

$$\langle u_i \otimes v_j, u_l \otimes u_k\rangle = \int \overline{u_i(x)v_j(y)}u_l(x)v_k(y)\mathrm{d}x\mathrm{d}y = \langle u_i, u_l\rangle \langle v_j, v_k\rangle = \delta_{il}\delta_{jk}.$$

- $(u_i \otimes v_j)_{i,j\in\mathbb{N}}$ is complete: Assume that $f \in L^2(\Omega_1 \times \Omega_2)$, $f \perp (u_i \otimes v_j)_{i,j\in\mathbb{N}}$. We prove that $f \equiv 0$. We have for all $i \in \mathbb{N}$

$$0 = \langle f, u_i \otimes v_j\rangle = \iint \overline{f(x, y)}u_i(x)v_j(y)\mathrm{d}x\mathrm{d}y = \int u_i(x) \underbrace{\int \overline{f(x, y)}v_j(y)\mathrm{d}y}_{g_j(x)} \mathrm{d}x$$

  Because $(u_i)_{i\in\mathbb{N}}$ is an ONB, for a.e. x we must have

$$\int \overline{f(x, y)}v_j(y) = 0$$

  for all $j \in \mathbb{N}$. However, as $(v_j)_{j\in\mathbb{N}}$ is an ONB it follows that for a.e. x, a.e. y $f(x, y) = 0$.

q.e.d.

Lemma 8.31. *a)* $L^2(\mathbb{R}^{dN}) = L^2(\mathbb{R}^d) \otimes L^2(\mathbb{R}^d) \otimes \cdots \otimes L^2(\mathbb{R}^{dN})$ *N-times and if* $(u_i)_{i\in\mathbb{N}}$ *is an ONB for* $L^2(\mathbb{R}^d)$*, then*

$$\left\{u_{i_1} \otimes \cdots \otimes u_{i_N} \,\middle|\, i_1, \ldots, i_N \in \mathbb{N}\right\}$$

is an ONB for $L^2(\mathbb{R}^{dN})$

b) $L^2_a(\mathbb{R}^{dN}) = P_N L^2(\mathbb{R}^{dN})$ *with the projection being defined by*

$$P_N \Psi_N(x_1, \ldots, x_N) = \frac{1}{N!} \sum_{\sigma \in \mathfrak{S}_n} \operatorname{sgn}(\sigma) \Psi_N\Big(x_{\sigma(1),\ldots,x_{\sigma(n)}}\Big)$$

for all $\Psi_N \in L^2(\mathbb{R}^d)$*. Consequently the Slater determinant*

$$\left\{u_{i_1} \wedge u_{i_2} \wedge \cdots \wedge u_{i_N} \,\middle|\, i_1, \ldots, i_N \in \mathbb{N}, i_1 < i_2 < \cdots < i_N\right\}$$

form an ONB for $L^2_a(\mathbb{R}^{dN})$*.*

□

Proof. a) By the previous lemma and induction.

b) P_N is a projection as $P_N^2 = P_N$ as

$$\begin{aligned}
P_N^2 \Psi_N(x_1, \ldots, x_N) &= P_N \frac{1}{N!} \sum_{\sigma \in \mathfrak{S}_n} \operatorname{sgn}(\sigma) \Psi_N\big(x_{\sigma(1)}, \ldots, x_{\sigma(N)}\big) = \\
&= \frac{1}{N!} \sum_{\sigma \in \mathfrak{S}_n} \operatorname{sgn}(\sigma) \frac{1}{N!} \sum_{\tau \in \mathfrak{S}_n} \operatorname{sgn}(\tau) \Psi_N\big(x_{\tau\circ\sigma(1)}, \ldots, x_{\tau\circ\sigma(N)}\big) = \\
&= \frac{1}{N!} \sum_{\sigma \in \mathfrak{S}_n} \frac{1}{N!} \underbrace{\sum_{\tau \in \mathfrak{S}_n} \operatorname{sgn}(\tau \circ \sigma) \Psi_N\big(x_{\tau\circ\sigma(1)}, \ldots, x_{\tau\circ\sigma(N)}\big)}_{\text{independent of } \sigma} = \\
&= \frac{1}{N!} N! \frac{1}{N!} \sum_{\tau \in \mathfrak{S}_n} \operatorname{sgn}(\tau) \Psi_N\big(x_{\sigma(1)}, \ldots, x_{\sigma(N)}\big) = P_N \Psi_N(x_1, \ldots, x_N)
\end{aligned}$$

q.e.d.

Proof of Theorem 8.25. We want to prove that if $u \in L^2(\mathbb{R}^d)$, $\|u\|_2 = 1$, then

$$\left\langle 0, \gamma_{\Psi_N}^{(1)} u \right\rangle \leqslant 1$$

Writing

$$\left\langle u, \gamma_{\Psi_N}^{(1)} u \right\rangle = \operatorname{Tr}\left(P_u \gamma_{\Psi_N}^{(1)}\right) = \left\langle \Psi_N, \sum_{j=1}^{N} (P_u)_{x_j} \Psi_N \right\rangle$$

where $P_u = |u\rangle \langle u|$. Thus we need to prove that

$$A = \sum_{j=1}^{N} (P_u)_{x_j} \leqslant 1$$

in $L_a^2(\mathbb{R}^d)$. Consider an ONB $(u_i)_{i \in \mathbb{N}}$ of $L^2(\mathbb{R}^d)$. We can choose $u_1 = u$. We claim that

$$Au_{i_1} \wedge \cdots \wedge u_{i_N} = \begin{cases} u_{i_1} \wedge \cdots \wedge u_{i_N}, & \text{if } 1 \in \{i_1, \ldots, i_N\} \\ 0, & \text{otherwise} \end{cases}$$

If the claim holds true

$$A = \sum_{1 \in \{i_1, \ldots, i_N\}} |u_{i_1} \wedge \cdots \wedge u_{i_N}\rangle \langle u_{i_1} \wedge \cdots \wedge u_{i_N}|$$

thus $0 \leqslant A \leqslant 1$. Let us check the claim

$$P_u = |u\rangle \langle u| \quad \therefore \quad P_u u_i = \delta_{i1} u_1$$

We have

$$
\begin{aligned}
Au_{i_1} \wedge \cdots \wedge u_{i_N} &= \sum_{j=1}^{N} (P_u)_{x_j} \sum_{\sigma \in \mathfrak{S}_N} \frac{1}{\sqrt{N!}} \operatorname{sgn}(\sigma) u_{i_{\sigma(1)}}(x_1) \cdots u_{i_{\sigma(N)}}(x_N) = \\
&= \sum_{j=1}^{N} \sum_{\sigma \in \mathfrak{S}_N} \frac{1}{\sqrt{N!}} \operatorname{sgn}(\sigma) u_{i_{\sigma(1)}}(x_1) \cdots \Big(P_u u_{i_{\sigma(j)}}(x_j) \Big) \cdots u_{i_{\sigma(N)}}(x_N) = \\
&= \sum_{j=1}^{N} \sum_{\sigma \in \mathfrak{S}_N} \frac{1}{\sqrt{N!}} \operatorname{sgn}(\sigma) \delta_{1\sigma(j)} u_{i_{\sigma(1)}}(x_1) \cdots u_1(x_j) \cdots u_{i_{\sigma(N)}}(x_N) = \\
&= \begin{cases} 0, & \text{if } 1 \notin \{i_1, \ldots, i_N\} \\ \sum_{j=1}^{N} \sum_{\substack{\sigma \in \mathfrak{S}_N \\ \sigma(j)=1}} \frac{1}{\sqrt{N!}} \operatorname{sgn}(\sigma) u_{i_{\sigma(1)}}(x_1) \cdots u_1(x_j) \cdots u_{i_{\sigma(N)}}(x_N) = u_{i_1} \wedge \cdots \wedge u_{i_N} \end{cases}
\end{aligned}
$$

q.e.d.

Example 8.32. Consider

$$H_N = \sum_{i=1}^{N} \left(-\Delta_{x_i} - \frac{Z}{|x_i|} \right)$$

with $x_i \in \mathbb{R}^3$, $Z > 0$ on $L^2_a(\mathbb{R}^{3N})$. What is $\inf \sigma(H_N)$?
By the Pauli exclusion principle

$$\inf \sigma(H_N) = \sum_{i=1}^{N} \mu_i \left(-\Delta - \frac{Z}{|x_i|} \right)$$

where μ_i is the i^{th} min-max value (eigenvalue) of $-\Delta - \frac{Z}{|x|}$ on $L^2(\mathbb{R}^3)$.
Recall that $-\Delta - \frac{Z}{|x|}$ has eigenvalues $-\frac{Z}{4n^2}$ with multiplicity n^2. Thus

$$\sum_{i=1}^{N} \mu_i \approx \sum_{1^2+2^2+\cdots+n^2} -\frac{Z^2}{4n^2} n^2 \approx -\frac{Z^2}{4} (3N)^{\frac{1}{3}}.$$

as

$$N \approx 1^2 + 2^2 + \cdots + n^2 = \frac{n(n+1)(2n+1)}{6} \approx \frac{n^3}{3}$$

thus $n \approx (3N)^{\frac{1}{3}}$. In the case $N = Z$, then

$$\inf \sigma(H_Z) = -\frac{3^{\frac{1}{3}}}{4} Z^{\frac{7}{3}} + o\Big(Z^{\frac{7}{3}} \Big)_{Z \to \infty}.$$

Remark 8.33. If we do not use the information on $\sigma\Big(-\Delta - \frac{Z}{|x|}\Big)$, then we can still prove (for $N = Z$)

$$\inf \sigma(H_Z) \geqslant -CZ^{\frac{7}{3}}$$

for all $Z \in \mathbb{N}$. To prove this

$$\sum_{i=1}^{N} \mu_i\left(-\Delta - \frac{Z}{|x|}\right) = \sum_{i=1}^{N} \mu_i\left(-\Delta - \frac{Z}{|x|} + L\right) - NL \geqslant -\operatorname{Tr}\left[-\Delta - \frac{Z}{|x|} + L\right]_- - LN$$

for $L > 0$. Using the Lieb-Thirring inequality $-\operatorname{Tr}[-\Delta + V]_- \geqslant -C \int\limits_{\mathbb{R}^d} V_-^{\frac{5}{2}}$. Then

$$-\operatorname{Tr}\left[-\Delta - \frac{Z}{|x|} + L\right]_- \geqslant -C \int\limits_{\mathbb{R}^3} \left[-\frac{Z}{|x|} + L\right]_-^{\frac{5}{2}} \mathrm{d}x = -C \int\limits_{|x| \leqslant \frac{Z}{L}} \left[-\frac{Z}{|x|} + L\right]_-^{\frac{5}{2}} \mathrm{d}x =$$
$$= c\left(\frac{Z}{L}\right)^3 L^{\frac{5}{2}} = c\frac{Z^3}{L^{\frac{1}{2}}}.$$

Thus we conclude that for all $L > 0$

$$\sum_{i=1}^{N} \mu_i\left(-\Delta - \frac{Z}{|x|}\right) \geqslant -C\frac{Z^3}{L^{\frac{1}{2}}} - LZ$$

Choosing $\frac{Z^3}{L^{\frac{1}{2}}} = LZ = \left(\left(\frac{Z^3}{L^{\frac{1}{2}}}\right)^2 LZ\right)^{\frac{1}{3}} = Z^{\frac{7}{3}}$. Thus we get the lower bound $-CZ^{\frac{7}{3}}$. For the Homework one can proceed via

$$\sum_{i=1}^{N} \mu_i\left(-\Delta + |x|^2\right) = \underbrace{\sum_{i=1}^{N} \mu_i\left(-\Delta + |x|^2 - L\right)}_{\text{Lieb-Thirring}} + LN \geqslant CN^{\frac{4}{3}}$$

$$\sum_{i=1}^{N} \langle u_i, (-\Delta + |x|^2) u_i \rangle \geqslant C \int \rho^{\frac{5}{3}} + \int |x|^2 \rho \mathrm{d}x$$

$\rho \geqslant 0$, $\int \rho = N$.

$\square$

Considering the atomic Hamiltonian

$$H_N = \sum_{i=1}^{\infty}\left(-\Delta_{x_i} - \frac{Z}{|x_i|}\right) + \sum_{i<j}^{N} \frac{1}{|x_i - x_j|}$$

on $L^2_a\big(\mathbb{R}^{3N}\big)$. H_N is self-adjoint on $H^2_a\big(\mathbb{R}^{3N}\big)$ with

$$E_N = \inf \sigma(H_N) = \inf_{\|\Psi_N\|_2} \langle \Psi_N, H_N \Psi_N \rangle$$

What does E_N look like? For $N \geqslant 2$ one already cannot solve this problem analytically. Even numerically considering 10 particle problem and solving it using the finite-elements method on a grid of 10-points per dimension we already get $10^3 0$ degrees of freedom. Hence the full problem quickly exceed current computational capabilities. Thus we need approximations to make E_N computable.

Definition 8.34 (Thomas-Fermi Theory)**.** Let $\rho_N(x)$ be the one-body density of Ψ_N as in Definition 8.22. Then we have

- $$\left\langle \Psi_N, \sum_{i=1}^{N} -\frac{Z}{|x|}\Psi_N \right\rangle = -Z \int\limits_{\mathbb{R}^3} \frac{\rho_N(x)}{|x|}$$

- From the kinetic Lieb-Thirring inequality we have

  $$\left\langle \Psi_N, \sum_{i=1}^{N} -\Delta_{x_i}\Psi_N \right\rangle \approx K_{\mathrm{cl}} \int\limits_{\mathbb{R}^3} \rho_N^{\frac{5}{3}}$$

  where $K_{\mathrm{cl}} = \frac{3}{5}(6\pi^2)^{\frac{2}{2}}$.

- $$\left\langle \Psi_N \frac{1}{2} \sum_{i \neq j}^{N} \frac{1}{|X_i - x_j|}\Psi_N \right\rangle \approx \frac{1}{2} \int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3} \frac{\rho_N(x)\rho_N(y)}{|x-y|} \mathrm{d}x \mathrm{d}y.$$

Thus we define the Thomas-Fermi functional

$$\mathcal{E}^{\mathrm{TF}}_Z(\rho) = K_{\mathrm{cl}} \int\limits_{\mathbb{R}^3} \rho^{\frac{5}{3}} - Z \int\limits_{\mathbb{R}^3} \frac{\rho(x)}{|x|} + \frac{1}{2}\int\limits_{\mathbb{R}^3}\int\limits_{\mathbb{R}^3} \frac{\rho(x)\rho(y)}{|x-y|}$$

with the Thomas-Fermi energy

$$E_Z^{\mathrm{TF}}(N) = \inf\left\{ \mathcal{E}_Z^{\mathrm{TF}}(\rho) \,\middle|\, \rho \in L^1 \cap L^{\frac{5}{3}}, \rho \geqslant 0, \int_{\mathbb{R}^3} \rho = N \right\}$$

□

Theorem 8.35 (TF Theory)**.** *Considering the case $N = Z$ (not necessarily an integer). Then*

(1) E_Z^{TF} has a unique minimiser. The minimiser is radial and

$$\frac{5}{3} K_{cl} (\rho_z^{TF})^{\frac{2}{3}} = \frac{Z}{|x|} - \rho_Z^{TF} * \frac{1}{|x|}.$$

(2) $E_Z^{TF} = Z^{\frac{7}{3}} E_1^{TF}$ and $\rho_Z^{TF}(x) = Z^2 \rho_1^{TF}\Big(Z^{\frac{1}{3}} x\Big)$.

□

Proof. (2) Assuming that $\rho \geqslant 0$, $\int \rho = Z$. Denote

$$\rho(x) = Z^2 f(Z^{\frac{1}{3}} x)$$

Then

$$\int \rho^{\frac{5}{3}} = \int Z^{\frac{10}{3}} \left| f(Z^{\frac{1}{3}} x) \right|^{\frac{5}{3}} \mathrm{d}x = \frac{Z^{\frac{10}{3}}}{Z} \int |f|^{\frac{5}{3}} \mathrm{d}x = Z^{\frac{7}{3}} \int f^{\frac{5}{3}}$$

$$Z \int \frac{\rho(x)}{|x|} \mathrm{d}x = Z^3 \int \frac{f(Z^{\frac{1}{3}} x)}{|x|} \mathrm{d}x = Z^{\frac{7}{3}} \int \frac{f(x}{|x|} \mathrm{d}x$$

$$\iint \frac{\rho(x)\rho(y)}{|x-y|} \mathrm{d}x\mathrm{d}y = Z^{\frac{7}{3}} \iint \frac{f(x) f(y)}{|x-y|} \mathrm{d}x\mathrm{d}y$$

Thus $\mathcal{E}_Z^{\mathrm{TF}}(\rho) = Z^{\frac{7}{3}} \mathcal{E}_1^{\mathrm{TF}}(f)$ and therefore $E_Z^{\mathrm{TF}} = Z^{\frac{7}{3}} E_1^{\mathrm{TF}}$.

(1) Step 1 Consider the case $Z = 1$, which is enough by the above.

$$\mathcal{E}^{\mathrm{TF}}(\rho) = K_{\mathrm{cl}} \int \rho^{\frac{5}{3}} - \int \frac{\rho(x)}{|x|} + \frac{1}{2} \iint \frac{\rho(x)\rho(y)}{|x-y|} \mathrm{d}x\mathrm{d}y$$

with $\rho \geqslant 0$, $\int \rho = 1$. Observe that

$$\int\limits_{\mathbb{R}^3} \frac{\rho(x)}{|x|}\mathrm{d}x = \int\limits_{|x|\leqslant 1} \frac{\rho(x)}{|x|} + \int\limits_{|x|\geqslant 1} \frac{\rho(x)}{|x|} \leqslant \left(\int \rho^{\frac{5}{3}}\right)^{\frac{3}{5}} \left(\int\limits_{|x|\leqslant 1} \frac{1}{|x|^{\frac{5}{2}}}\right)^{\frac{2}{5}} + \int \rho(x) \leqslant$$
$$\leqslant C\left(\int \rho^{\frac{5}{3}}\right)^{\frac{3}{5}} + 1 \leqslant \frac{1}{2}\int \rho^{\frac{5}{3}} + C$$

Thus

$$\mathcal{E}^{\mathrm{TF}}(\rho) \geqslant \frac{1}{2}\int \rho^{\frac{5}{3}} - C$$

for all $\rho \in L^1 \cap L^{\frac{5}{3}}$, $\int \rho = 1$.

Thus $E^{\mathrm{TF}} > -\infty$. Thus there exists a minimising sequence ρ_n such that $\rho_n \geqslant 0$, $\int \rho_n = 1$ and $\mathcal{E}^{\mathrm{TF}}(\rho_n) \to E^{\mathrm{TF}}$. Since

$$E^{\mathrm{TF}} \longleftarrow \mathcal{E}^{\mathrm{TF}}(\rho_n) \geqslant \frac{1}{2}\int \rho_n^{\frac{5}{3}} - C$$

thus ρ_n us bounded in $L^{\frac{5}{3}}$ independently of n. Thus we can go to a subsequence (if necessary) and assume that $\rho_n \rightharpoonup \rho_0$ in $L^{\frac{5}{3}}$, i.e. for all $\varphi \in L^{\frac{5}{2}}$

$$\int \rho_n\varphi \longrightarrow \int \rho_0\varphi.$$

We have to prove that ρ_0 is a minimiser.

Step 2 The mapping $\rho \mapsto \mathcal{E}^{\mathrm{TF}}(\rho)$ is strictly convex, i.e.

$$\mathcal{E}^{\mathrm{TF}}\left(\frac{f+g}{2}\right) \leqslant \frac{\mathcal{E}^{\mathrm{TF}}(f) + \mathcal{E}^{\mathrm{TF}}(g)}{2}$$

with equality iff $f \equiv g$.

To show this note that $f \mapsto f^{\frac{5}{3}}$ is convex and $f \mapsto \frac{f}{|x|}$ is linear. The non-trivial thing is to show that

$$f \mapsto \frac{1}{2}\iint \frac{f(x)f(y)}{|x-y|}\mathrm{d}x\mathrm{d}y =: D(f)$$

is convex. This follows from

$$\frac{D(f_1)+D(f_2)}{2} - D\left(\frac{f_1+f_2}{2}\right) = D\left(\frac{f_1-f_2}{2}\right) \geqslant 0$$

as

$$D(f) = C\int \frac{\left|\widehat{f_1-f_2}(k)\right|^2}{|k|^2}\mathrm{d}k \geqslant 0.$$

Thus

- If $\mathcal{E}^{\mathrm{TF}}$ has a minimiser, then it is unique. Moreover, the minimiser (if it exists) is radial as
$$\mathcal{E}^{\mathrm{TF}}(\rho(\cdot)) = \mathcal{E}^{\mathrm{TF}}(\rho(R\cdot))$$
for all $R \in SO(3)$.

- We can assume that the minimising sequence ρ_n in Step 1 are radial
$$\mathcal{E}^{\mathrm{TF}}(\rho) = \mathcal{E}^{\mathrm{TF}}(\rho(R\cdot)) = \int\limits_{SO(3)} \mathcal{E}^{\mathrm{TF}}(\rho(R\cdot))\mathrm{d}R \geqslant \mathcal{E}^{\mathrm{TF}}\left(\int\limits_{SO(3)} \rho(R\cdot)\mathrm{d}R\right) =: \mathcal{E}^{\mathrm{TF}}(\tilde{\rho})$$
There $\mathrm{d}R$ is the Haar measure on $SO(3)$, which is the only measure that on $SO(3)$ that is invariant under $SO(3)$ and $\int_{SO(3)} \mathrm{d}R = 1$.
Note that $\tilde{\rho} \geqslant 0$, $\int \tilde{\rho} = 1$ and $\tilde{\rho}$ is radial. In particular as $\mathcal{E}^{\mathrm{TF}}(\rho_n) \geqslant \mathcal{E}^{\mathrm{TF}}(\tilde{\rho}_n)$ and ρ is a minimising sequence, weakly converging to ρ_0 it follows that $\tilde{\rho}_n \rightharpoonup \rho_0$, hence ρ is also radial.

Step 3 We need to prove that ρ_0 is a minimiser. We check that $\liminf_{n\to\infty} \mathcal{E}^{\mathrm{TF}}(\rho_n) \geqslant \mathcal{E}^{\mathrm{TF}}(\rho)$.

- Since $\rho_n \rightharpoonup \rho_0$ weakly in $L^{\frac{5}{3}}$ it follows that $\liminf \int \rho_n^{\frac{5}{3}} \geqslant \int \rho_0^{\frac{5}{3}}$, as
$$\|f\|_p^p = \sup_{\substack{g\in L^q\\ \|g\|_q=1}} \left|\int fg\right|$$
with $\frac{1}{p}+\frac{1}{q}=1$.

- $$\int \frac{\rho_n(x)}{|x|} \to \int \frac{\rho_0(x)}{|x|}$$

as

$$\left|\int \frac{\rho_n(x)-\rho_0(x)}{|x|}\right| = \left|\int\limits_{|x|\leqslant R} \frac{\rho_n(x)-\rho_0(x)}{|x|}\right| + \left|\int\limits_{|x|\geqslant R} \frac{\rho_n(x)-\rho_0(x)}{|x|}\right| \leqslant$$
$$\leqslant \left|\int\limits_{|x|\leqslant R} \frac{\rho_n(x)-\rho_0(x)}{|x|}\right| + \frac{C}{R}$$

Since $\frac{1}{|x|}\mathbf{1}_{\{|x|\leqslant R\}} \in L^{\frac{5}{2}} = \left(L^{\frac{5}{3}}\right)^*$, it follows that

$$\int\limits_{|x|\leqslant R} \frac{\rho_n(x)}{|x|} \xrightarrow{n\to\infty} \int\limits_{|x|\leqslant R}$$

as $\rho_n \rightharpoonup \rho_0$ weakly in $L^{\frac{5}{3}}$. Thus

$$\limsup_{n\to\infty} \left|\int\limits_{\mathbb{R}^3} \frac{\rho_n-\rho_0}{|x|}\right| \leqslant \frac{C}{R}$$

Taking $R\to\infty$ yields the result.

- $$\iint \frac{\rho_n(x)\rho_n(y)}{|x-y|} \xrightarrow{n\to\infty} \iint \frac{\rho_0(x)\rho_0(y)}{|x-y|} \iff \iint \frac{\rho_n(x)\rho_n(y)}{\max\{|x|,|y|\}} \xrightarrow{n\to\infty} \iint \frac{\rho_0(x)\rho_0(y)}{\max\{|x|,|y|\}}$$

  This can be done by separating the two cases $\max\{|x|,|y|\} \leqslant R$ and $\max\{|x|,|y|\} \geqslant R$.

Thus we may conclude that

$$E^{\mathrm{TF}} = \liminf_{n\to\infty} \mathcal{E}^{\mathrm{TF}}(\rho_n) \geqslant \mathcal{E}^{\mathrm{TF}}(\rho_0)$$

We yet cannot follows that ρ_0 is a minimiser as we have to show that $\int \rho_0 = 1$. Note that as $\rho_n \rightharpoonup \rho_0$ in $L^{\frac{5}{3}}$ thus

$$1 = \liminf \int \rho_n \geqslant \rho_0$$

Thus we have to prove that $\int \rho_0 = 1$ and this is non-trivial.

Step 4 Consider the problem

$$E_{\leqslant}^{\mathrm{TF}} := \inf\left\{\mathcal{E}^{\mathrm{TF}}(\rho)\,\middle|\,\rho \geqslant 1, \int \rho \leqslant 1\right\}$$

for which $E_{\leqslant}^{\mathrm{TF}} \leqslant E^{\mathrm{TF}}$.

By the same argument, we can prove that $E_{\leqslant}^{\mathrm{TF}}$ has a minimiser. Denote g_0 the minimiser $E_{\leqslant}^{\mathrm{TF}}$. We will prove that $\int g_0 = 1$ thus g_0 is also a minimiser for E^{TF} and therefore

$$E^{\mathrm{TF}} \leqslant \mathcal{E}^{\mathrm{TF}}(g_0) \leqslant E_{\leqslant}^{\mathrm{TF}} \leqslant E^{\mathrm{TF}}$$

and $g_0 = \rho_0$.

Let us prove that $\int g_0 = 1$. Assume that $\int g_0 < 1$, ten $\mathcal{E}^{\mathrm{TF}}(g_0) \leqslant \mathcal{E}^{\mathrm{TF}}(g_0) \leqslant \mathcal{E}^{\mathrm{TF}}(f)$ or all $f \geqslant 0$, $\int f \leqslant 1$. Take $\varphi \geqslant -Cg_0$. Then $g_\varepsilon = g_0 + \varepsilon\varphi \geqslant 0$ if $\varepsilon > 0$ is small enough and $\int g_\varepsilon = \int g_0 + \varepsilon \int \varphi \leqslant 1$ if $\varepsilon > 0$ small.

Thus $\mathcal{E}^{\mathrm{TF}}(g_0) \leqslant \mathcal{E}^{\mathrm{TF}}(g_\varepsilon)$ for all $\varepsilon > 0$ small.

Therefore we have

$$0 \leqslant \frac{d}{d\varepsilon}\mathcal{E}^{\mathrm{TF}}(g_\varepsilon)\bigg|_{\varepsilon=0} = \frac{5}{3}K_{\mathrm{cl}}\int g_0^{\frac{2}{3}}\varphi - \int \frac{\varphi}{|x|}\mathrm{d}x + \iint \frac{g_0(x)\varphi(y)}{|x-y|}\mathrm{d}x\mathrm{d}y = \int W\varphi$$

where

$$W = \frac{5}{3}K_{\mathrm{cl}}g_0^{\frac{2}{3}} - \frac{1}{|x|} + g_0 * \frac{1}{|x|}.$$

and one has to justify the interchanging of the derivative and the integration.

Therefore $W\varphi \geqslant 0$ for all $\varphi \geqslant -Cg_0$, in particular we get

$$\begin{cases} W \geqslant 0, & \text{for a.e. } x \\ W(x) = 0 & \text{if } g_0(x) > 0 \end{cases}$$

We have

$$\frac{5}{3}K_{\mathrm{cl}}g_0^{\frac{2}{3}} \geqslant \frac{1}{|x|} - g_0 * \frac{1}{|x|} \geqslant \underbrace{\left(1 - \int \rho\right)}_{>0}\frac{1}{|x|}$$

as g_0 is radial and by Newton's theorem

$$g_0 * \frac{1}{|x|} = \int \frac{g_0(y)}{|x-y|}\ y = \int \frac{g_0(y)}{\max\{|x|,|y|\}}\mathrm{d}y \leqslant \frac{\int \rho_0}{|x|}$$

i.e. $g_0^{\frac{2}{3}} \geqslant \frac{C}{|x|}$ for a.e. x, however, this is impossible as $g_0 \in L^1$ and $\frac{1}{|x|^{\frac{3}{2}}}$ is not.

We can conclude that $\int g_0 = 1$, i.e. $g_0 = \rho$ is the unique minimiser for E^{TF} (and $E^{\mathrm{TF}} = E^{\mathrm{TF}}_{\leqslant}$).

Step 5 We need to prove that

$$\frac{5}{3} K_{\mathrm{cl}} g_0^{\frac{2}{3}} = \frac{1}{|x|} - g_0 * \frac{1}{|x|}, \qquad \text{for a.e. } x$$

i.e. $W \equiv 0$. We can mimic the proof in Step 4. We have for all $\varphi \geqslant -C g_0$, $\int \varphi \leqslant 0$.

$$\int W\varphi \geqslant 0$$

Choosing $\varphi(x) = h(x) - \left(\int h\right) g_0(x)$ which has satisfies $\int \varphi_0 = 0$ and $\varphi \geqslant -C g_0$ if $h \geqslant -C g_0$.

Thus

$$0 \leqslant \int W\left(h - \left(\int h\right) g_0(x)\right) = \int (W + \mu) h$$

with $\mu = -\int Wh \in \mathbb{R}$ a constant. Thus $\int (W+\mu) h \geqslant 0$ for all $h \geqslant -c g_0$. Thus

$$\begin{cases} W + \mu \geqslant 0, & \text{for a.e. } x \\ W + \mu = 0, & \text{if } g_0(x) > 0 \end{cases}$$

Recalling that

$$W + \mu = \frac{5}{3} K_{\mathrm{cl}} g_0^{\frac{2}{3}} - \frac{1}{|x|} + g_0 * \frac{1}{|x|} + \mu$$

We can see that $\mu \geqslant 0$. Indeed

$$\frac{5}{3} K_{\mathrm{cl}} g_0^{\frac{2}{3}} \geqslant \underbrace{\frac{1}{|x|} - g_0 * \frac{1}{|x|}}_{\geqslant 0} - \mu \geqslant -\mu$$

and $g_0 \in L^1$ thus $-\mu \leqslant 0$ and $\mu \geqslant 0$.

We prove that $\mu = 0$. Assume that $\mu > 0$. Because $W + \mu \geqslant -\frac{1}{|x|} + \mu > 0$ if $|x| \geqslant \frac{1}{|\mu|}$ it follows that $g_0(x) = 0$ if $|x| \geqslant \frac{1}{|\mu|}$, i.e. g_0 has compact support. Take $R > 0$ the smallest number such that $\operatorname{supp} g_0 \subset B_R(0)$.

Note that for all $R' \leqslant |x| \leqslant R$

$$-\frac{1}{|x|} + g_0 * \frac{1}{|x|} \geqslant \frac{-1 + \int_{|x| \leqslant R'} g_0}{R'}$$

Thus

$$-\frac{1}{|x|} + g_0 * \frac{1}{|x|} \xrightarrow{|x| \to R} 0$$

i.e. for all $\varepsilon > 0$ there exists a $R' < R$ such that

$$-\frac{1}{|x|} + g_0 * \frac{1}{|x|} \geqslant -\varepsilon$$

Thus $W + \mu \geqslant -\varepsilon + \mu > 0$ if $\varepsilon < \mu$ and $|x| \geqslant R'$, i.e. $g_0(x) = 0$ if $|x| \geqslant R'$. This a contradiction to $\operatorname{supp} g_0 \subset B_R(0)$ with R smallest.

Because $\mu = 0$, $W \geqslant 0$ a.e. and thus we have

$$\frac{5}{3} K_{\mathrm{cl}} g_0^{\frac{2}{3}} \geqslant \frac{1}{|x|} - g_0 * \frac{1}{|x|} > 0.$$

for all x. Thus $g_0 > 0$ for all x and therefore $W = 0$ and

$$\frac{5}{3} K_{\mathrm{cl}} g_0^{\frac{2}{3}} = \frac{1}{|x|} - g_0 * \frac{1}{|x|}.$$

q.e.d.