Math 212b Lecture 5.

Bound states and scattering states.

From W.O. Amrein and V. Georgescu,
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W. Hunziker and I. Sigal
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It is a truism in atomic physics or quantum chemistry courses that the eigenstates of the Schrödinger operator are the bound states, the ones that remain bound to the nucleus, and that the “scattering states” which fly off in large positive or negative times correspond to the continuous spectrum. The purpose of today’s lecture is to give a mathematical justification for this truism. The key result is due to Ruelle, (1969), using ergodic theory methods. The more streamlined version presented in today’s lecture comes from the two papers mentioned in the title. The ergodic theory used is limited to the mean ergodic theorem of von-Neumann which has a very slick proof due to F. Riesz (1939) which I shall give.

The mean ergodic theorem.

We will need the continuous time version: Let H be a self-adjoint operator on a Hilbert space $\mathcal{H}$ and let

$$V_t = \exp(-itH)$$

be the one parameter group it generates (by Stone's theorem). von Neumann's mean ergodic theorem asserts that for any $f \in \mathcal{H}$ the limit

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T V_t f \, dt$$

exists, and the limit is an eigenvector of H corresponding to the eigenvalue 0.

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T V_t f\,dt$$

Clearly, if $Hf = 0$, then $V_t f = f$ for all t and the above limit exists trivially and is equal to f. If f is orthogonal to the image of H, i.e. if

$$Hg = 0\ \forall g \in \mathrm{Dom}(H)$$

then $f \in \mathrm{Dom}(H^*) = \mathrm{Dom}(H)$ and $H^* f = Hf = 0$. So if we decompose $\mathcal{H}$ into the zero eigenspace of H and its orthogonal complement, we are reduced to the following version of the theorem which is the one we will actually use:

Theorem 2 *Let H be a self-adjoint operator on a Hilbert space $\mathcal{H}$, and assume that H has no eigenvectors with eigenvalue 0, so that the image of H is dense in $\mathcal{H}$. Let $V_t = \exp(-itH)$ be the one parameter group generated by H. Then*

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T V_t f \, dt = 0$$

for all $f \in \mathcal{H}$.

Proof. If $h = -iHg$ then

$$V_t h = \frac{d}{dt} V_t g$$

so

$$\frac{1}{T}\int_0^T V_t h dt = \frac{1}{T}(V_t g - g) \to 0.$$

By hypothesis, for any $f \in \mathcal{H}$ we can, for any $\epsilon > 0$, find an h of the above form such that $\|f - h\| < \frac{1}{2}\epsilon$ so

$$\left\| \frac{1}{T}\int_0^T V_t f dt \right\| \leq \frac{1}{2}\epsilon + \left\| \frac{1}{T}\int_0^T V_t h dt \right\|.$$

By then choosing T sufficiently large we can make the second term less than $\frac{1}{2}\epsilon$. $\square$

Cores and relative bounds.

Recall that a symmetric operator T is called essentially self-adjoint if its closure is self adjoint.

If A is a self-adjoint operator with domain $D(A)$, a subspace $\mathcal{D} \subset D(A)$ is called a **core** for A if the closure of the restriction of A to $\mathcal{D}$ is A. We will give a variant of this definition when we study quadratic forms.

Let A and B be densely defined operators on a Hilbert space $\mathcal{H}$. We say that B is A-**bounded** if

- $D(B) \supset D(A)$ and
- There exist real numbers a and b such that

$$\|B\phi\| \leq a\|A\phi\| + b\|\phi\| \quad \forall\ \phi \in D(A). \tag{1}$$

$$\|B\phi\| \leq a\|A\phi\| + b\|\phi\| \quad \forall\ \phi \in D(A). \qquad (1)$$

Notice that if

$$\|B\phi\|^2 \leq a^2\|A\phi\|^2 + b^2\|\phi\|^2 \qquad (2)$$

then (1) holds. On the other hand, if (1) holds, then for any $\epsilon > 0$, then

$$\|B\phi\|^2 \leq a^2\|A\phi\|^2 + b^2\|\phi\|^2 + 2ab\|A\phi\|\phi\|.$$

Writing $ab = (a\epsilon)(b\epsilon^{-1})$ we get

$$2ab\|A\phi\|\phi\| \leq a^2\epsilon^2\|A\phi\|^2 + b^2\epsilon^{-2}\|\phi\|^2.$$

So (1) implies (2) with a replaced by $a+\epsilon$ and b replaced by $b+\epsilon^{-1}$. Thus the infimum of a over all (a,b) such that (1) holds is the same as the infimum of a over all (a,b) such that (2) holds.

So (1) implies (2) with a replaced by $a+\epsilon$ and b replaced by $b+\epsilon^{-1}$. Thus the infimum of a over all (a,b) such that (1) holds is the same as the infimum of a over all (a,b) such that (2) holds.

This common infimum is called the **relative bound** of B with respect to A. If this relative bound is 0 we say that B is **infinitesimally small** with respect to A. In verifying (1) or (2) it is sufficient to do so for all ϕ belonging to a core of A.

The following theorem was proved by Rellich in 1939 and was extensively used by Kato in the 1960's and is known as the **Kato-Rellich theorem**.

Theorem 1 *Let A be a self-adjoint operator and B a symmetric operator which is relatively A-bounded with relative bound $a < 1$. Then $A + B$ is self-adjoint on $D(A)$ and is essentially self-adjoint on any core of A. If A is bounded below by M then $A + B$ is bounded below by*

$$M - \max\left\{\frac{b}{1-a}, a|M| + b\right\}$$

for any (a, b) for which (1) holds.

To prove that $A + B$ is self-adjoint, it is enough to show that for some $\mu > 0$ we have that $\text{Range}(A+B \pm i\mu I) = \mathcal{H}$. For *any* $\mu > 0$ and any $\phi \in D(A)$ we have

$$\|(A \pm i\mu I)\phi\|^2 = \|A\phi\|^2 + \mu^2\|\phi\|^2.$$

We may write $\phi = (A + i\mu I)^{-1}\psi$ and rewrite the above equality (with $\pm = +$) as

$$\|\psi\|^2 = \|A(A + i\mu I)^{-1}\psi\|^2 + \mu^2\|(A + i\mu)^{-1}\psi\|^2.$$

In particular,

$$\|A(A + i\mu I)^{-1}\psi\| \leq \|\psi\| \quad \text{and} \quad \|(A + i\mu I)^{-1}\psi\| \leq \frac{1}{\mu}\|\psi\|.$$

$$\|B\phi\| \leq a\|A\phi\| + b\|\phi\| \quad \forall\, \phi \in D(A). \qquad (1)$$

$$\|A(A+i\mu I)^{-1}\psi\| \leq \|\psi\| \quad \text{and} \quad \|(A+i\mu I)^{-1}\psi\| \leq \frac{1}{\mu}\|\psi\|.$$

Substituting $\phi = (A+i\mu I)^{-1}\psi$ into (1) gives

$$\|B(A+i\mu I)^{-1}\psi\| \leq \left(a + \frac{b}{\mu}\right)\|\psi\|.$$

Now $a < 1$ by assumption. So for μ sufficiently large the operator $C := B(A+i\mu I)^{-1}$ has norm < 1. Hence -1 is not in the spectrum of C and so $I + C$ is invertible and so $\text{Range}(I+C) = \mathcal{H}$. Also $\text{Range}(A+i\mu I) = \mathcal{H}$ since A is self-adjoint. Hence $\text{Range}(I+C)(A+i\mu I) = \mathcal{H}$. But

$$(I+C)(A+i\mu I)\phi = (A+B+i\mu I)\phi.$$

The same argument with $-\mu$ implies that $A+B$ is self-adjoint.

If $\mathcal{D}$ is a core of A then follows from (1) that the domain of the closure $A+B$ restricted to $\mathcal{D}$ contains the closure of the domain of A restricted to $\mathcal{D}$. this shows that $A+B$ is essentially self-adjoint on any core of A.

The lower bound part is proved the same way.

The point spectrum and the continuous spectrum.

Let H be a self-adjoint operator on a separable Hilbert space $\mathcal{H}$ and let V_t be the one parameter group generated by H so

$$V_t := \exp(-iHt).$$

Let

$$\mathcal{H} = \mathcal{H}_p \oplus \mathcal{H}_c$$

be the decomposition of $\mathcal{H}$ into the subspaces corresponding to pure point spectrum and continuous spectrum of H.

Increasing projections.

Let $\{F_r\}$, $r = 1, 2, \ldots$ be a sequence of self-adjoint projections. (In the application we have in mind we will let $\mathcal{H} = L_2(\mathbb{R}^n)$ and take F_r to be the projection onto the completion of the space of continuous functions supported in the ball of radius r centered at the origin, but in this section our considerations will be quite general.) We let F'_r be the projection onto the subspace orthogonal to the image of F_r so

$$F'_r := I - F_r.$$

The spaces $\mathcal{M}_0$ and $\mathcal{M}_\infty$.

Let

$$\mathcal{M}_0 := \{f \in \mathcal{H} | \lim_{r\to\infty} \sup_{t\in\mathbb{R}} \|(I - F_r)V_t f\|^2 = 0\}, \qquad (1)$$

and

$$\mathcal{M}_\infty := \left\{ f \in \mathcal{H} \middle| \lim_{T\to\infty} \frac{1}{T} \int_0^T \|F_r V_t f\|^2 dt = 0, \text{ for all } r = 1, 2, \dots \right\}. \qquad (2)$$

Proposition 1 *The following hold:*

1. *$\mathcal{M}_0$ and $\mathcal{M}_\infty$ are linear subspaces of $\mathcal{H}$.*
2. *The subspaces $\mathcal{M}_0$ and $\mathcal{M}_\infty$ are closed.*
3. *$\mathcal{M}_0$ is orthogonal to $\mathcal{M}_\infty$.*
4. *$\mathcal{H}_p \subset \mathcal{M}_0$.*
5. *$\mathcal{M}_\infty \subset \mathcal{H}_c$.*

The following inequality will be used repeatedly: For any $f, g \in \mathcal{H}$

$$\|f+g\|^2 \leq \|f+g\|^2 + \|f-g\|^2 = 2\|f\|^2 + 2\|g\|^2 \quad (5)$$

where the last equality is the theorem of Appolonius.

1. $\mathcal{M}_0$ and $\mathcal{M}_\infty$ are linear subspaces of $\mathcal{H}$.

Proof of 1. Let $f_1, f_2 \in \mathcal{M}_0$. Then for any scalars a and b and any fixed r and t we have

$$\|(I-F_r)V_t(af_1+bf_2)\|^2 \leq 2|a|^2\|((I-F_r)V_t f_1\|^2+2|b|^2\|(I-F_r)V_t f_2\|^2$$

by (3). Taking separate sups over t on the right side and then over t on the left shows that

$$\sup_t \|(I-F_r)V_t(af_1+bf_2)\|^2$$

$$\leq 2|a|^2 \sup_t \|((I-F_r)V_t f_1\|^2 + 2|b|^2 \sup_t \|((I-F_r)V_t f_2\|^2$$

for fixed r. Letting $r \to \infty$ then shows that $af_1 + bf_2 \in \mathcal{M}_0$.

Let $f_1, f_2 \in \mathcal{M}_\infty$. For fixed r we use (3) to conclude that

$$\frac{1}{T}\int_0^T \|F_r V_t(af_1 + bf_2)\|^2 dt$$

$$\leq \frac{2|a|^2}{T}\int_0^T \|F_r V_t f_1\|^2 dt + \frac{2|b|^2}{T}\int_0^T \|F_r V_t f_2\|^2 dt.$$

Each term on the right converges to 0 as $T \to \infty$ proving that $af_1 + bf_2 \in \mathcal{M}_\infty$. This proves 1).

2. The subspaces $\mathcal{M}_0$ and $\mathcal{M}_\infty$ are closed.

Proof of 2. Let $f_n \in \mathcal{M}_0$ and suppose that $f_n \to f$. Given $\epsilon > 0$ choose N so that $\|f_n - f\|^2 < \frac{1}{4}\epsilon$ for all $n > N$. This implies that

$$\|(I - F_r)V_t(f - f_n)\|^2 < \frac{1}{2}\epsilon$$

for all t and n since V_t is unitary and $I - F_r$ is a contraction. Then

$$\sup_t \|(I - F_r)V_t f\|^2 \leq \frac{1}{2}\epsilon + 2\sup_t \|(I - F_r)V_t f_n\|^2$$

for all $n > N$ and any fixed r. We may choose r sufficiently large so that the second term on the right is also less that $\frac{1}{2}\epsilon$. This proves that $f \in \mathcal{M}_0$.

Let $f_n \in \mathcal{M}_\infty$ and suppose that $f_n \to f$. Given $\epsilon > 0$ choose N so that $\|f_n - f\|^2 < \frac{1}{4}\epsilon$ for all $n > N$. Then

$$\frac{1}{T}\int_0^T \|F_r V_r f\|^2 dt \leq \frac{2}{T}\int_0^T \|F_r V_r (f - f_n)\|^2 dt$$

$$+\frac{2}{T}\int_0^T \|F_r V_r f_n\|^2 dt$$

$$\leq \frac{1}{2}\epsilon + \frac{2}{T}\int_0^T \|F_r V_r f_n\|^2 dt.$$

Fix n. For any given r we can choose T_0 large enough so that the second term on the right is $< \frac{1}{2}\epsilon$. This shows that for any fixed r we can find a T_0 so that

$$\frac{1}{T}\int_0^T \|F_r V_r f\|^2 dt < \epsilon$$

for all $T > T_0$, proving that $f \in \mathcal{M}_\infty$. This proves 2).

3. $\mathcal{M}_0$ is orthogonal to $\mathcal{M}_\infty$.

Proof of 3. Let $f \in \mathcal{M}_0$ and $g \in \mathcal{M}_\infty$ both $\neq 0$. Then

$$
\begin{aligned}
|(f,g)|^2 &= \frac{1}{T}\int_0^T |(f,g)|^2 dt \\
&= \frac{1}{T}\int_0^T |(V_t f, V_t g|^2 dt \\
&= \frac{1}{T}\int_0^T |(F_r' V_t f, g) + (V_t f, F_t g)|^2 dt \\
&\leq \frac{2}{T}\int_0^T |(F_r' V_t f, V_t g)|^2 dt + \frac{2}{T}\int_0^T |(V_t f, F_t g)|^2 dt \\
&\leq \frac{2}{T}\|g\|^2 \int |F_r' V_t f\|^2 dt + \frac{2}{T}\|f\|^2 \int_0^T \|F_r V_t g\|^2 dt
\end{aligned}
$$

where we used the Cauchy-Schwarz inequality in the last step.

$$|(f,g)|^2 \quad \leq \quad \frac{2}{T}\|g\|^2 \int |F_r' V_t f\|^2 dt + \frac{2}{T}\|f\|^2 \int_0^T \|F_r V_t g\|^2 dt$$

For any $\epsilon > 0$ we may choose r so that

$$\|F_r' V_t f\|^2 \leq \frac{\epsilon}{4\|g\|^2}$$

for all t. We can choose a T such that

$$\frac{1}{T}\int_0^T \|F_r V_t g\|^2 dt < \frac{\epsilon}{4\|f\|^2}.$$

Plugging back into the last inequality shows that

$$|(f,g)|^2 < \epsilon.$$

Since this is true for any $\epsilon > 0$ we conclude that $f \perp g$. This proves 3.

4. $\mathcal{H}_p \subset \mathcal{M}_0$.

Proof of 4. Suppose $Hf = E$. Then

$$\|F_r' V_t f\|^2 = \|F_r'(e^{-iEt} f)\|^2 = \|e^{-iEt} F_r' f\|^2 = \|F_r' f\|^2.$$

But we are assuming that $F_r' \to 0$ in the strong topology. So this last expression tends to 0 proving that $f \in \mathcal{M}_0$ which is the assertion of 4).

3. *$\mathcal{M}_0$ is orthogonal to $\mathcal{M}_\infty$.*

4. *$\mathcal{H}_p \subset \mathcal{M}_0$.*

5. *$\mathcal{M}_\infty \subset \mathcal{H}_c$.*

Proof of 5. By 3) we have $\mathcal{M}_\infty \subset \mathcal{M}_0^\perp$. By 4) we have $\mathcal{M}_0^\perp \subset \mathcal{H}_p^\perp = \mathcal{H}_c$. □

Goal.

Proposition 1 is valid without any assumptions whatsoever relating H to the F_r. The only place where we used H was in the proof of 4) where we used the fact that if f is an eigenvector of H then it is also an eigenvector of of V_t and so we could pull out a scalar.

The goal is to impose sufficient relations between H and the F_r so that

$$\mathcal{H}_c \subset \mathcal{M}_\infty. \tag{4}$$

3. *$\mathcal{M}_0$ is orthogonal to $\mathcal{M}_\infty$.*

4. *$\mathcal{H}_p \subset \mathcal{M}_0$.*

5. *$\mathcal{M}_\infty \subset \mathcal{H}_c$.*

If we prove this then part 5) of Proposition 1 implies that

$$\mathcal{H}_c = \mathcal{M}_\infty$$

and then part 3) says that

$$\mathcal{M}_0 \subset \mathcal{M}_\infty^\perp = \mathcal{H}_c^\perp = \mathcal{H}_p.$$

Then part 4) gives

$$\mathcal{M}_0 = \mathcal{H}_p.$$

Using the mean ergodic theorem.

The mean ergodic theorem implies that if U_t is a unitary one parameter group acting without (non-zero) fixed vectors on a Hilbert space $\mathcal{G}$ then

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T U_t\psi dt = 0$$

for all $\psi \in \mathcal{G}$. Let

$$\mathcal{G} = \mathcal{H}_c \hat{\otimes} \mathcal{H}_c.$$

We know from our discussion of the spectral theorem that $H \otimes I - I \otimes H$ does not have zero as an eigenvalue acting on $\mathcal{G}$. We may apply the mean ergodic theorem to conclude that

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T e^{-itH} f \otimes e^{itH} e dt = 0$$

for any $e, f \in \mathcal{H}_c$. We have

$$|(e, e^{-itH} f)|^2 = (e \otimes f, e^{-itH} f \otimes e^{itH} e).$$

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T e^{-tH} f \otimes e^{itH} e dt = 0$$

for any $e, f \in \mathcal{H}_c$. We have

$$|(e, e^{-itH} f)|^2 = (e \otimes f, e^{-tH} f \otimes e^{itH} e).$$

We conclude that

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T |(e, V_t f)|^2 dt = 0 \quad \forall\, e \in \mathcal{H}, \quad f \in \mathcal{H}_c. \qquad (5)$$

Indeed, if $e \in \mathcal{H}_c$ this follows from the above, while if $e \in \mathcal{H}_p$ the integrand is identically zero.

The Amrein-Georgescu theorem.

We continue with the previous notation, and let $E_c : \mathcal{H} \to \mathcal{H}_c$ denote orthogonal projection.

We let S_n and S be a collection of bounded operators on $\mathcal{H}$ such that

- $[S_n, H] = 0$,
- $S_n \to S$ in the strong topology,
- The range of S is dense in $\mathcal{H}$, and
- $F_r S_n E_c$ is compact for all r and n.

Theorem 1 [Armein-Georgescu.] *Under the above hypotheses (4) holds.*

$$\mathcal{H}_c \subset \mathcal{M}_\infty. \tag{4}$$

Proof. Since $\mathcal{M}_\infty$ is a closed subspace of $\mathcal{H}$, to prove that (4) holds, it is enough to prove that

$$\mathcal{D} \subset \mathcal{H}_c$$

for some set $\mathcal{D}$ which is dense in $\mathcal{H}_c$. Since S leaves the spaces $\mathcal{H}_p$ and $\mathcal{H}_c$ invariant, the fact that the range of S is dense in $\mathcal{H}$ by hypothesis, says that $S\mathcal{H}_c$ is dense in $\mathcal{H}_c$. So we have to show that

$$g = Sf, \quad f \in \mathcal{H}_c \ \Rightarrow \ \lim_{T\to\infty} \frac{1}{T} \int_0^T \|F_r V_t g\|^2 dt = 0$$

for any fixed r. We may assume $f \neq 0$.

Let $\epsilon > 0$ be fixed. Choose n so large that

$$\|(S - S_n)f\|^2 < \frac{\epsilon}{6}.$$

Any compact operator in a separable Hilbert space is the norm limit of finite rank operators. So we can find a finite rank operator T_N such that

$$\|F_r S_n E_c - T_N\|^2 < \frac{\epsilon}{12\|f\|^2}.$$

Writing $g = (S - S_n)f + S_n f$ we conclude that

$$\frac{1}{T}\int_0^T \|F_r V_t g\|^2 dt$$

$$\leq \quad \frac{2}{T}\int_0^T \|F_r V_t (S - S_n) f\|^2 dt + \frac{2}{T}\int_0^T \|F_r V_t S_n f\|^2 dt$$

$$\frac{1}{T}\int_0^T \|F_r g\|^2 dt \quad \leq$$

$$\begin{aligned}
&\leq \frac{2}{T}\int_0^T \|F_r V_t(S-S_n)f\|^2 dt + \frac{2}{T}\int_0^T \|F_r V_t S_n f\|^2 dt \\
&\leq \frac{\epsilon}{3} + \frac{4}{T}\int_0^T \|F_r S_n E_c - T_N\|^2 \|V_t f\|^2 dt + \frac{4}{T}\int_0^T \|T_N V_t\|^2 dt \\
&\leq \frac{2}{3}\epsilon + \frac{4}{T}\int_0^T \|T_N V_t\|^2 dt.
\end{aligned}$$

To say that T_N is of finite rank means that there are $g_i, h_i \in \mathcal{H},\ i = 1, \ldots N < \infty$ such that

$$T_N f = \sum_{i=1}^{N} (f, h_i) g_i.$$

Substituting this into $\frac{4}{T}\int_0^T \|T_N V_t\|^2 dt.$ gives

$$\frac{4}{T}\int_0^T \|T_N V_t\|^2 dt = \frac{4}{T}\int_0^T \left\| \sum_{i=0}^{N} (V_t f, h_i) g_i \right\|^2 dt$$

$$\leq 2^{N-1} \cdot 4 \cdot \sum \|g_i\|^2 \frac{1}{T}\int_0^T |(h_i, V_t f)|^2 dt.$$

$$\frac{4}{T}\int_0^T \|T_N V_t\|^2 dt = \frac{4}{T}\int_0^T \left\| \sum_{i=0}^{N} (V_t f, h_i) g_i \right\|^2 dt$$

$$\leq 2^{N-1} \cdot 4 \cdot \sum \|g_i\|^2 \frac{1}{T} \int_0^T |(h_i, V_t f)|^2 dt.$$

By (5) we can choose T_0 so large that this expression is $< \frac{\epsilon}{3}$ for all $T > T_0$. $\square$

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T |(e, V_t f)|^2 dt = 0 \quad \forall\, e \in \mathcal{H}, \quad f \in \mathcal{H}_c. \qquad (5)$$

Remark.

Of course a special case of the theorem will be where all the $S_n = S$ as will be the case for Ruelle's theorem for Kato potentials.

Kato potentials.

Let $X = \mathbb{R}^n$ for some n. A locally L_2 real valued function on X is called a **Kato potential** if for any $\alpha > 0$ there is a $\beta = \beta(\alpha)$ such that

$$\|V\psi\| \leq \alpha\|\Delta\psi\| + \beta\|\psi\| \tag{6}$$

for all $\psi \in C_0^\infty(X)$.

Clearly the set of all Kato potentials on X form a real vector space.

We give some examples of Kato potentials.

$$V \in L_2(\mathbb{R}^3).$$

For example, suppose that $X = \mathbb{R}^3$ and $V \in L_2(X)$. We claim that V is a Kato potential. Indeed,

$$\|V\psi\| := \|V\psi\|_2 \leq \|V\|_2 \|\psi\|_\infty.$$

So we will be done if we show that for any $a > 0$ there is a $b > 0$ such that

$$\|\psi\|_\infty \leq a\|\Delta\psi\|_2 + b\|\psi\|_2.$$

By the Fourier inversion formula we have

$$\|\psi\|_\infty \leq \|\hat{\psi}\|_1$$

where $\hat{\psi}$ denotes the Fourier transform of ψ. Now the Fourier transform of $\Delta\psi$ is the function

$$\xi \mapsto \|\xi\|^2 \hat{\psi}(\xi)$$

where $\|\xi\|$ denotes the Euclidean norm of ξ. Since $\hat{\psi}$ belongs to the Schwartz space $\mathcal{S}$, the function

$$\xi \mapsto (1 + \|\xi\|^2)\hat{\psi}(\xi)$$

belongs to L_2 as does the function

$$\xi \mapsto (1 + \|\xi\|^2)^{-1}$$

in three dimensions.

Let λ denote the function

$$\xi \mapsto \|\xi\|.$$

By the Cauchy-Schwarz inequality we have

$$\|\hat{\psi}\|_1 = |((1+\lambda^2)^{-1}, (1+\lambda^2)\hat{\psi})|$$

$$\leq c\|(\lambda^2+1)\hat{\psi}\| \leq c\|\lambda^2\hat{\psi}\|_2 + c\|\hat{\psi}\|_2$$

where

$$c^2 = \|(1+\lambda^2)^{-1}\|_2.$$

For any $r > 0$ and any function $\phi \in \mathcal{S}$ let ϕ_r be defined by

$$\hat{\phi}_r(\xi) = r^3 \hat{\phi}(r\xi).$$

Then

$$\|\hat{\phi}_r\|_1 = \|\hat{\phi}\|_1, \ \ \|\hat{\phi}_r\|_2 = r^{\frac{3}{2}} \|\hat{\phi}\|_2, \ \text{and} \ \ \|\lambda^2 \hat{\phi}_r\|_2 = r^{-\frac{1}{2}} \|\lambda^2 \phi\|_2.$$

Applied to ψ this gives

$$\|\hat{\psi}\|_1 \leq c r^{-\frac{1}{2}} \|\lambda^2 \hat{\psi}\|_2 + c r^{\frac{3}{2}} \|\hat{\psi}\|_2.$$

By Plancherel

$$\|\lambda^2 \hat{\psi}\|_2 = \|\Delta \psi\|_2 \quad \text{and} \quad \|\hat{\psi}\|_2 = \|\psi\|_2.$$

This shows that any $V \in L_2(\mathbb{R}^3)$ is a Kato potential.

$$V \in L_\infty(X).$$

Indeed

$$\|V\psi\|_2 \leq \|V\|_\infty \|\psi\|_2.$$

If we put these two examples together we see that if $V = V_1 + V_2$ where $V_1 \in L_2(\mathbb{R}^3)$ and $V_2 \in L_\infty(\mathbb{R}^3)$ then V is a Kato potential.

4.1.3 The Coulomb potential.

The function

$$V(x) = \frac{1}{\|x\|}$$

on $\mathbb{R}^3$ can be written as a sum $V = V_1 + V_2$ where $V_1 \in L_2(\mathbb{R}^3)$ and $V_2 \in L_\infty(\mathbb{R}^3)$ and so is Kato potential.

Kato potentials from subspaces.

Suppose that $X = X_1 \oplus X_2$ and V depends only on the X_1 component where it is a Kato potential. Then Fubini implies that V is a Kato potential if and only if V is a Kato potential on X_1.

So if $X = \mathbb{R}^{3N}$ and we write $x \in X$ as $x = (x_1, \dots, x_N)$ where $x_i \in \mathbb{R}^3$ then

$$V_{ij} = \frac{1}{\|x_i - x_j\|}$$

are Kato potentials as are any linear combination of them. So the total Coulomb potential of any system of charged particles is a Kato potential.

By example 4.1.4, the restriction of this potential to the subspace $\{x | \sum m_i x_i = 0\}$ is a Kato potential. This is the "atomic potential" about the center of mass.

Applying the Kato-Rellich theorem.

Theorem 2 *Let V be a Kato potential. Then*

$$H = \Delta + V$$

is self-adjoint with domain $\mathcal{D} = \mathrm{Dom}(\Delta)$ and is bounded from below. Furthermore, we have an operator bound

$$\Delta \leq aH + b \tag{7}$$

where

$$a = \frac{1}{1-\alpha} \quad \text{and } b = \frac{\beta(\alpha)}{1-\alpha}, \quad 0 < \alpha < 1.$$

$$\|V\psi\| \leq \alpha\|\Delta\psi\| + \beta\|\psi\| \tag{8}$$

for all $\psi \in C_0^\infty(X)$.

Proof. As a multiplication operator, V is closed on its domain of definition consisting of all $\psi \in L_2$ such that $V\psi \in L_2$. Since $C_0^\infty(X)$ is a core for Δ, we can apply the Kato condition (8) to all $\psi \in \mathrm{Dom}(\Delta)$. Thus H is defined as a symmetric operator on $\mathrm{Dom}(\Delta)$. For Re $z < 0$ the operator $(z-\Delta)^{-1}$ is bounded. So for Re $z < 0$ we can write

$$zI - H = [I - V(zI-\Delta)^{-1}](zI-\Delta).$$

By the Kato condition (8) we have

$$\|V(zI-\Delta)^{-1}\| \leq \alpha + \beta|\mathrm{Re} z|^{-1}.$$

$$\|V(zI-\Delta)^{-1}\| \leq \alpha + \beta|\mathrm{Re} z|^{-1}.$$

If we choose $\alpha < 1$ and then Re z sufficiently negative, we can make the right hand side of this inequality < 1. For this range of z we see that $R(z, H) = (zI - H)^{-1}$ is bounded so the range of $zI - H$ is all of L_2. This proves that H is self-adjoint and that its resolvent set contains a half plane Re $z << 0$ and so is bounded from below. Also, for $\psi \in \mathrm{Dom}(\Delta)$ we have

$$\Delta\psi = H\psi - V\psi$$

so

$$\|\Delta\psi\| \leq \|H\psi\| + \|V\psi\| \leq \|H\psi\| + \alpha\|\Delta\psi\| + \beta\|\psi\|$$

which proves (9). □

Using the inequality (9).

$$\Delta \leq aH + b \tag{9}$$

Proposition 2 *Let H be a self-adjoint operator on $L_2(X)$ satisfying (9) for some constants a and b. Let $f \in L_\infty(X)$ be such that $f(x) \to 0$ as $x \to \infty$. Then for any z in the resolvent set of H the operator*

$$fR(z, H)$$

is compact, where, as usual, f denotes the operator of multiplication by f,

Proof. Let $p_j = \frac{1}{i}\frac{\partial}{\partial x_j}$ as usual, and let $g \in L_\infty(X^*)$ so the operator $g(p)$ is defined as the operator which send ψ into the function whose Fourier transform is $\xi \mapsto g(\xi)\hat{\psi}(\xi)$. The operator $f(x)g(p)$ is the norm limit of the operators $f_n g_n$ where f_n is obtained from f by setting $f_n = \mathbf{1}_{B_n} f$ where B_n is the ball of radius 1 about the origin, and similarly for g. The operator $f_n(x)g_n(p)$ is given by the square integrable kernel

$$K_n(x, y) = f_n(x)\hat{g}_n(x - y)$$

and so is compact. Hence $f(x)g(p)$ is compact. We will take

$$g(p) = \frac{1}{1 + p^2} = (1 + \Delta)^{-1}.$$

$$\Delta \leq aH + b \tag{9}$$

The operator $(1+\Delta)R(z,H)$ is bounded. Indeed, by (9)

$$\|(1+\Delta)(zI-H)^{-1}\psi\| \leq (1+a)\|H(zI-H)^{-1}\psi\|+b\|(R(z,H)\psi)\|$$
$$\leq \|(1+a)\psi\| + (a+b)\|R(z,H)\psi\|.$$

So

$$f(x)R(z,H) = f(x)\frac{1}{1+p^2} \cdot (1+\Delta)R(z,H)$$

is compact, being the product of a compact operator and a bounded operator.

Ruelle's theorem.

$$\Delta \leq aH + b \tag{9}$$

Let us take $H = \Delta + V$ where V is a Kato potential. Let F_r be the operator of multiplication by $\mathbf{1}_{B_r}$ so F_r is projection onto the space of functions supported in the ball B_r of radius r centered at the origin. Take $S = R(z, H)$, where z has sufficiently negative real part. Then $F_r S E_c$ is compact, being the product of the operator $F_r R(z, H)$ (which is compact by Proposition 2) and the bounded operator E_c. Also the image of S is all of $\mathcal{H}$. So we may apply the Amrein Georgescu theorem to conclude that $\mathcal{M}_0 = \mathcal{H}_p$ and $\mathcal{M}_\infty = \mathcal{H}_c$.

Facts used about compact operators.

Proposition 3 *The norm limit of a sequence of compact operators is compact.*

Suppose that $\|T_n - T\| \to 0$ with T_n compact. Let f_n be a sequence of elements with $\|f_j\|$. By Cantor diagonalization we can pass to a subsequence (which we will rename as f_j such that $T_n f_j$ is Cauchy for all n. Then $\|Tf_j - Tf_k\| \le 2\|T - T_n\| + \|T_n(f_j - f_k)\|$ so Tf_j is Cauchy and so converges to some limit g.

Proposition 4 *Every compact operator on a separable Hilbert space is the norm limit of a sequence of operators of finite rank.*

Let $\{\phi_j\}$ b an orthonormal basis. Let

$$a_n := \sup_{\psi \perp \{\phi_1,\ldots,\phi_n \|\psi\|=1} \|T\psi\|.$$

The a_n are monotone decreasing and so tend to a limit ≥ 0. This limit must be zero. Indeed, choose ψ_n with $\psi \perp \{\phi_1, \ldots, \phi_n \ \|\psi\| = 1$ and $\|T\psi_n\| \geq \frac{1}{2}a_n$. The ψ_n converge weakly to 0, hence the $T\psi_n$ converge weakly to 0. This implies that the $T\psi_n$ converge strongly to 0. For if not, we can choose a subsequence which converges to some $\psi \neq 0$ which is impossible. so $a_n \to 0$.

But a_n is the norm of $\sum_{j=1}^n (\cdot, \phi_j) T\phi_j - T$. $\square$