

Spectral Theory

Percy Deift

Transcribed by Ron Wu

This is a graduate course, offered in fall 2013 at New York University. Course textbooks are four volumes of *Methods of Modern Mathematical Physics* by Reed and Simon. Suggested exercises would be given but there would be no midterm or final. Textbooks used in functional analysis I, last semester, may be good for review. They are *Principles of Functional Analysis* by Martin Schechter, and *Functional Analysis* by Peter Lax.

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1 Introduction

1.1 Course Outline

Lecture 1
(9/6/13)

(1) Strun-Liouville Theory; Weyl limit point theory and limit circle theory; Schrodinger operators with potentials that decay at infinity; periodic Schrodinger operators; some inverse theory.

(2) Spectral theory of a particle in n -dimension; scattering theory.

(3) Stability of matter for system of electrons.

[We ended up only half way finished (1).]

This is the second semester of full year functional analysis course. In the first semester, we described some very general methods, techniques, results for self-adjoint operators in a Hilbert space. The goal of this semester is to illustrate the general theory with concrete examples.

1.2 Review From Last Semester

We consider *densely defined* linear operators in a *separable* Hilbert space \mathcal{H} with inner product (\cdot, \cdot) .

Example 1. Hilbert spaces $\mathcal{H} = L^2(\mathbb{R}^n)$, $\mathcal{H} = \mathbb{C}^n$, $\mathcal{H} = L^2(a, b)$, $\mathcal{H} = l^2(\mathbb{Z})$.

Definition 2. A (densely defined) linear operator A with domain $D(A) \subset \mathcal{H}$ is *closed* if

$$\begin{cases} x_n \rightarrow x \\ Ax_n \rightarrow y \end{cases}$$

$x_n \in D(A)$ implies

$$x \in D(A), y = Ax.$$

Definition 3. An operator A with $D(A) = \mathcal{H}$ is *continuous* if

$$x_n \rightarrow x \implies Ax_n \rightarrow Ax.$$

Proposition 4. A is continuous iff A is bounded i.e.

$$\|A\| \equiv \sup_{\substack{x \neq 0 \\ x \in H}} \frac{\|Ax\|}{\|x\|} < \infty.$$

Proposition 5. *A is continuous $\implies A$ is closed (by the closed graph theorem)*

Proposition 6. *Conversely A closed operator A with $D(A) = \mathcal{H}$ is bounded (or equivalently continuous).*

Note 7. Here $D(A) = \mathcal{H}$ is very important!

Definition 8. A is *symmetric* if

$$(Ax, y) = (x, Ay) \quad \forall x, y \in D(A).$$

Definition 9. The adjoint A^* of an operator A is defined as follows: $y \in D(A^*)$ iff $\exists f \in \mathcal{H}$ s.t.

$$(y, Ax) = (f, x)$$

$\forall x \in D(A)$. In that case, then

$$A^*y \equiv f.$$

Definition 10. B is an *extension* of A , written $A \subset B$, if $D(A) \subset D(B)$ and $Ax = Bx$, $x \in D(A)$.

Proposition 11. *If A is symmetric, then A^* extends A , i.e. $A \subset A^*$.*

Definition 12. We say A is *self-adjoint* if $A = A^*$.

Proposition 13. *If A is bounded and symmetric, then it is self-adjoint.*

In particular a bounded symmetric matrix is s.adj.

But if A is un-bounded and symmetric, it may not be s.adj,

Example 14. Let

$$Af = if'$$

with domain $D(A) = \{f \in L^2(0, \infty) : f \text{ absolutely continuous, } f' \in L^2(0, \infty), f(0) = 0\}$. Then A is a closed, symmetric operator in $L^2(0, \infty)$, but it is not s.adj.

Absolutely continuous is required for integration by parts to work.

Definition 15. A symmetric operator A is *closable* i.e. it has a smallest closed extension, denoted \bar{A} . i.e. $A \subset \bar{A}$ if $B \supset A$, B closed, then $B \supset \bar{A}$.

Definition 16. A symmetric operator A is *essentially self-adjoint* (e.s.a) if its closure \bar{A} is self-adjoint.

Example 17. If $Af = -f''$, $D(A) = C_0^\infty(\mathbb{R})$, then A is symmetric, and $\bar{A}f = -f''$, $D(\bar{A}) = \{f \in L^2(\mathbb{R}), f, f' \text{ abs cont}, f'' \in L^2(\mathbb{R})\}$ and \bar{A} is s.adj.

The self-adjoint operators (or more general the essentially s.adj) operators are *distinguished* amongst the symmetric operators by the fact that they have a unitary *spectral resolution*, which is stated in the following theorem.

Theorem 18. (*Spectral Theorem*) If A is a s.adj operator in a separable Hilbert space \mathcal{H} then \exists Borel measures $\{\mu_k\}_{k=1}^N$, called the spectral measures, $N \leq \infty$, on \mathbb{R} and a unitary map

$$U : \mathcal{H} \rightarrow \bigoplus_{n=1}^N L^2(\mathbb{R}, d\mu_n)$$

such that

$$\psi \mapsto \phi = (\phi(x, 1), \dots, \phi(x, n), \dots) = U\psi$$

$$\|\psi\|_{\mathcal{H}}^2 = \sum_{n=1}^N \int_{\mathbb{R}} |\phi(x, n)|^2 d\mu_n(x)$$

which turns A into multiplication by x in each space $L^2(\mathbb{R}, d\mu_n)$, i.e.

$$(UA\psi)(x, n) = x(U\psi)(x, n) = x\phi(x, n), \quad n \geq 1$$

and

$$\psi \in D(A) \iff \sum_{n=1}^N \int_{\mathbb{R}} |U\psi(x, n)|^2 x^2 d\mu_n(x) < \infty$$

More if $F(x)$ is a bounded Borel function, then

$$(UF(A)\psi)(x, n) = F(x)(U\psi)(x, n), \quad m \geq 1.$$

Example 19. If $F(x) = e^{itx}$, $t \in \mathbb{R}$, then $(Ue^{itA}\psi)(x, n) = e^{itx}(U\psi)(x, n)$, so that

$$\begin{aligned} \|e^{itA}\psi\|_{\mathcal{H}}^2 &= \|Ue^{itA}\psi\|_{\bigoplus_n L^2(d\mu_n)}^2 = \sum_{n=1}^N \int_{\mathbb{R}} |e^{itx}|^2 |U\psi(x, n)|^2 d\mu_n(x) \\ &= \sum_{n=1}^N \int_{\mathbb{R}} |U\psi(x, n)|^2 d\mu_n(x) = \|\psi\|_{\mathcal{H}}^2 \end{aligned}$$

Hence e^{itA} is an isometry and in fact a unitary map. In this way we see that if A is s.adj, then it generates a *unitary group* $\{e^{itA}\}_{t \in \mathbb{R}}$. Clearly if $\psi \in D(A)$, then $\psi_t = e^{-itA}\psi$ is a solution of

$$\begin{aligned} i \frac{d}{dt} \psi_t &= A\psi_t \\ \psi_{t=0} &= \psi \end{aligned}$$

In particular if A is a Schrodinger operator in \mathbb{R}^n

$$A = -\Delta + V(x)$$

for some potential $V(x)$, V real, which is s.adj on some domain $D(A) \subset \mathcal{H}$, then $\psi_t = e^{-itA}\psi$ solves the Schrodinger equation in $L^2(\mathbb{R}^n)$

$$\begin{aligned} i \frac{d}{dt} \psi_t &= -\Delta \psi_t + V \psi_t \\ \psi_{t=0} &= \psi \end{aligned}$$

and preserves *probabilities* i.e. $\|\psi_t\| = \|\psi\|$.

If A is only symmetric, and not e.s.a, then the above construction fails. (Converse statement is not true, see **Stone's Theorem**).

So the issue of s.adjointness is really just the question of obtaining estimates to ensure a “good” solution for an associated differential equation.

Definition 20. A point $\lambda \in \text{spectrum of } A$, $\sigma(A)$, if $A - \lambda$ is *not* a bijection from $D(A)$ onto \mathcal{H} .

Example 21. λ is an eigenvalue of A if $\exists \psi \neq 0$ in $D(A)$ s.t. $(A - \lambda)\psi = 0$. Clearly $\lambda \in \sigma(A)$ and we say $\lambda \in \text{point spectrum of } A$.

Definition 22. The *resolvent* of A , $\rho(A)$, is the complement of $\sigma(A)$.

Proposition 23. If A is a closed operator and $\lambda \in \rho$, then $(A - \lambda)^{-1}$, the resolvent of A , is a bounded operator from \mathcal{H} onto $D(A)$. Moreover $\sigma(A)$ is a closed set in \mathbb{C} , and $\rho(A)$ is open.

Exercise 24. Prove the above proposition by Closed Graph Theorem.

1.3 What does Spectral Analysis do?

Spectral Analysis consists of 2 principal parts:

1. determine $\sigma(A)$. **Theorem.** If A is s.adj, $\sigma(A) \subset \mathbb{R}$.

2. determine the nature of the measures. Any measure $d\mu$ on \mathbb{R} can be decomposed as a sum of 3 measures with disjoint support,

$$d\mu \equiv d\mu_{s.cont} \oplus d\mu_{pp} \oplus d\mu_{ac}$$

where $d\mu_{ac}$ is abs. cont w.r.t. Lebesgue measure, $d\mu_{pp}$ is a countable sum of delta function/measures, $d\mu_{s.cont}$ is a singular continuous measure (like the Cantor measure!)

Given A with spectrum measure $\{d\mu_n\}_{n=1}^N$, the task is to determine the singular continuous, pure points and abs. continuous parts of each $d\mu_n$. These parts determine the behavior of the solution $e^{itA}\psi$ of the associated equation

$$\begin{aligned} i \frac{d}{dt} \psi_t &= A \psi_t \\ \psi_{t=0} &= \psi \end{aligned}$$

Example 25. Let $\bar{A}f = -f''$, $D(\bar{A}) = \{f \in L^2 : f, f' \text{ abs cont}, f'' \in L^2\}$. As noted in example 17 \bar{A} is s.adj. Now the Fourier transform

$$\mathcal{F}f(s) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-isx} f(x) dx$$

is a *unitary map* from $L^2(dx) \rightarrow L^2(ds)$.

$$\int |\mathcal{F}f(s)|^2 ds = \int |f(x)|^2 dx$$

with inverse map

$$\mathcal{F}^{-1}g(x) = \frac{1}{\sqrt{2\pi}} \int e^{ixs} g(s) ds$$

which is also unitary. \mathcal{F} turns \bar{A} into multiplication by s^2 . i.e.

Exercise 26. Show if $f \in D(\bar{A})$, then

$$\mathcal{F}\bar{A}f(s) = s^2(\mathcal{F}f)(s)$$

Example 27. Let $d\mu_1(y) = d\mu_2(y) = \frac{dy}{2\sqrt{y}}$ on \mathbb{R}_+ and consider the map $U : L^2(\mathbb{R}) \rightarrow L^2(\mathbb{R}_+, d\mu_1) \oplus L^2(\mathbb{R}_+, d\mu_2)$ which takes

$$f \mapsto (\phi(y, 1), \phi(y, 2)) = ((\mathcal{F}f)(\sqrt{y}), (\mathcal{F}f)(-\sqrt{y}))$$

hence

$$\begin{aligned}
\int_0^\infty |\phi(y, 1)|^2 d\mu_1(y) &+ \int_0^\infty |\phi(y, 2)|^2 d\mu_2(y) \\
&= \int_0^\infty |\mathcal{F}f(\sqrt{y})|^2 \frac{dy}{2\sqrt{y}} + \int_0^\infty |\mathcal{F}f(-\sqrt{y})|^2 \frac{dy}{2\sqrt{y}} \\
&= \int_0^\infty |\mathcal{F}f(s)|^2 ds + \int_0^\infty |\mathcal{F}f(-s)|^2 ds \quad (s \equiv \sqrt{y}) \\
&= \int_{-\infty}^\infty |\mathcal{F}f(s)|^2 ds = \|f\|_{L^2(\mathbb{R})}^2
\end{aligned}$$

So U is unitary. Also for $f \in D(\bar{A})$

$$\begin{aligned}
L^2(\mathbb{R}) \ni \bar{A}f = -f'' &\mapsto ((\mathcal{F}\bar{A}f)(\sqrt{y}), (\mathcal{F}\bar{A}f)(-\sqrt{y})) \\
&= ((\sqrt{y})^2(\mathcal{F}f)(\sqrt{y}), (-\sqrt{y})^2(\mathcal{F}f)(-\sqrt{y})) \\
&= (y\phi(y, 1), y\phi(y, 2))
\end{aligned}$$

So U is the spectral map for \bar{A} , i.e. it turns A into multiplication by y in $L^2(\mathbb{R}_+, d\mu_1) \oplus L^2(\mathbb{R}_+, d\mu_2)$. Here $N = 2$ so \bar{A} has uniform multiplicity 2.

1.4 Criteria for Extension

Question 28. *Given a symmetric operator A , does it have self-adjoint extensions, and if so, how many?*

Let's first examine Example 14. The operator $Af = if'$ acting in $L^2(\mathbb{R}_+)$ with $D(A) = \{f \in L^2(\mathbb{R}_+) : f \text{ abs cont, } f' \in L^2, f(0) = 0\}$ is a closed, symmetric operator, but it has *no* s.adj. extension.

This is easy to understand physically, for if A had such an extension, \tilde{A} say, then we could solve the equation

$$i \frac{d}{dt} \psi_t = \tilde{A} \psi_t, \quad \psi_{t=0} = \psi$$

with $\|\psi_t\| = \|\psi\|$. We would have $\psi_t = e^{-it\tilde{A}}\psi$ and so if $\psi \in C_0^\infty[0, \infty) \subset D(A) \subset D(\tilde{A})$ we would see that

$$i \frac{d}{dt} \psi_t = i \frac{\partial}{\partial x} \psi_t$$

hence $\psi_t(x) = \psi(x + t)$, so ψ_t is just transporting $\psi(x)$ to the left. Since $\psi(x)$ is compact supported smooth function, and $\psi(0) = 0$. For

$t \gg 1$, ψ_t disappear through the “wall” and $\psi_t(x) = 0$ in $L^2(\mathbb{R}_+)$. So $\|\psi_t\| \neq \|\psi\| \forall t$.

If A is a *closed* symmetric operator, its symmetric extensions are described in the following way: for any λ let $N_\lambda(A) = \{u \in D(A^*) : (A^* - \lambda)u = 0\}$, set

$$n_+ = \dim N_\lambda(A), \operatorname{Im} \lambda > 0$$

$$n_- = \dim N_\lambda(A), \operatorname{Im} \lambda < 0$$

notice n_+, n_- are constant in \mathbb{C}_+ and \mathbb{C}_- respectively. The symmetric extensions of A are parametrized by the *partial isometrics* of $N_i(A)$ into $N_{-i}(A)$.

Theorem 29. *A has s.adj extension iff $n_+ = n_-$. And if $n_+ = n_-$, then the s.adj extensions of A are parametrized by the unitary maps from $N_i(A)$ onto $N_{-i}(A)$.*

Proposition 30. *A s.adj operator is maximally symmetric i.e. if S is s.adj and T is symmetric, $T \subset T^*$, then $S \subset T \implies S = T$.*

Proof. If $S \subset T$ and by adjointness, $T^* \subset S^*$ then $T \subset T^* \subset S^* = S$ i.e. $T \subset S$ so $T = S$. \square

In terms of Theorem 29, this means that

Proposition 31. *A is closed, s.adj $\iff n_+ = n_- = 0$.*

Example 32. Let's first reexamine Example 14. We showed that $Af = if'$ acting in $\{f \in L^2(0, \infty) : f \text{ abs cont, } f' \in L^2, f(0) = 0\}$ has no self adj extension. $D(A^*) = \{f \in L^2(0, \infty) : f \text{ abs cont, } f' \in L^2\}$.

$$(A^* - i)f = 0 \implies i(f' - f) = 0 \implies f = ce^x \notin L^2(0, \infty)$$

$$(A^* + i)f = 0 \implies i(f' + f) = 0 \implies f = ce^{-x} \in L^2(0, \infty)$$

So $n_+ = 0 \neq n_- = 1$.

Let $A = i\frac{d}{dx}$ acting in $L^2(0, 1)$ with domain $D(A) = \{f \in L^2 : f \text{ abs cont, } f' \in L^2, f(0) = f(1) = 0\}$. Then A is a closed symmetric operator. One can show that $A^*f = i\frac{d}{dx}f$ with domain $D(A^*) = \{f \in L^2(0, 1) : f \text{ abs cont, } f' \in L^2\}$. Then

$$f \in \operatorname{Null}(A^* - i) \iff if' - if = 0 \implies f = ce^x$$

$$f \in \text{Null}(A^* + i) \iff if' + if = 0 \implies f = ce^{-x}$$

then $n_+ = n_- = 1$, and the s.adj extensions of A must be all unitary maps U from a 1 dimension space onto a 1 dimensional space. Such maps are just multiplications by a scalar of modulus 1 i.e. $c = e^{i\alpha}$. So the s. adj extensions of A are parametrized by a circle. What are these extension look like? They have the form $A_\alpha f = if'$, $D(A_\alpha) = \{f \in L^2(0, 1) : f \text{ abs cont, } f' \in L^2, f(1) = e^{i\alpha}f(0)\}$ and the circle parametrization is clear.

1.5 Quadratic Form Representation of an Operator

Definition 33. A quadratic form $q(\cdot, \cdot)$ is a map of

$$Q(q) \times Q(q) \rightarrow \mathbb{C}$$

where $Q(q)$ is a dense linear subspace of \mathcal{H} called the form domain, such that $q(\cdot, \psi)$ is linear and $q(\phi, \cdot)$ is conjugate linear (anti-linear) $\forall \phi, \psi \in Q(q)$.

Definition 34. If $q(\phi, \psi) = \overline{q(\psi, \phi)}$, we say q is *symmetric*.

Definition 35. If $q(\psi, \psi) \geq 0 \forall \psi \in Q$, q is called *positive*.

Definition 36. If $q(\psi, \psi) \geq -M \|\psi\|^2 \forall \psi \in Q$, for some $-\infty < M < \infty$, we say that q is *semibounded*.

Proposition 37. If q is positive, then it is symmetric.

Example 38. (1) $q(f, g) = \int_0^1 \bar{f}'g' + \int_0^1 \bar{f}g$. $Q(q) = C^1[0, 1]$; (2) $q(f, g) = \bar{f}(0)g(0)$. $Q(q) = C_0^\infty(\mathbb{R}) \subset L^2(\mathbb{R})$. (1), (2) are both semi-bounded quadratic forms.

Definition 39. If A is a s.adj operator in \mathcal{H} with *diagonalizing unitary* map

$$U : \mathcal{H} \rightarrow \bigoplus_{n=1}^N L^2(\mathbb{R}, d\mu_n),$$

let

$$Q(q) = \left\{ \psi : \sum_{n=1}^N \int_{-\infty}^{\infty} x^2 \underbrace{|\phi(x, n)|^2}_{U\psi} d\mu_n(x) < \infty \right\}$$

and for $\psi, \varphi \in Q(q)$, define the symmetric quadratic form

$$q(\psi, \varphi) = \sum_{n=1}^N \int_{-\infty}^{\infty} \underbrace{x \overline{\phi(x, n)}}_{U\psi} \underbrace{\tilde{\phi}(x, n)}_{U\varphi} d\mu_n(x)$$

we call q the *quadratic form* associated with A and write

$$Q(q) = Q(A)$$

$Q(A)$ is called the *form domain* of the operator A .

Definition 40. Let q be a semibounded quadratic form, $q(\psi, \psi) \geq -M \|\psi\|^2$, we say that q is *closed* if $Q(q)$ is complete in the norm

$$\|\psi\|_{+1} = \sqrt{q(\psi, \psi) + (M + 1) \|\psi\|^2}.$$

The important result is the following:

Theorem 41. If q is a closed semi-bounded quadratic form, then q is the quadratic form of a unique s.adj. operator A . And the domain $D(A)$ is determined in the following way

$$D(A) = \{\psi \in Q(q) : q(\phi, \psi) = (\phi, \chi_\psi)\}$$

for some unique $\chi_\psi \in \mathcal{H}$ and $\forall \phi \in Q(q)$. And if $\psi \in D(A)$, $A\psi = \chi_\psi$.

Idea of proof:

$$(\phi, A\psi) = (U\phi, UA\psi) = x(U\phi, U\psi) = x(\phi, \psi) = q(\phi, \psi)$$

Exercise 42. Let $q(f, g) = \overline{f(0)}g(0)$, $Q(q) = C_0^\infty(\mathbb{R}) \subset L^2(\mathbb{R})$, then q is a densely defined positive quadratic form. Show it has no closed extensions.

On the other hand

Theorem 43. If A is a densely defined positive operator in \mathcal{H} , i.e.

$$(\psi, A\psi) \geq 0, \forall \psi \in D(A) \subset \mathcal{H}$$

then the quadratic form

$$q(\phi, \psi) \leq (\phi, A\psi), \psi, \phi \in D(A)$$

always has a closure \hat{q} , i.e. a smallest, closed extension of q . \hat{q} is positive and hence \exists a unique associated s.adj operator \hat{A} with $D(\hat{A}) \subset Q(\hat{q}) = Q(\hat{A})$ s.t. $q(\phi, \psi) = (\phi, \hat{A}\psi) \forall \psi \in D(\hat{A})$ and $\forall \phi \in Q(\hat{q})$.

\hat{A} is an extension of A and is called the *Friedrichs extension* of A .

Example 44. Let $A = -\frac{d^2}{dx^2}$ with $D(A) = \{f \in C_0^\infty(0,1)\}$. Then the Friedrichs extension \hat{A} of A is $-\frac{d^2}{dx^2}$ in $D(\hat{A}) = \{f \in L^2, f, f' \text{ abs cont}, f'' \in L^2(0,1), f(0) = f(1) = 0\}$.

Example 45. Let $q(\phi = Uf, \psi = Ug) = \int_0^1 \bar{f}'g'dx$ is a closed, semi-bounded quadratic form with form domain $Q(q) = \{f \in L^2(0,1) : f \text{ abs cont}, f' \in L^2(0,1)\}$. Then the operator A associated with q is the *Neumann operator* $Af = -f''$ with

$$D(A) = \{f \in L^2(0,1) : f, f' \text{ abs cont}, f'' \in L^2(0,1), f'(0) = f'(1) = 0\}$$

Proposition 46. *If a symmetric operator A commutes with its complex conjugation, then it has s.adj extension.*

This is because conjugation sets up a bijection from $N_i(A) \rightarrow N_{-i}(A) \implies n_+(A) = n_-(A)$.

This is the case, in particular, for Schrodinger operators

$$H = -\Delta + V(x)$$

with real potentials $V(x)$. Thus such operators always have s.adj extensions.

Note 47. Recall $A = i\frac{d}{dx}$, $D(A) = C_0^\infty(0,\infty)$ has no s.adj extension.

1.6 Min-Max Theorem

The min-max theorem is very important in many different kinds of spectral situations.

Definition 48. The *discrete spectrum*, $\sigma_{disc}(A)$, of A are isolated points in $\sigma(A)$ corresponding to eigenvalues of finite multiplicity. The essential spectrum $\sigma_{ess}(A)$ is its complement. $\sigma_{ess}(A) = \sigma(A) \setminus \sigma_{disc}(A)$.

Definition 49. Multiplicity of λ , $\lambda \in \sigma(A)$, is $\dim \text{Null}(A - \lambda)$.

Theorem 50. *Let q be a closed, semi-bounded quadratic form and let A be the associated s.adj operator. Define*

$$\mu_n = \sup_{\psi_1, \dots, \psi_{n-1}} \inf_{\substack{\psi \perp \langle \psi_1, \dots, \psi_{n-1} \rangle \\ \psi \in Q(A), \|\psi\| = 1}} q(\psi, \psi)$$

where $\langle \psi_1, \dots, \psi_{n-1} \rangle$ denotes the span of $\psi_1, \dots, \psi_{n-1}$. Then for each n , either

(a) There are at least n eigenvalues (counting degenerate eigenvalues a number of times equal to their multiplicity) below the bottom of the essential spectrum of A and $\mu_n(A)$ is the n th eigenvalue counting multiplicity

or

(b) μ_n is the bottom of the essential spectrum i.e. $\mu_n = \inf\{\lambda : \lambda \in \sigma_{\text{ess}}(A)\}$ and in that case $\mu_n = \mu_{n+1} = \mu_{n+2} = \dots$ and there are at most $n - 1$ eigenvalues (counting multiplicity) below μ_n .

As we will see that the great utility of the min-max theorem is that it only involves the form domains of the operators, not the operator domains. In practice, as we will see, operators may have very different operator domains, but their form domains are related. This allows us to use known results for one operator, in analyzing other operators.

Note 51. A compact self adjoint operator A has pure point spectrum $\{\lambda_i\}$, accumulating only at 0. The non-zero eigenvalues have finite multiplicity, i.e. $\dim(\text{Null}(A - \lambda_i)) < \infty$, if $0 \neq \lambda_i \in \sigma(A)$. and the eigenvectors $\{\psi_j\}$ associated with the λ_i 's form a complete orthonormal sequence for \mathcal{H} . Thus $\sigma(A) = \sigma_{pp}(A)$.

Definition 52. If A and B are bounded self adj operators in \mathcal{H} . We write $A \leq B$ if

$$(\psi, A\psi) \leq (\psi, B\psi), \forall \psi \in \mathcal{H}$$

We want to extend the definition of $A \leq B$ to unbounded operators.

Definition 53. Let A and B be s.a. positive operators where A is defined on a dense subspace of \mathcal{H} and B is defined on a dense Hilbert subspace $\tilde{\mathcal{H}}$ of \mathcal{H} . We write $0 \leq A \leq B$ iff

(i) $Q(B) \subset Q(A)$; (ii) For any $\psi \in Q(B) \subset Q(A)$, $0 \leq (\psi, A\psi) \leq (\psi, B\psi)$.

Example 54. $q_N = \int_0^1 |f'|^2$, $Q(q_N) = \{f \text{ abs cont on } (0, 1), f' \in L^2(0, 1)\}$; $q_D = \int_0^1 |f'|^2$, $Q(q_D) = \{f \text{ abs cont on } (0, 1), f' \in L^2, f(0) = f(1) = 0\}$. Then $0 \leq -(d^2/dx^2)_N \leq -(d^2/dx^2)_D$.

Example 55. Let Ω be a bounded region in \mathbb{R}^n . Let $-\Delta_\Omega$ be the Friedrichs extension of $-\Delta$ acting on $C_0^\infty(\Omega) \subset L^2(\Omega)$. $-\Delta_\Omega$ is the

Dirichlet operator for Ω . Let S_L be any square box $S_L = \{|x_i| < L : i = 1, \dots, n\}$ containing Ω . Let $-\Delta_{S_L}$ be the Friedrichs extension of $-\Delta$ acting on $C_0^\infty(S_L) \subset L^2(S_L)$. As $C_0^\infty(\Omega) \subset C_0^\infty(S_L)$, it follows that

$$0 \leq -\Delta_{S_L} \leq -\Delta_\Omega \quad (1.1)$$

It then follows from (1.1) that

$$\mu_n(-\Delta_{S_L}) \leq \mu_n(-\Delta_\Omega) \quad (1.2)$$

$m = 1, 2, \dots$ where $\mu_n(-\Delta_{S_L})$, $\mu_n(-\Delta_\Omega)$ are defined in Min-Max theorem.

Now for any n -tuple $k = (k_1, \dots, k_n)$ with $k_i \in \mathbb{N}^{\geq 1}$, $i = 1, \dots, n$.

Exercise 56. Show the functions

$$\Phi_{k;L}(x) = L^{-n/2} \prod_{i=1}^n \psi_{k_i} \left(\frac{x_i}{L} \right)$$

with

$$\begin{aligned} \psi_j(x) &= \cos \frac{j\pi x}{2}, \quad j = 1, 3, 5, \dots \\ \psi_j(x) &= \sin \frac{j\pi x}{2}, \quad j = 2, 4, 6, \dots \end{aligned}$$

are eigenvectors (i.e. $\Phi_{k;L} \in D(-\Delta_{S_L})$) for $-\Delta_{S_L}$ with eigenvalues

$$E_k(L) = \left(\frac{\pi}{2L} \right)^2 \sum_{i=1}^n k_i^2$$

Example. (continued) Moreover, by Fourier analysis, the $\Phi_{k;L}$'s are a complete orthonormal set for $L^2(S_L)$. Hence

$$\sigma(-\Delta_{S_L}) = \{E_k(L) : k = (k_1, \dots, k_n), k_i \geq 1\}$$

Now it follows that $\mu_n(-\Delta_{S_L}) \rightarrow \infty$, as $n \rightarrow \infty$. (clearly, the $\mu_n(-\Delta_{S_L})$'s are non-decreasing with n). Because if $\mu_n(-\Delta_{S_L}) \nrightarrow \infty$, then by part (b) of Min-Max, the $\sigma_{ess}(-\Delta_{S_L}) \neq \emptyset$. But then $\mu_n(-\Delta_\Omega) \rightarrow \infty$ by (1.2). But then again by part (b) of Min-Max, $-\Delta_\Omega$ must have purely discrete spectrum!

In other words, $-\Delta_\Omega$ must have a complete orthonormal set of eigenvectors $\{\phi_m^\Omega\}$ with eigenvalue $E_m^\Omega \rightarrow \infty$, $-\Delta_\Omega \phi_m^\Omega = E_m^\Omega \phi_m^\Omega$.

Definition 57. Let A, B be densely defined operators in a Hilbert space \mathcal{H} . Suppose that

- (i) $D(A) \subset D(B)$; (ii) for some a and b in \mathbb{R} and $\forall \psi \in D(A)$

$$\|B\psi\| \leq a \|A\psi\| + b \|\psi\|$$

then B is A -bounded. The infimum of such a is called the relative bound of B w.r.t A .

Theorem 58. (*Kato-Rellich Theorem*) Suppose that A is s. adj, B is symmetric and B is A -bounded with relative bound $a < 1$. Then $A + B$ is s. adj on $D(A)$.

Example 59. Let $A = -d^2/dx^2$ with $D(A) = \{f \in L^2(\mathbb{R}) : f, f' \text{ abs cont, } f'' \in L^2(\mathbb{R})\}$. let $Bf(x) = V(x)f(x)$ where $V(x)$ is real valued and $V \in L^2(\mathbb{R})$. Claim B is A -bounded with relative bound < 1 . Indeed, for all $f \in D(A)$, we have the *classical inequality* on \mathbb{R} , for any $\epsilon > 0$,

$$\begin{aligned} |f(x)|^2 &\leq \frac{1}{\epsilon} \|f\|_{L^2}^2 + \epsilon \|f'\|_{L^2}^2 \\ \|Bf\|_{L^2}^2 &\leq \|B\|_{L^2}^2 \left(\frac{1}{\epsilon} \|f\|_{L^2}^2 + \epsilon \|f'\|_{L^2}^2 \right) \\ &\leq \|B\|_{L^2}^2 \left(\frac{1}{\sqrt{\epsilon}} \|f\|_{L^2} + \sqrt{\epsilon} \|f'\|_{L^2} \right)^2 \end{aligned}$$

So

$$\|Bf\|_{L^2} \leq \frac{1}{\sqrt{\epsilon}} \|B\|_{L^2} \|f\|_{L^2} + \|B\|_{L^2} \sqrt{\epsilon} \|f'\|_{L^2}$$

Now choose $\epsilon < 1/\|B\|_{L^2}^2$. So

$$\|Bf\|_{L^2} \leq \|f'\|_{L^2} + \frac{1}{\sqrt{\epsilon}} \|B\|_{L^2} \|f\|_{L^2} \quad (1.3)$$

Again by a classical inequality

$$\|f'\| \leq \frac{1}{2} \|f\| + \frac{1}{2} \|f''\|$$

it follows that $H = -\frac{d^2}{dx^2} + V(x)$ is s.adj on $D(A) = D(-\frac{d^2}{dx^2})$.

We also have by (1.3),

$$\begin{aligned} |(f, Bf)| &\leq \|f\| \|Bf\| \\ &\leq \|f\|^2 \|B\|_{L^2} \frac{1}{\sqrt{\epsilon}} + \|f\| \|f'\| \|B\|_{L^2} \sqrt{\epsilon} \\ &\leq \frac{1}{\epsilon} \|f\|^2 + \|f\| \|f'\| \\ &\leq \left(1 + \frac{1}{\epsilon}\right) \|f\|^2 + \frac{1}{2} \|f'\|^2 \end{aligned}$$

Let $b = 1 + \frac{1}{\epsilon}$. Hence for $f \in D(A)$

$$\begin{aligned}(f, A + Bf) &= \|f'\|^2 + (f, Bf) \\ &\geq \|f'\|^2 - \frac{1}{2}\|f'\|^2 - b\|f\|^2 \\ &= \frac{1}{2}\|f'\|^2 - b\|f\|^2\end{aligned}$$

i.e.

$$(f, A + Bf) \geq \frac{1}{2}(f, Af) - b\|f\|^2$$

$\forall f \in D(A)$ and in fact for all $f \in Q(A) = \{f \in L^2 : f \text{ abs cont, } f' \in L^2\}$.

The same inequality is true for $H = -\frac{d^2}{dx^2} + V(x)$ in $L^2(0, 1)$ where $D(H) = D(-\frac{d^2}{dx^2}) = \{f \in L^2(0, 1) : f, f' \text{ a.cont. } f'' \in L^2, f(0) = f(1) = 0\}$, but as we showed $-\frac{d^2}{dx^2}$ with such Dirichlet boundary condition at $x = 0$ and $x = 1$ has pure point spectrum $E_k^{(0,1)} \rightarrow \infty$. But then we conclude from min-max theorem, that $-\frac{d^2}{dx^2} + V(x)$ also has pure point spectrum with eigenvalue $E_k^V \geq \frac{1}{2}E_k^{(0,1)} - b \rightarrow \infty$, if V is real valued and $V \in L^2(0, 1)$.

Exercise 60. Show that the Hamiltonian for the Hydrogen atom

$$H = -\Delta - \frac{e^2}{|x|}$$

is s.adj on $D(-\Delta) = \{f \in L^2(\mathbb{R}^3) : |\vec{k}|^2 \hat{f}(\vec{k}) \in L^2(\mathbb{R}^3)\}$.

2 One Dimension Schrodinger Operator

We are now ready to consider 1-dim Schrodinger operator

$$H = -\frac{d^2}{dx^2} + V(x)$$

in more detail. We will *always* assume that $V(x)$ is real valued and $L_{loc}^2(I)$ on any interval under consideration. $I = (0, 1)$, $(0, \infty)$ or $(-\infty, \infty)$. (Much of the theory goes through for $V \in L_{loc}^1$, but there are certain technicalities which we can avoid by assuming $V \in L_{loc}^2$)

2.1 On finite interval

On a finite interval, say $[0, b]$, the following s.adj realizations of $H = -\frac{d^2}{dx^2} + V(x)$ are of interest:

Let $D = \{f \in L^2(0, b) : f, f' \text{ abs cont, } f'' \in L^2(0, b)\}$

Dirichlet

$$H_D = H$$

$$D_D = D \cap \{f(0) = f(b) = 0\}$$

Neumann

$$H_N = H$$

$$D_N = D \cap \{f'(0) = f'(b) = 0\}$$

Floquet α ($0 \leq \alpha < 2\pi$)

$$H_\alpha = H$$

$$D_\alpha = D \cap \{f(b) = f(0)e^{i\alpha}, f'(b) = f'(0)e^{i\alpha}\}$$

If $\alpha = 0$, $H_\alpha = H_{\text{periodic}}$. If $\alpha = \pi$, $H_\alpha = H_{\text{antiperiodic}}$.

Dirichlet-Neumann

$$H_{DN} = H$$

$$D_{DN} = D \cap \{f(0) = 0, f'(b) = 0\}$$

Neumann-Dirichlet

$$H_{ND} = H$$

$$D_{ND} = D \cap \{f'(0) = 0, f(b) = 0\}$$

Robin

$$H_{\alpha\beta} = H$$

$$D_{\alpha\beta} = D \cap \{f'(0) = \alpha f(0), f'(b) = \beta f(b)\}$$

Each of these operators is indeed s.adj on its domain. One can either check this directly or use the Kato-Rellich Theorem. In each case the operator $H = -d^2/dx^2$ is s.adj on its domain by a simple calculation and the result follows as above from the classical inequality on $(0, b)$.

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$$|f(x)|^2 \leq d \|f\|^2 + c \|f''\|^2, \quad d > 0, 0 < c < 1$$

for any $f \in D$.

The proof of Robin on $(0, b)$ is more complicated than the proof above on \mathbb{R} , where we can use the Fourier transform to make the estimates very simple.

One way to prove Robin is the following. For $x, y \in (0, b)$,

$$\begin{aligned} |f(x)|^2 &= |f(y)|^2 + \int_y^x (\bar{f}f' + \bar{f}'f) \\ &\leq |f(y)|^2 + 2\|f\|_{L^2(0,b)}\|f'\|_{L^2(0,b)} \end{aligned}$$

here x, y are independent, so we can choose y that gives $\inf_y |f(y)|^2$ then use integration w.r.t y , we find

$$\begin{aligned} |f(x)|^2 &\leq \frac{1}{b}\|f\|^2 + 2\|f\|\|f'\| \\ \|f\|_\infty^2 &\leq \left(\frac{1}{b} + \frac{1}{\epsilon}\right)\|f\|^2 + \epsilon\|f'\|^2, \quad \text{any } \epsilon > 0 \end{aligned}$$

similarly

$$|f'(x)|^2 \leq \left(\frac{1}{b} + \frac{1}{\epsilon}\right)\|f'\|^2 + \epsilon\|f''\|^2, \quad \text{any } \epsilon > 0$$

But

$$\begin{aligned} \|f'\|^2 &= \int_0^b \bar{f}'f' \\ &= \bar{f}'f'|_0^b - \int_0^b \bar{f}f'' \\ &\leq \frac{1}{\epsilon'}\|f\|_\infty^2 + \epsilon'\|f'\|_\infty^2 + \frac{1}{\epsilon}\|f\|_{L^2(0,b)}^2 + \epsilon\|f''\|_{L^2(0,b)}^2 \\ &\leq \frac{1}{\epsilon'}\|f\|_\infty^2 + \epsilon'\left(\left(\frac{1}{b} + 1\right)\|f'\|^2 + \|f''\|^2\right) + \frac{1}{\epsilon}\|f\|^2 + \epsilon\|f''\|^2 \end{aligned}$$

Then we have

$$\begin{aligned} [1 - \epsilon'\left(\frac{1}{b} + 1\right)]\|f'\|^2 &\leq \frac{1}{\epsilon'}\|f\|_\infty^2 + \epsilon'\|f''\|^2 + \frac{1}{\epsilon}\|f\|^2 + \epsilon\|f''\|^2 \\ &\leq \frac{1}{\epsilon'}\left[\left(\frac{1}{b} + 1\right)\|f\|^2 + \epsilon\|f'\|^2\right] + \frac{1}{\epsilon}\|f\|^2 + (\epsilon + \epsilon')\|f''\|^2 \\ [1 - \epsilon'\left(\frac{1}{b} + 1\right) - \frac{\epsilon}{\epsilon'}]\|f'\|^2 &\leq \left(\frac{1}{\epsilon'}\left(\frac{1}{b} + \frac{1}{\epsilon}\right) + \frac{1}{\epsilon}\right)\|f\|^2 + (\epsilon + \epsilon')\|f''\|^2 \end{aligned} \tag{2.1}$$

take $\epsilon < \frac{\epsilon'}{4} < \min\{(\frac{1}{b} + 1)^{-1} \frac{1}{16}, \frac{1}{5}\}$, that is $\epsilon'(\frac{1}{b} + 1) + \frac{\epsilon}{\epsilon'} < \frac{1}{4} + \frac{1}{4} = \frac{1}{2}$, and $\epsilon + \epsilon' < \frac{1}{4}$, so (2.1) becomes

$$\frac{1}{2} \|f'\|^2 \leq \frac{1}{4} \|f''\|^2 + \left(\frac{1}{\epsilon'} \left(\frac{1}{b} + \frac{1}{\epsilon} \right) + \frac{1}{\epsilon} \right) \|f\|^2$$

then combining (1.3) by Rellich, Rabin is s. adj.

Note 61. More generally one can show $|f(x)|^2 \leq d \|f\|^2 + c \|f^{(k)}\|^2$ where (k) is the k th derivative. and d is depended only on k , see *Sobolev Spaces* by Robert Adam.

Exercise 62. Check each of the six operators listed at the beginning of this section has discrete spectrum $E_k \rightarrow \infty$. This can be done by direct computation for $V(x) \equiv 0$. And for $V \neq 0$ by min-max. To use min-max, one need use the quadratic forms. Show the quadratic forms associated with the first five operators is given by

$$q(f) = \int_0^b |f'|^2 dx$$

and

$$Q(q_D) = T \cap \{f(0) = f(b) = 0\}$$

$$Q(q_N) = T$$

$$Q(q_\alpha) = T \cap \{f(b) = e^{i\alpha} f(0)\}$$

$$Q(q_{DN}) = T \cap \{f(0) = 0\}$$

$$Q(q_{ND}) = T \cap \{f(b) = 0\}$$

and for Robin

$$q_{\alpha\beta}(f) = \int_0^b |f'|^2 - \beta |f(b)|^2 + \alpha |f(0)|^2$$

$$Q(q_D) = T$$

where $T = \{f \in L^2(0, b) : f \text{ a cont, } f' \in L^2(0, b)\}$.

2.2 On Positive Real

We have shown Schrodinger operator on \mathbb{R} and $(0, b)$. We now want to investigate

$$H = -\frac{d^2}{dx^2} + V(x)$$

on positive real with

$$D(H) = C_0^\infty(0, \infty) \subset L^2(0, \infty)$$

and $V(x)$ is real valued and $V \in L_{loc}^2(0, \infty)$. What can we say about its s.adj extensions, if any?

Theorem 63. *Let $H = -\frac{d^2}{dx^2} + V(x)$ be as above. Then*

(a) *H is symmetric*

(b) *$D(H^*) = D \equiv \{f \in L^2 : f, f' \text{ abs cont, } -f'' + Vf \in L^2(0, \infty)\}$ and $H^*f = -f'' + Vf$ for $f \in D(H^*)$*

(c) *H has equal deficiency indices $n_+(H) = n_-(H)$. (hence H has s.adj extension.)*

(d) *If \tilde{H} is a s.adj extension of H , then $\tilde{H} \subset H^*$. In particular, $D(\tilde{H}) \subset D(H^*)$ and they have the same action on $D(\tilde{H})$.*

Note 64. In part (b), if $f \in D(H^*)$, then f is continuous and hence $Vf \in L_{loc}^2(0, \infty) \implies f'' \in L_{loc}^2(\mathbb{R}_+)$.

Proof. (a) is obvious.

(b) Let \hat{H} be the operator $-d^2/dx^2 + V$ acting on $D(\hat{H}) = D$ given above. We show that $\hat{H} = H^*$. Let $f \in D$ and $g \in C_0^\infty(\mathbb{R}_+) = D(H)$, then

$$(Hg, f) = \int_0^\infty \overline{-g'' + Vf} f = - \int \bar{g} f'' + \int V \bar{g} f$$

as f, f', g, g' are abs cont. and g has compact support. Thus $(Hg, f) = (g, -f'' + Vf)$, $\forall g \in C_0^\infty(\mathbb{R})$. But as $f \in D$, $\hat{H}f = -f'' + Vf \in L^2$ and so $f \in D(H^*)$ as $H^*f = \hat{H}f$. Thus $\hat{H} \subset H^*$.

Now suppose that $f \in D(H^*)$. Then $\forall g \in C_0^\infty(\mathbb{R}_+)$, $(Hg, f) = (g, h)$ for some $h \in L^2(\mathbb{R}_+)$ and $h = H^*f$. Thus $\int_0^\infty \overline{-g'' + Vf} f = \int_0^\infty \bar{g} h$. Set $y = h - Vf$. As $V \in L_{loc}^2$ and $h, f \in L^2$, we see that $y \in L_{loc}^1(\mathbb{R}_+)$. Hence

$$\begin{aligned} \int_0^\infty \overline{-g''} f &= \int_0^\infty \bar{g}(x) y(x) dx \\ &= [\bar{g}(x) \int_1^x y(t) dt]_{x=0}^{x=\infty} - \int_0^\infty [\bar{g}'(x) \int_1^x y(t) dt] dx \\ &= [-\bar{g}'(x) \int_1^x dt]_{x=0}^{x=\infty} + \int_0^\infty [\bar{g}''(x) \int_1^x dt \int_1^t y(s) ds] dx \end{aligned}$$

Hence

$$\int_0^\infty dx g''(x) [f + \int_1^x dt \int_1^t y(s) ds] = 0$$

$\forall g \in C_0^\infty(\mathbb{R}_+)$.

Exercise show it follows that $f(x) = -\int_1^x dt \int_1^t y(s) ds + a + bx$, for some a, b .

In particular we see that f is abs cont. and $f'(x) = -\int_1^x y(s) ds + b$ and so f' is abs cont. and $f''(x) = -y(x) = -h + Vf$. Thus $-f'' + Vf = h \in L^2$, and so $f \in D$. Thus $\hat{H}f = h = H^*f \implies H^* \subset \hat{H}$. This shows that H^* is indeed given as in (b).

(c) follows as H commutes with complex conjugation, by proposition 46.

(d) is an abstract fact. If $\tilde{H} = \tilde{H}^*$ and $\tilde{H} \supset H$, then $\tilde{H} = \tilde{H}^* \subset H^*$. \square

2.3 Wronskian

Now as $u \in \text{Null}(H^* \pm i) \iff u$ is a solution of $-u'' + (V \pm i)u = 0$, and there are at most 2 independent solutions of each of these equations, we see as above that $n_+ = n_- \leq 2$.

A crucial object in analyzing the spectrum of Schrodinger operator in 1-dim is the *Wronskian*.

Definition 65. It is given by

$$W(f, g) = f'(x)g(x) - f(x)g'(x)$$

of two C^1 functions f, g .

Fact 66. The key fact is that f, g are solutions $Hf = \lambda f$, $Hg = \lambda g$ of Schrodinger equation with energy λ , then

$$W(f, g) = \text{const.}$$

Proof. Indeed,

$$\frac{d}{dx} (f'g - fg') = f''g - fg'' = (V - \lambda)f g - f(V - \lambda)g = 0$$

We are really requiring f, f', g, g' to be abs. cont. so that $dW/dx = 0 \implies W = \text{constant}$. \square

The converse is true in the following sense:

Fact 67. *If $Hf = \lambda f$, $f \neq 0$, and $W(f, g) = \text{const}$, then $Hg = \lambda g$.*

Proof. Indeed, if

$$0 = f''g - fg'' = (V - \lambda)gf - fg''$$

then dividing out f , we get the result. \square

Fact 67 tells us that given f , we can construct a second solution g whenever $f \neq 0$. We have $f'g - fg' = c$, thus

$$\frac{d}{dx} \frac{g}{f} = \frac{g'}{f} - \frac{gf'}{f^2} = -\frac{W(f, g)}{f^2} = -\frac{c}{f^2}$$

so

$$\frac{g(x)}{f(x)} = c' - c \int^x \frac{dt}{f^2}$$

or

$$g(x) = c'f(x) - cf(x) \int^x \frac{dt}{f^2(t)} \quad (2.2)$$

Fact 68. *If $g = c'f$, then $W(f, g) = 0$. Conversely if $W(f, g) = 0$, by the equation above, $g(x) = c'f(x)$ on the set $f \neq 0$.*

Proof. Equation (1.1) works well to prove $W(f, g) = 0 \iff f = cg$, but it fails when $f(x_0) = 0$ for some x_0 . It is well known that as f solves a 2nd order equation, the zero's of f cannot accumulate at a finite point. Suppose $f(x_0) = 0$ then $f(x) \neq 0$ for $0 < |x - x_0| < \delta$ for some $\delta > 0$. Suppose $g(x) = c_+f(x)$, $g(x) = c_-f(x)$ for $x_0 < x < x_0 + \delta$ and $x_0 - \delta < x < x_0$ respectively. But then by the continuity of f, g, f', g' at x_0 and the fact that $f'(x_0) \neq 0$, we conclude that $c_+ = c_-$ and so we see that $g = cf \forall x$ for some constant c . Thus $W(f, g) = 0 \iff f = cg$. \square

We are not assuming f and g here are solutions of $(H - \lambda)f = 0$ or $(H - \lambda)g = 0$. But if $f \neq 0$ and $(H - \lambda)f = 0$, then

$$(H - \lambda) = -\frac{1}{f} \frac{d}{dx} f^2 \frac{d}{dx} \frac{1}{f}$$

This formula is true in any dimension as

$$(H - \lambda) = -\frac{1}{f} \nabla \cdot f^2 \nabla \frac{1}{f}$$

From above (2.2) we clearly see that

$$(H - \lambda)g = -c(H - \lambda)f \int^x \frac{dt}{f^2} = c \frac{1}{f} \frac{d}{dx} f^2 \frac{d}{dx} \frac{1}{f} f \int^x \frac{dt}{f^2} = 0$$

This formula makes (2.2) transparent.

The following result is basic.

Proposition 69. *Consider the differential equation*

$$-\psi'' + V\psi = \lambda\psi \quad (2.3)$$

for $\lambda \in \mathbb{C}$, where $V(x)$ is real valued and is in $L^2_{loc}(0, \infty)$ and $\psi, \psi' \in \text{abs cont on } (0, \infty)$.

(a) If $\text{Im}\lambda \neq 0$, then \exists at least 1 non-zero solution of (2.3) which is in L^2 near 0 and at least 1 solution in L^2 near ∞ .

(b) If for some $\lambda \in \mathbb{C}$, both solutions of (2.3) in L^2 near ∞ (resp. 0), then for all $\lambda \in \mathbb{C}$, both solutions of (2.3) are in L^2 near ∞ (resp. near 0).

Proof. (a) Suppose $\text{Im}\lambda \neq 0$. Let f be $C^2_0[1, \infty) = \{f \in C^2[1, \infty) : f(x) = 0 \text{ for } x \text{ suff large}\}$ with $f(1) = 0, f'(1) \neq 0$. Set

$$g(x) = \begin{cases} -f''(x) + (V(x) - \lambda)f & x \geq 1 \\ 0 & 0 < x < 1 \end{cases}$$

Clearly $g \in L^2(0, \infty)$ and $g(x) \not\equiv 0$. Indeed if $g(x) = 0 \forall x \geq 1$, then $-f'' + Vf = \lambda f$ on $(1, \infty)$ and so the s.adj Dirichlet problem on $[0, b]$ for some sufficiently large $b > 1$. ($f(x) = 0$ for $x > \hat{b}$.) has a non-real eigenvalue λ , which is a contradiction. Hence $g \not\equiv 0$.

Now let \tilde{H} be s. adj extension of H (such extensions exist as $n_+ = n_-$). As $\lambda \notin \mathbb{R}$, by Propersition 23 $(\tilde{H} - \lambda)^{-1}$ exists. Set

$$h = (\tilde{H} - \lambda)^{-1}g \in L^2(0, \infty)$$

thus $(\tilde{H} - \lambda)h = g(x) = 0$ for $0 < x < 1$. But $\tilde{H} \subset H^* \implies (\tilde{H} - \lambda)h = -h'' + (V - \lambda)h = 0$ for $0 < x < 1$.

Now suppose that $h(x) \equiv 0$ for $0 < x < 1$. As $h \in D(\tilde{H}) \subset D(H^*)$, we have by continuity, $h(1) = h'(1) = 0$. We will show this leads to

a contradiction. Now observe first that as \tilde{H} is s.adj and in particular symmetric, and as $h \in D(\tilde{H})$,

$$\begin{aligned}
0 &= (h, \tilde{H}h) - (\tilde{H}h, h) \\
&= \lim_{\epsilon \downarrow 0} \int_{\epsilon}^{1/\epsilon} \left(\bar{h} \tilde{H}h - \overline{\tilde{H}h} h \right) dx \\
&= \lim_{\epsilon \downarrow 0} \int_{\epsilon}^{1/\epsilon} [\bar{h} (-h'' + Vh) - \overline{-h'' + Vh} h] \\
&= \lim_{\epsilon \downarrow 0} \int_{\epsilon}^{1/\epsilon} \bar{h}'' h - h'' \bar{h} \\
&= \lim_{\epsilon \downarrow 0} (\bar{h}' h - h' \bar{h})_{\epsilon}^{1/\epsilon} \\
&= \lim_{x \rightarrow \infty} \bar{h}'(x) h(x) - h'(x) \bar{h}(x)
\end{aligned}$$

as $h(x) = 0$ for $0 < x < 1$. i.e.

$$\lim_{x \rightarrow \infty} \bar{h}'(x) h(x) - h'(x) \bar{h}(x) = 0 \quad (2.4)$$

Next note that for $x \geq 1$, $l(x) \equiv h(x) - f(x)$ solves $-l'' + (V - \lambda)l = 0$ with $l(1) = 0$. Thus for $b > 1$

$$\begin{aligned}
0 &= \int_1^b \left[\bar{l} (-l'' + (V - \lambda)l) - \overline{-l'' + (V - \lambda)l} l \right] \\
&= (\bar{\lambda} - \lambda) \int_1^b |l|^2 + \int_1^b (\bar{l}'' l - \overline{l''} \bar{l}) dx \\
&= (\bar{\lambda} - \lambda) \int_1^b |l|^2 + (\bar{l}' l - \overline{l'} \bar{l})_1^b \\
&= (\bar{\lambda} - \lambda) \int_1^b |l|^2 + \bar{l}'(b) l(b) - \overline{l'(b)} \bar{l}(b) \\
&= (\bar{\lambda} - \lambda) \int_1^b |l|^2 + (\bar{h}' h - \overline{h'} \bar{h})(b)
\end{aligned}$$

as $l(1) = 0$, for b suff large. Letting $b \rightarrow \infty$ we conclude from (2.4) that

$$0 = (\bar{\lambda} - \lambda) \int_1^{\infty} |l(x)|^2 dx$$

and so $l(x) \equiv 0$, $\forall x \geq 1$ as $\lambda \neq \bar{\lambda}$. Thus $h(x) = f(x)$ $x \geq 1$. But $h'(1) = 0 \neq f'(1)$, which is a contradiction.

Thus $h(x) \neq 0$ for $0 < x < 1$. This shows that there exists a non-zero solution of (2.3) which is L^2 near 0. A similar proof, choose $f \in C_0^2(0, 1]$, $f(1) = 0$, $f'(1) \neq 0$ shows that \exists a non-zero solution of (2.3) which is in L^2 near ∞ .

(b) Suppose ψ_1, ψ_2 are two independent solutions of (2.3) for some $\lambda_0 \in \mathbb{C}$, normalized so that

$$W(\psi_1, \psi_2) = \psi_1' \psi_2 - \psi_1 \psi_2' = 1$$

Let $u(x)$ be any solution of (2.3) with $\lambda = \lambda_1 \neq \lambda_0$ and fix $c > 0$. Then an explicit computation shows that

$$u(x) - (\lambda_1 - \lambda_0) \int_c^x (\psi_1(x)\psi_2(\xi) - \psi_1(\xi)\psi_2(x)) u(\xi) d\xi$$

solves (2.3) with $\lambda = \lambda_0$, so

$$u(x) = c_1 \psi_1(x) + c_2 \psi_2(x) + (\lambda_1 - \lambda_0) \int_c^x (\psi_1(x)\psi_2(\xi) - \psi_1(\xi)\psi_2(x)) u(\xi) d\xi$$

for some constants c_1 and c_2 . Suppose $\psi_1, \psi_2 \in L^2(\infty)$. Let

$$M = \max \left\{ \left(\int_c^\infty |\psi_1|^2 dx \right)^{1/2}, \left(\int_c^\infty |\psi_2|^2 dx \right)^{1/2} \right\}$$

then by the Schwartz inequality

$$|u(x)| \leq |c_1| |\psi_1(x)| + |c_2| |\psi_2(x)| + |\lambda_1 - \lambda_0| (|\psi_1(x)| + |\psi_2(x)|) M \|u\|_{[c,x]}$$

where $\|u\|_{[c,x]} = \left(\int_c^x |u|^2 d\xi \right)^{1/2}$, thus

$$\|u\|_{[c,x]} \leq (|c_1| + |c_2|) M + (\lambda_1 - \lambda_0) 2M^2 \|u\|_{[c,x]}$$

so that if $|\lambda_1 - \lambda_0| < 1/4M^2$, we have $\|u\|_{[c,x]} \leq 2(|c_1| + |c_2|) M$, $\forall x \geq c$, thus $u \in L^2(\infty)$.

Now we can choose M as small as we like by choosing c large. By choosing c_1, c_2 independently, we find two independent solutions of (2.3) with $\lambda = \lambda_1$. It follows that we have proven (b) at ∞ . The case at 0 is similar. This completes the proof of proposition 69. \square

Remark 70. For $V = 0$, $-\psi'' = \lambda\psi$ has solutions $\psi = e^{\pm i\sqrt{\lambda}x}$. For real positive λ , we see that there are no L^2 solutions of (2.3) at ∞ for any λ .

2.4 Limit Circle-Limit Point Criterion

Definition 71. We say that $V(x)$ is in the *limit circle case* at ∞ (resp. at 0) if for some λ and hence for all λ , all solutions of

$$-\psi'' + V\psi = \lambda\psi$$

are in L^2 at ∞ (resp. at 0). If $V(x)$ is not in the limit circle case at ∞ (resp. at 0) it is said to be in the *limit point case* at ∞ (resp. at 0).

We will explain this terminology later. This terminology is due to Weyl. The basic result is the following.

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Theorem 72. (*Weyl's limit point - limit circle criterion*) Let $V(x)$ be real valued and in $L^2_{loc}(\mathbb{R}_+)$. Then $H = -\frac{d^2}{dx^2} + V(x)$ is *ess.s.adj* on $C_0^\infty(0, \infty) \iff V(x)$ is in the limit point case at both 0 and ∞ .

Proof. (\implies) If V is limit circle at both 0 and ∞ , then $N(H^* + i)$ and $N(H^* - i)$ each has 2 independent solutions and have $n_\pm = 2$. If V is limit circle at one end, but not at the other, then $n_\pm = 1$. Thus if V is not limit point at ∞ and at 0, then it is not e.s.a.

(\impliedby) Now suppose V is limit point at both 0 and ∞ . For $f, g \in D(H^*)$, we set

$$W_x(f, g) = \overline{f(x)}g'(x) - \overline{f'(x)}g(x)$$

W_x is continuous and for $0 < a < b < \infty$,

$$W_b - W_a = \int_a^b (\overline{H^* f}g - \overline{f}H^* g) dx$$

Since the integrand on the RHS is in L^1 , and $W_\infty = \lim_{b \rightarrow \infty} W_b$, $W_0 = \lim_{a \downarrow 0} W_a$ exist,

$$W_\infty - W_0 = (H^* f, g) - (f, H^* g) \quad (2.5)$$

If we can show LHS of (2.5) = 0, then H^* is symmetric and so H is e.s.a.

One can prove that H^* is symmetric implies H is e.s.a. in 2 ways.
(i) If T is a closable operator, then $\bar{T} = T^{**}$. In particular as every symmetric operator is closable, we must have $\bar{S} = S^{**}$. In particular if S^* is symmetric, i.e. $S^* \subset (S^*)^* = S^{**}$, then $S \subset \bar{S} \subset S^* \subset S^{**} = \bar{S}$, i.e. $\bar{S} = S^* = \bar{S}^*$ (note: $S^* = (\bar{S})^*$ for any closable operator S). Then S is e.s.a.

(ii) Alternatively if S^* is symmetric and $(S^* - i)f = 0$, then $(S^*f, f) = (f, S^*f) \implies -i(f, f) = i(f, f)$, so $f = 0$. Then $n_+(S) = n_-(S) = 0$, so S is e.s.a.

Now let $A = -d^2/dx^2 + V$ on

$$D(A) = \{\psi \in C_0^\infty[1, \infty) : \psi(1) = 0\} \in L^2(0, \infty)$$

A is symmetric on $D(A)$ and by a familiar computation $A^* = -d^2/dx^2 + V$ on $D(A^*) = \{\psi \in L^2(1, \infty) : \psi, \psi' \text{ abs cont, } -\psi'' + V\psi \in L^2(1, \infty), \psi(1) = 0\}$

Now if $0 \neq \hat{f} \in D(A^*)$, $(A^* - i)\hat{f} = 0$, then \hat{f} must be proportional to the unique non-zero solution f of

$$-f'' + (V - i)f = 0$$

which lies in L^2 at ∞ . Now f can be constructed as similar to proof of proposition 69, choose $f \in C_0^2(0, 1]$, $f(1) = 0$, $f'(1) \neq 0$ from $h = (\bar{A} - i)^{-1}g$ for some g with compact support. Here again, \bar{A} is some s.adj extension of A . Therefore take $f(x) = h(x)$ for x beyond the support of g . A similar computation to equation (2.4), (use $\hat{f} \in D(A^*)$, so $\hat{f}(1) = 0$) show that $\hat{f} \equiv 0$. Thus $n_+(A) = 0$ and so $n_-(A) = 0$. Thus A is e.s.a.

Now let $f, g \in D(H^*)$ and choose $f_1, g_1 \in C_0^\infty(0, \infty)$, s.t.

$$f(1) + f_1(1) = 0 = g(1) + g_1(1)$$

set $f_2 = f + f_1$, $g_2 = g + g_1$, then

$$\begin{aligned} W_\infty(f, g) &= W_\infty(f_2, g_2) \\ &= W_\infty(f_2, g_2) - W_1(f_2, g_2) \\ &= (A^* f_2, g_2) - (f_2, A^* g_2) \end{aligned}$$

as f_2, g_2 clearly $\in D(A^*)$. But $A^* = (\bar{A})^* = \bar{A}$ as \bar{A} is s.adj. Thus RHS of above equation is 0, so $W_\infty(f, g) = 0$. Similarly we find $W_0(f, g) = 0$, and we are done. \square

Remark 73. The heart of the above proof is really the following fact that we proved: Suppose $A = -d^2/dx^2 + V(x)$ is limit point at ∞ , and suppose $D(A) = \{\psi \in C_0^\infty[1, \infty) : \psi \text{ satisfies some s.adj boundary condition at } x = 1\}$ e.g. $\psi(1) = 0$ or $\psi'(1) = 0$ or $\alpha\psi(1) + \beta\psi'(1) = 0$ $\alpha, \beta \in \mathbb{R}$. Then A is e.s.a.

Exercise 74. Suppose V is real and in $L^2(0, \infty)$, then show $H = -d^2/dx^2$ is e.s.a on $C_0^\infty[0, \infty) \cap \{f(0) = 0\}$. Hence V is limit point at ∞ .

2.5 Classical Motion

We now want to investigate when $V(x)$ is limit point at both ends. Here it is useful to consider the *classical motion* generated by the Hamiltonian $H(x, p) = p^2 + V(x)$ on \mathbb{R}_+ i.e.

$$\dot{x} = H_p = 2p$$

$$\dot{p} = -H_x = -V'(x)$$

$$x(t=0) = x_0, p(t=0) = p_0$$

Assumption 75. We assume (i) V is in $C^1(0, \infty)$; (ii) $V'(x)$ is uniformly Lipschitz on compact subsets of $(0, \infty)$. i.e. $|V'(x) - V'(y)| \leq L_{(x_0, x_1)} |x - y|$ for $0 < x_0 \leq x, y \leq x_1 < \infty$.

Note 76. $\ddot{x} = 2\dot{p} = -2V'(x)$ and that energy $p(t)^2 + V(x(t))$ is conserved for the system given above. Use standard argument, one can show local existence and uniqueness for solutions of classical motion given above.

Proposition 77. Suppose that a global solution of classical motion given above does not exist for some (x_0, p_0) . i.e. the maximal interval on which the solution exists is $[0, \tau)$ for some $\tau < \infty$. Then

either

$$\lim_{t \uparrow \tau} x(t) = 0$$

or

$$\lim_{t \uparrow \tau} x(t) = \infty$$

Exercise 78. Prove this proposition.

Definition 79. We say that the classical motion generated by V is *complete* at 0 (resp. ∞) if there is no $(x_0, p_0) \in \mathbb{R}_+ \times \mathbb{R}$ so that the solution with $x(0) = x_0, p(0) = p_0$ runs off to $x(t) = 0$ (resp. ∞) in finite time t .

Thus if V is complete at 0 and at ∞ , global solutions exist for all initial conditions (x_0, p_0) . The following result settles the question of when V is complete.

Theorem 80. Let $V(x)$ satisfying assumption 75 above, then the classical motion generated by $V(x)$,

(i) is not complete at 0 $\iff V(x)$ is bounded above near zero.

(ii) is not complete at ∞ $\iff V(x)$ is bounded above for $x \geq 1$ and $\int_1^\infty \frac{dx}{\sqrt{K - V(x)}} < \infty$ for some $K > \sup_{x \geq 1} V(x)$.

Proof. (i) Suppose V is not bounded above at 0. Then $\exists x_n \downarrow 0$ s.t. $V(x_n) \rightarrow \infty$. By conservation of energy

$$V(x(t)) \leq p(t)^2 + V(x(t)) = p_0^2 + V(x_0)$$

Thus $x(t)$ cannot equal x_n for n suff large and so $x(t)$ can never get near zero. Conversely, suppose $V(x) \leq M < \infty$ on $(0, 1)$. Let $x(0) = x_0 = 1$ and choose $p_0 < 0$ s.t. $p_0^2 + V(1) = 1 + M$. Then $p(t)^2 + V(x(t)) = p_0^2 + V(1) = 1 + M$, that follows that $p(t)^2 \geq 1 + M - V(x(t)) \geq 1$. As $p(0) < 0$, this means that $p(t) < 0$ for all $t \geq 0$. As $dx/dt = 2p(t)$, it follows that for all t for which the solution exists, $0 < x(t) < 1$ and $p(t) < -1$. hence $x(t)$ must reach 0 in finite time. Indeed

$$x(t) = 1 + 2 \int_0^t p(s) ds \leq 1 - 2t$$

Thus $x(t)$ must reach zero before time $1/2$.

(ii) If $V(x)$ is not bounded above on $(1, \infty)$, then the same argument as in (a) shows that V is complete at ∞ . So suppose $V(x) \leq M$ for $x \geq 1$ and that

$$\int_1^\infty \frac{dx}{\sqrt{K - V(x)}} < \infty, \text{ for some } K > \sup_{x \geq 1} V(x).$$

Choose $x(0) = x_0 = 1$, $p(0) = p_0 = \frac{1}{2}\dot{x}(0) > 0$, s.t. $p_0^2 + V(x) = K$, then arguing as above $x(t) \geq 1$ and $p(t) > 0 \forall t \geq 0$ and $\dot{x} = 2p(t) = 2\sqrt{K - V(x(t))}$. Now

$$t = \int_1^{x(t)} \frac{dx}{2\sqrt{K - V(x)}} \leq \int_1^\infty \frac{dx}{2\sqrt{K - V(x)}} < \infty$$

thus $x(t)$ must reach ∞ at time $T = \int_1^\infty \frac{dx}{2\sqrt{K - V(x)}} < \infty$ Thus we have incompleteness at ∞ .

Finally suppose that $V(x) \leq M$ for $x \geq 1$ and

$$\int_1^\infty \frac{dx}{\sqrt{K - V(x)}} = \infty \tag{2.6}$$

for all $K > \sup_{x \geq 1} V(x)$. Let $(x(t), p(t))$ be the solution of classical motion with arbitrary initial data $(x_0, p_0) \in \mathbb{R}_+ \times \mathbb{R}$. Suppose that for some $t_0 > 0$, $x(t_0) \geq 1$ and $p(t_0) > 0$. There are now 2 possibilities: either

(α) $p(t_1) = 0$ for some $t_1 > t_0$ or (β) $p(t) > 0$ for all $t > t_0$ for which the solution exists.

In case (α), we have $V(x(t_1)) = H = p_0^2 + V(x_0)$. If $V'(x(t_1)) = 0$ then $x(t) = x(t_1)$, $p(t) = 0$, $\forall t$. Recall $\ddot{x} = -2V'(x(t))$. If $V'(x(t_1)) > 0$, then the particle cannot move to the right of $x(t_1)$ for $t > t_1$. Otherwise $p(t)^2 + V(x(t)) > V(x(t_1)) = H$. On the other hand, if $V'(x(t_1)) < 0$, then for $t < t_1$, $p(t)^2 + V(x(t)) > V(x(t_1)) = E$ and the particle could not have gotten to $x(t_1)$ in the first place. Thus we see that in case (α), we have completeness at ∞ .

In case (β), $\dot{x}(t) = 2p(t) = \sqrt{E - V(x(t))} > 0 \forall t > t_0$. Hence for $t > t_0$, $x(t) > x(t_0) > 1$ and $t - t_0 = \int_{x(t_0)}^{x(t)} \frac{dx}{2\sqrt{E - V(x)}}$. Now let $K > \max(E, \sup_{x \geq 1} V(x))$. Then $K - V(x) > E - V(x) \implies t - t_0 \geq \int_{x(t_0)}^{x(t)} \frac{dx}{2\sqrt{K - V(x)}}$ which implies by (2.6) that we cannot have $\lim_{t \uparrow \tau} x(t) = \infty$ for some finite τ . Again we have completeness at ∞ . This proves the theorem. \square

2.6 Semi-Classical Limit

We know that in the “semi-classical limit”, quantum mechanics is described by classical mechanics. \hbar Planck’s constant $\rightarrow 0$. The question here is whether the essential self-adjointness of

$$H = -\frac{d^2}{dx^2} + V(x)$$

is correlated with the completeness of the classical Hamiltonian system generated by the Hamiltonian $H(x, p) = p^2 + V(x)$. More precisely we expect that $H = -d^2/dx^2 + V(x)$ is e.s.a. on $C_0^\infty(0, \infty) \subset L^2(0, \infty)$ iff in the classical motion generated by $H(x, p)$ is complete. The particle stays away from 0 and ∞ , so that we need not specify boundary conditions at 0 or infinity.

The relevant result is the following.

Theorem 81. *Let $V(x)$ be differentiable on $(0, \infty)$ and suppose $K > \sup_{x \geq 1} V(x)$, for some $K \geq 0$. Suppose that*

$$(i) \int_0^\infty \frac{dx}{\sqrt{K - V(x)}} = \infty; \quad (ii) \frac{V'(x)}{|V(x)|^{3/2}} \text{ is bounded near } \infty.$$

Then V is limit point at ∞ .

Proof. We will show that both solutions of $Hu = 0$ cannot be in L^2 near ∞ . If $0 < c_1 < c < \infty$ and $u(x)$ is a real solution in L^2 near ∞ , then as $V(x) \geq -(K - V(x))$,

$$I_1 \equiv - \int_{c_1}^c u^2(x) dx \leq \int_{c_1}^c u^2(x) \frac{V(x)}{K - V(x)} dx = \int_{c_1}^c u''(x) \frac{u(x)}{K - V(x)} dx$$

integrating by parts, we find

$$I_1 \leq \underbrace{u'(x) \frac{u(x)}{K - V(x)} \Big|_{c_1}^c}_{I_2} - \underbrace{\int_{c_1}^c \frac{u'(x)^2}{K - V(x)} dx}_{I_3} - \underbrace{\int_{c_1}^c \frac{u'(x)u(x)V'(x)}{(K - V(x))^2} dx}_{I_4}$$

Now by Cauchy-Schwarz

$$|I_4|^2 \leq (I_5)^2 \underbrace{\int_{c_1}^c u(x)^2}_{I_1} \underbrace{\int_{c_1}^c \frac{u'(x)^2}{K - V(x)}}_{I_3}$$

where

$$I_5 = \sup_{x \geq 1} \left| \frac{V'(x)}{(K - V(x))^{3/2}} \right|$$

If $V(x) > 0$ for some $x \geq 1$, and $0 < V(x) < K$, so $\frac{|V'(x)|}{|V(x)|^{3/2}} \geq \frac{|V'(x)|}{K^{3/2}}$. But as $\sup_{x \geq 1} V(x) < K$, for that x , we have $K - V(x) \geq \delta$ for some $\delta > 0$ and so

$$\frac{|V'(x)|}{|K - V(x)|^{3/2}} \leq \frac{1}{\delta^{3/2}} |V'(x)| \leq \frac{K^{3/2}}{\delta^{3/2}} \sup \frac{|V'(x)|}{|V(x)|^{3/2}}$$

On the other hand if $V(x) < 0$, for some $x \geq 1$, then $K - V(x) \geq |V(x)|$ and so $\frac{|V'(x)|}{|K - V(x)|^{3/2}} \leq \frac{|V'(x)|}{|V(x)|^{3/2}}$. It follows from these observations that $I_5 < \infty$.

Now suppose that $\lim_{x \rightarrow \infty} u'(x)u(x) = \infty$, so that eventually $u(x)$ and $u'(x)$ have the same sign. Thus if $u(x_0) > 0$ for some $x_0 \gg 1$, then $u(x) \geq u(x_0) > 0 \forall x > x_0$, which is impossible as $u \in L^2(\infty)$. Similarly if $u(x_0) < 0$ for some $x_0 \gg 1$, also is impossible, thus $I_2 < \infty$. Therefore $\int_{c_1}^{\infty} \frac{u'(x)^2}{K - V(x)} < \infty$.

Now suppose that ψ and ϕ are independent solutions of $H\psi = 0$, without lost of generality, we can assume that $W(\psi, \phi) = 1 = \psi'\phi - \psi\phi'$. Then

$$\frac{1}{\sqrt{K - V(x)}} = \frac{\psi'\phi}{\sqrt{K - V(x)}} - \frac{\psi\phi'}{\sqrt{K - V(x)}} \in L^1(\infty)$$

for by Cauchy-Schwarz $\left| \int \frac{\psi' \phi}{\sqrt{K-V(x)}} \right|^2 \leq \int \frac{\psi'(x)^2}{K-V(x)} \int \phi^2 < \infty$. That contradicts (i) in theorem 81. \square

Corollary 82. *In particular, if V on $(0, 1) \in L^2(0, 1)$, then the Dirichlet operator $-d^2/dx^2 + V(x)$ on $C_0^\infty[0, \infty) \cap \{\psi(0) = 0\}$ is e.s.a.*

Exercise 83. Prove this corollary. (cf. Exercise 74)

Remark 84. A classical particle moving with momentum p has a de-Broglie wavelength $\lambda = h/p$. If the particle moves into a region with a typical length scale L , then the particle will act classically if $\lambda/L \ll 1$, and quantum effects will be apparent if $\lambda/L \gg 1$.

Now for a particle moving with energy 0, say, $H = p^2 + V = 0$. We have $|p| = \sqrt{-V}$ and so

$$\lambda = h/\sqrt{-V(x)} \implies \left| \frac{d\lambda}{dx} \right| = |\text{const.}| \left| \frac{V'}{(-V)^{3/2}} \right|$$

Thus condition (ii) in theorem 81 is just the requirement that quantum effects are bounded. So theorem 81 says that if quantum effects are bounded, a particle is classically complete at $\infty \iff$ it is limit point at infinity, i.e. quantum mechanically complete at ∞ .

Example 85. Let $c > 0$ and consider $H = -d^2/dx^2 - cx^\alpha$. Then it follows theorem 81 that if $-2 \leq \alpha \leq 2$, then it is limit point at ∞ . Actually a more refined result (see Reed Simon Vol II page 159) gives it is e.s.a $\iff \alpha \leq 2$.

Exercise 86. Clearly if $V(x)$ is bounded then theorem 81 implies V is limit point at ∞ . We are familiar with this result by Kato-Rellich. Why?

2.7 Classical Break Down

The quantum-classical analogy may break down if V oscillates too rapidly, i.e. big V' .

Example 87. (Reed Simon Vol II page 155) V is quantum mechanically complete but classically incomplete.

Example 88. (Reed Simon Vol II page 157) V is classically complete but quantum mechanically incomplete.

Exercise 89. Work through these examples.

2.8 Limit Circle-Limit Point Theory

Finally we explain the terminology limit point, limit circle. The standard reference is Coddington and Levinson, *Theory of Ordinary Differential Equations*, chapter 9.

Suppose for convenience that V is continuous on $[0, \infty)$ and consider $H = -d^2/dx^2 + V$ acting on smooth function. Fix $\lambda \in \mathbb{C} \setminus \mathbb{R}$ and let y_1, y_2 be the solutions of $Hy_i = \lambda y_i$, $i = 1, 2$, with

$$\begin{aligned} y_1(x=0, \lambda) &= 1 & y_2(x=0, \lambda) &= 0 \\ y_1'(x=0, \lambda) &= 0 & y_2'(x=0, \lambda) &= 1 \end{aligned}$$

For a fixed $b > 0$, the set $\{m = m(\lambda, b)\}$ for which $\chi = y_1 + my_2$ obeys

$$\chi(b) \cos \beta + \chi'(b) \sin \beta = 0 \quad (2.7)$$

for β runs over $[0, \pi)$ forms a circle C_b . Indeed

$$(y_1(b, \lambda) + my_2(b, \lambda)) \cos \beta + (y_1'(b, \lambda) + my_2'(b, \lambda)) \sin \beta = 0$$

gives

$$\begin{aligned} m &= -\frac{y_1(b, \lambda) \cot \beta + y_1'(b, \lambda)}{y_2(b, \lambda) \cot \beta + y_2'(b, \lambda)} \\ &= -\frac{y_1(b, \lambda)z + y_1'(b, \lambda)}{y_2(b, \lambda)z + y_2'(b, \lambda)} \end{aligned} \quad (2.8)$$

Now $y_1(b, \lambda) \neq 0$, for otherwise the s.adj problem for H on $L^2(0, b)$ with $y_1'(0, \lambda) = y_1(b, \lambda) = 0$ would have a non-real eigenvalue. Hence as β runs over $[0, \pi)$, $z = \cot \beta$ runs over the real line and hence by arguments of conformal mapping, $m = m(\lambda, b)$, λ, b fixed, runs over a circle $C_b = C_b(\lambda)$. It is an easy **Exercise** to see that the equation for C_b has the form

$$[\chi\chi](b) = 0$$

where $[fg] = f\bar{g}' - f'\bar{g} = W(\bar{g}, f)$. As

$$\begin{aligned} \frac{d}{dx}[\chi\chi](x) &= \frac{d}{dx}(\chi\bar{\chi}' - \chi'\bar{\chi}) \\ &= \chi\bar{\chi}'' - \chi''\bar{\chi} \\ &= \chi(V - \bar{\lambda})\bar{\chi} - (V - \lambda)\chi\bar{\chi} \\ &= (\lambda - \bar{\lambda})|\chi|^2 \end{aligned}$$

we have as $\chi(0) = 1$, $\chi'(0) = m$.

$$\begin{aligned}
[\chi\chi](b) &= [\chi\chi](0) + 2i\text{Im}\lambda \int_0^b |\chi|^2 dx \\
&= (\bar{m} - m) + 2i\text{Im}\lambda \int_0^b |\chi|^2 dx \\
&= -2i\text{Im}m + 2i\text{Im}\lambda \int_0^b |\chi|^2 dx
\end{aligned} \tag{2.9}$$

Now the interior of C_b is given by (**Exercise**)

$$\frac{[\chi\chi](b)}{[y_2y_2](b)} < 0$$

and

$$[y_2y_2](b) = 2i\text{Im}\lambda \int_0^b |y_2|^2 dx$$

and so the interior of C_b takes the form

$$\int_0^b |\chi|^2 dx \leq \frac{\text{Im}m}{\text{Im}\lambda}, \quad \text{Im}\lambda \neq 0$$

Moreover m is on the circle C_b iff

$$\int_0^b |\chi|^2 dx = \frac{\text{Im}m}{\text{Im}\lambda} \tag{2.10}$$

Moreover the radius r_b of the circle is given by (**Exercise**)

$$r_b = \frac{1}{|[y_2y_2](b)|} \tag{2.11}$$

and so for $\text{Im}\lambda > 0$

$$\frac{1}{r_b} = 2\text{Im}\lambda \int_0^b |y_2(x, \lambda)|^2 dx \tag{2.12}$$

More let $0 < a < b < \infty$. Then m lies inside or on C_b if

$$\int_0^a |\chi|^2 < \int_0^b |\chi|^2 \leq \frac{\text{Im}m}{\text{Im}\lambda}$$

and therefore m is inside C_a . This means that C_b lies inside C_a if $a < b$. Thus for a given λ , $\text{Im}\lambda > 0$, as $b \rightarrow \infty$, the circles C_b converge either

to a circle C_∞ or to a point m_∞ . If the C_b converge to a circle, then its radius $r_\infty = \lim r_b$ is positive, and from equation (2.12), this implies $y_2 \in L^2(0, \infty)$. If \hat{m}_∞ is any point on C_∞ , then \hat{m}_∞ is inside any C_b for $b > 0$. Hence

$$\int_0^b |y_1 + \hat{m}_\infty y_2|^2 < \frac{\text{Im} \hat{m}_\infty}{\text{Im} \lambda}$$

and letting $b \rightarrow \infty$, one sees that $y_1 + \hat{m}_\infty y_2 \in L^2(0, \infty)$. The same argument holds if \hat{m}_∞ reduces to the point m_∞ . Therefore, if $\text{Im} \lambda \neq 0$, there always exists a solution of $Hf = \lambda f$ of class $L^2(0, \infty)$. In the case $C_b \rightarrow C_\infty$, all solutions are in $L^2(0, \infty)$, for $\text{Im} \lambda \neq 0$, since both y_2 and $y_1 + \hat{m}_\infty y_2$ are, and this identifies the limit circle case with the existence of the limit circle C_∞ . Correspondingly, the limit point case is identified with the existence of the point m_∞ . In the case $C_b \rightarrow m_\infty$, these results $\lim r_b = 0$ and so by equation (2.12), $y_2(x, \lambda) \notin L^2(0, \infty)$. Therefore in this situation there is one and only one independent solution of class $L^2(0, \infty)$ for $\text{Im} \lambda \neq 0$.

In the limit circle case (so y_1 and $y_2 \in L^2(0, \infty)$), it follows from equation (2.10) that $m \in C_\infty \iff$

$$\text{Im} \lambda \int_0^\infty |\chi|^2 = \text{Im} m \quad (2.13)$$

It follows then from equation (2.9) that

$$[\chi\chi](\infty) = 0$$

The following basic result has been proved.

Theorem 90. *If $\text{Im} \lambda \neq 0$ and y_1, y_2 are as above, then the solution $x = y_1 + my_2$ satisfies the real boundary condition (2.7) $\iff m$ lies on the circle*

$$[\chi\chi](b) = 0$$

As $b \rightarrow \infty$ either $C_b \rightarrow C_\infty$, a limit circle, or $C_b \rightarrow m_\infty$, a limit point. All solutions are in $L^2(0, \infty)$ in the former case, and if $\text{Im} \lambda \neq 0$, exactly one independent solution in $L^2(0, \infty)$ in the latter case. Moreover in the limit-circle case, a point is on the limit $C_\infty(\lambda) \iff [\chi\chi](\infty) = 0$.

The Green's function G associated with the s.adj. boundary problem

$$Hf = \lambda f \quad f(0) = 0$$

$$\cos \beta f(b) + \sin \beta f'(b) = 0$$

is given by

$$G(x, y; \lambda) = y_2(x, \lambda) (y_1(y, \lambda) + m(\lambda, b, \beta)y_2(y, \lambda)) \quad (2.14)$$

for $0 \leq x \leq y \leq b$. And

$$G(x, y; \lambda) = y_2(y, \lambda) (y_1(x, \lambda) + m(\lambda, b, \beta)y_2(x, \lambda)) \quad (2.15)$$

for $0 \leq y < x \leq b$.

Exercise 91. Check directly that G is indeed the kernel for $(H - \lambda)^{-1}$, i.e.

$$(H - \lambda)^{-1}f(x) = \int_0^b G(x, y)f(y)dy.$$

In the limit-point case, it follows from the above theorem that G on $(0, \infty)$ is given by equations (2.14), (2.15), with $m(\lambda, b, \beta)$ replaced by m_∞ , an irrespective of the boundary condition given by β in (2.7), as $b \rightarrow \infty$. (see remark 92 below). In other words, the operator H on $C_0^\infty[0, \infty) \cap \{y(0) = 0\}$ is e.s.adj. In the limit circle case, there are an infinite number of limit functions to which G may tend, depending on how β varies as $b \rightarrow \infty$. In other words, the operator H on $C_0^\infty[0, \infty) \cap \{y(0) = 0\}$ is not e.s.adj.

Each point \hat{m}_∞ on the limit circle C_∞ corresponds to a different s.adj extension of H . Note that we see again, now in a concrete form, that the s.adj. extensions of H are parametrized by a circle, as dictated by von Neumann's general theory.

Remark 92. There is a parallel limit point/limit circle theory for discretization of Schrodinger operators, i.e. for tri-diagonal operators T on $l_{2,+} = \{u : u = (u_1, u_2, \dots), \sum_1^\infty |u_i|^2 < \infty\}$,

$$\begin{cases} (Tu)_i = b_{i-1}u_{i-1} + a_iu_i + b_iu_{i+1} & i \geq 2 \\ (Tu)_1 = a_1u_1 + b_1u_2 \end{cases} \quad (2.16)$$

with $b_i > 0$, $i \geq 1$, $a_i \in \mathbb{R}$. The extension of Weyl limit-point/limit-circle theory is due to Hellinger. (See Akhiezer *the Classical Moment Problem and Some Related Questions in Analysis*)

Exercise 93. Every bounded s.adj operator in a separable Hilbert space is unitarily equivalent to a countable orthogonal sum of tridiagonal operator of type (2.16) with $\sup_i (|a_i| + |b_i|) < \infty$.

Before we return to limit-point/limit-circle theory we note that these one dimensional methods also give rise to results in n -dimensions if the potential is spherically symmetric i.e. $V(x) = V(r)$, $r = |x|$. We have (Reed-Simon II p161)

Theorem 94. *Let $V = V(r)$ be a continuous spherically symmetric potential in $\mathbb{R}^n \setminus \{0\}$.*

- (i) *If $V(r) + \frac{(n-1)(n-3)}{4} \frac{1}{r^2} \geq \frac{3}{4r^2}$, then $-\Delta + V(r)$ is e.s.a. on $C_0^\infty(\mathbb{R}^n \setminus \{0\})$.*
(ii) *If $0 \leq V(r) + \frac{(n-1)(n-3)}{4} \frac{1}{r^2} \leq \frac{c}{r^2}$, $c < 3/4$, then $-\Delta + V$ is not e.s.a on $C_0^\infty(\mathbb{R}^n \setminus \{0\})$.*

Proof. The idea of the proof rests on the fact that $\mathcal{H} = L^2(\mathbb{R}^n)$ can be decomposed according to the eigenspace K_l of the Laplace-Beltrami operator on S^{n-1} , i.e.

$$\mathcal{H} = L^2(\mathbb{R}_+, r^{n-1} dr) \otimes L^2(S^{n-1}, d\Omega) = \bigoplus_{l=0}^{\infty} L_l$$

where $L_l = L^2(\mathbb{R}_+, r^{n-1} dr) \otimes K_l$ (see Reed-Simon II, p160-161)

Now $-\Delta + V(r)$ acting on L_l is

$$-\Delta + V(r) = -\frac{d^2}{dr^2} - \frac{n-1}{r} \frac{d}{dr} + V(r) - \frac{k_l}{r^2} \quad (2.17)$$

where k_l is the corresponding l th eigenvalue of the Laplace-Beltrami operator on K_l , and it is enough to show that the right side of (2.17) is e.s.a in $L^2(\mathbb{R}_+, r^{n-1} dr)$ on $C_0^\infty(\mathbb{R}_+)$ (**Exercise** why?)

But this operator is unitarily equivalent to

$$h_l = -\frac{d^2}{dr^2} - \frac{(n-1)(n-3)}{4r^2} + V(r) - \frac{k_l}{r^2}$$

in $L^2(\mathbb{R}_+, dr)$ on $C_0^\infty(\mathbb{R}_+)$ (**Exercise** why?) In other words, the problem is reduced to show that the 1-dim Schrodinger operator h_l are e.s.a. on $C_0^\infty(\mathbb{R}_+)$, a problem amenable to limit point/limit circle theory. This completes the proof of this theorem. \square

Remark 95. In the above considerations we always took Dirichlet Boundary conditions at 0. We could equally have taken general Robin boundary conditions at 0, i.e.

$$\sin \alpha y(0, \lambda) + \cos \alpha y'(0, \lambda) = 0$$

for any $0 \leq \alpha < \pi$ and then everything goes through as before (see Coddington and Levinson Chap 9).

We will do limit piont case below. We will show in the limit point case, we still have

$$\int_0^\infty |y_1 + m_\infty y_2|^2 = \frac{\text{Im} m_\infty}{\text{Im} \lambda} \quad (2.18)$$

but this is a little more complicated to prove as y_1, y_2 are not both in $L^2(0, \infty)$.

In the limit circle case, we have too

$$\text{Im} \lambda \int_0^\infty |y_1 + m y_2|^2 dx = \text{Im} m$$

for any $m \in C_\infty$. Proof is similar.

Proof. (2.18) We have by Faton's Lemma, that the LHS in (2.18) is \leq RHS, but consider $h = \bar{h} \in C_0^\infty(0, \infty)$, $h(x) = 0$ for $x < 1$, $h(x) = 1$ for $x > 2$, then for $g_\varepsilon(x) = h(\frac{x}{\varepsilon})$,

$$g_\varepsilon \chi(x) = g_\varepsilon(y_1 + m_\infty y_2)(x)$$

lies in

$$D(H^*) = \{a \in L^2(0, \infty) : u, u' \text{ abs cont}, -u'' + V u \in L^2(0, \infty), y(0) = 0\}$$

As H is e.s.a on $C_0^\infty[0, \infty) \cap \{u(0) = 0\}$, H^* is symmetric and so

$$(g_\varepsilon \chi, H^*(g_\varepsilon \chi)) - (H^*(g_\varepsilon \chi), g_\varepsilon \chi) = 0$$

i.e.

$$\int_0^\infty \overline{g_\varepsilon \chi} [-(g_\varepsilon \chi)'' + V(g_\varepsilon \chi)] - \int_0^\infty \overline{-(g_\varepsilon \chi)'' + V \chi} g_\varepsilon g_\varepsilon \chi = 0$$

But $(g_\varepsilon \chi)'' = g_\varepsilon \chi'' + 2g'_\varepsilon \chi' + g''_\varepsilon \chi$. Thus

$$\begin{aligned} 0 &= \int \overline{g_\varepsilon \chi} [g_\varepsilon (-\chi'' + V \chi)] - [g_\varepsilon (-\bar{\chi}'' + V \bar{\chi}) \bar{g}_\varepsilon \chi] \\ &\quad + \int \overline{g_\varepsilon \chi} (-g''_\varepsilon \chi) - \int -\bar{g}''_\varepsilon \bar{\chi} g_\varepsilon \chi - 2 \int [\bar{g}_\varepsilon \bar{\chi} g'_\varepsilon \chi' - \bar{g}'_\varepsilon \bar{\chi}' g_\varepsilon \chi] \end{aligned}$$

i.e.

$$0 = \int g_\varepsilon^2 |\chi|^2 (\lambda - \bar{\lambda}) - 2 \int g_\varepsilon g'_\varepsilon (\bar{\chi} \chi' - \bar{\chi}' \chi) \quad (2.19)$$

Now $g'_\varepsilon = \frac{1}{\varepsilon} h'(\frac{x}{\varepsilon})$ is supported between ε and 2ε , and for $x < 2\varepsilon$,

$$\chi(x) = y_1 + m_\infty y_2 = 1 + o(\varepsilon)$$

$$\chi'(x) = y_1' + m_\infty y_2' = m_\infty + o(\varepsilon)$$

Thus

$$\begin{aligned} -2 \int g_\varepsilon g_\varepsilon' (\bar{\chi} \chi' - \bar{\chi}' \chi) &= -\frac{2}{\varepsilon} \int h\left(\frac{x}{\varepsilon}\right) h'\left(\frac{x}{\varepsilon}\right) [m_\infty - \bar{m}_\infty + o(\varepsilon)] dx \\ &= -\frac{2}{\varepsilon} \left[\int h\left(\frac{x}{\varepsilon}\right) h'\left(\frac{x}{\varepsilon}\right) dx (m_\infty - \bar{m}_\infty) \right] + o(1) \end{aligned}$$

as $\varepsilon \downarrow 0$. □

But $\frac{2}{\varepsilon} \int h\left(\frac{x}{\varepsilon}\right) h'\left(\frac{x}{\varepsilon}\right) dx = h^2(\infty) - h^2(0) = 1$. Thus it follows from (2.19) that as $\varepsilon \downarrow 0$

$$2\operatorname{Im}\lambda \int_0^\infty |\chi|^2 - 2\operatorname{Im}m_\infty = 0$$

i.e. $\int_0^\infty |\chi|^2 = \frac{\operatorname{Im}m_\infty}{\operatorname{Im}\lambda}$, as desired.

In the limit-point case the Green's function for $\bar{H} = \bar{H}^* = H$ for $H = C_0^\infty[0, \infty) \cap \{f(0) = 0\}$ is given by (same as (2.14), (2.15))

$$G(x, y) = \begin{cases} y_2(x)\chi(y) & x \leq y \\ \chi(x)y_2(y) & x > y \end{cases}$$

To show that $(\bar{H} - \lambda)^{-1}f(x) = \int_0^\infty G(x, y)f(y)dy \forall f \in L^2(0, \infty)$, first consider f with compact support on $[0, \infty)$. Then let

$$\begin{aligned} Tf(x) &\equiv \int_0^\infty G(x, y)f(y)dy \\ &= y_2(x) \int_x^\infty \chi(y)f(y)dy + \chi(x) \int_0^x y_2(y)f(y)dy \\ &= \chi(x) \int_0^\infty y_2(y)f(y)dy \end{aligned}$$

for x sufficiently large.

So $Tf \in L^2(0, \infty)$ as $\chi \in L^2(0, a)$, when $x \gg 1$. Note that if f is a general $f \in L^2(0, \infty)$, $Tf(x)$ exists $\forall x \geq 0$, but it is not clearly in $L^2(0, \infty)$. However, a direct calculation as before (see exercise 91) shows that $Tf \in D(\bar{H})$ and

$$(\bar{H} - \lambda)Tf = f \tag{2.20}$$

But as \bar{H} is s.adj and $\operatorname{Im}\lambda \neq 0$, and $(\bar{H} - \lambda)^{-1}$ exists as

$$\|(\bar{H} - \lambda)^{-1}\|_{L^2(0, \infty)} \leq \frac{1}{|\operatorname{Im}\lambda|}$$

applying $(\bar{H} - \lambda)^{-1}$ to (2.20), we find for f with compact support that $Tf = (\bar{H} - \lambda)^{-1}f$ and so $\|Tf\| \leq \frac{\|f\|}{\text{Im}\lambda}$.

Thus $Tf(x) = \int_0^\infty G(x, y)f(y)dy$ extends to a bounded operator, in fact $T = (\bar{H} - \lambda)^{-1}$, for all $f \in L^2(0, \infty)$ by Fatou's Lemma.

3 Spectral Theory

We now begin the explicit construction of the unitary map that transforms $\bar{H} = \bar{H}^*$ into a multiplication operator.

Again we assume for simplicity that $V(x)$ is real valued and continuous on $[0, \infty)$. Fix $0 \leq \beta < \pi$, then for any $b > 0$ the operator H_b with domain $D_b = \{u \in L^2(0, b) : u, u' \text{ abs cont, } u'' \in L^2, u(0) = 0, \cos \beta y(b) + \sin \beta y'(b) = 0\}$ is s.adj. Moreover as we showed earlier (see min-max) H_b pure point spectrum with eigenvalues $\mu_1^b < \mu_2^b < \dots < \mu_k^b \rightarrow \infty$ as $k \rightarrow \infty$, with associated normalized eigenvectors,

$$\begin{aligned} H_b y_k^b &= \mu_k^b y_k^b \\ y_k^b(0) &= 0 \\ \cos \beta y_k^b(b) + \sin \beta y_k^{b'}(b) &= 0 \\ \int_0^b \left(y_k^b(x)\right)^2 dx &= 1 \end{aligned}$$

The eigenvalues are indeed simple, for if

$$H_b f = \mu f \quad H_b g = \mu g$$

then we can choose γ so that $h \equiv f + \gamma g$ satisfies $h(0) = 0$ and $h'(0) = 0$ and so $h(x) \equiv 0$, as H_b is 2nd order and so f, g are proportional.

If $y_2(x, \lambda)$ is the standard solution of $H y_2 = \lambda y_2$, $y_2(0, \lambda) = 0$, $y_2'(0, \lambda) = 1$, then up to a constant multiple,

$$y_k^b(x) = y_2(x, \mu_k^b) \tag{3.1}$$

$k = 1, 2, \dots$. As the set $\{y_2(x, \mu_k^b)\}$ is a complete orthonormal set, it follows that for any $f \in L^2(0, b)$

$$\int_0^b |f(t)|^2 dt = \sum_{k=1}^{\infty} \frac{|\hat{f}(\mu_k^b)|^2}{\int_0^b y_2^2(x, \mu_k^b) dx} = \int_{-\infty}^{\infty} |\hat{f}(\lambda)|^2 d\rho_b(\lambda) \tag{3.2}$$

where $\hat{f}(\lambda) = \int_0^b y_2(x, \lambda) f(x) dx$, and $d\rho_b(\lambda) = \sum_{k=1}^{\infty} \frac{\delta(\lambda - \mu_k^b)}{\int_0^b y_2^2(x, \mu_k^b) dx}$.

Here

$$\rho_b(\lambda) = \int_{-\infty}^{\lambda} d\rho_b(s) = \int_{-\infty}^{\infty} \chi_{(-\infty, \lambda]}(s) d\rho_b(s) \quad (3.3)$$

is the *spectral function* for the problem. Note that $\rho_b(\lambda)$ is non-decreasing and is continuous from the right.

3.1 Spectral Theory (Limit-Point Case)

We will first consider the limit point case for V , then we will prove the following result for limit circle case later. The proof will take 3 lectures.

Theorem 96. *Suppose $V(x)$ is limit point at ∞ . Then*

(i) $\exists \rho(x) \uparrow$ on $(-\infty, \infty)$ s.t.

$$\rho(\lambda) - \rho(\mu) = \lim_{b \rightarrow \infty} \rho_b(\lambda) - \rho_b(\mu)$$

at points of continuity λ, μ of ρ , and ρ_b is defined in (3.3).

(ii) If $f \in L^2(0, \infty)$, then

$$\hat{f}(\lambda) = l.i.m. \int_0^b y_2(x, \lambda) f(x) dx$$

exists, i.e. as $b \rightarrow \infty$,

$$\int_0^b y_2(x, \lambda) f(x) dx$$

converges in $L^2(\rho(d\lambda))$, and

$$\int_0^{\infty} |f(t)|^2 dt = \int_{-\infty}^{\infty} |\hat{f}(\lambda)|^2 d\rho(\lambda) \quad (3.4)$$

(iii) If $g(\lambda) \in L^2(d\rho(\lambda))$, then

$$\check{g}(x) = l.i.m. \int_{\lambda=-\infty}^{\infty} y_2(x, \lambda) g(\lambda) d\rho(\lambda)$$

exists, i.e. as $n \rightarrow \infty$

$$\int_{-n}^n y_2(x, \lambda) g(\lambda) d\rho(\lambda)$$

converges in $L^2(0, \infty)$.

Moreover

$$\left(\hat{f}\right)^\vee = f \quad (\check{g})^\wedge = g$$

thus $f \rightarrow \hat{f}$ is onto, providing an isometry, $L^2(0, \infty) \rightarrow L^2(d\rho)$.

(iv)

$$(\bar{H}f)^\wedge(\lambda) = \lambda \hat{f}(\lambda)$$

for $f \in D(\bar{H}) = D(H^*)$.

(v) If $m_\infty(\lambda)$ is the limit point, $\lambda \in \mathbb{C} \setminus \mathbb{R}$, then

$$\rho(\lambda) - \rho(\mu) = \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_\mu^\lambda \text{Im} m_\infty(\nu + i\varepsilon) d\nu \quad (3.5)$$

at points of continuity λ, μ of ρ and conversely

$$m_\infty(z) - m_\infty(z_0) = \int_{-\infty}^\infty \left(\frac{1}{\nu - z} - \frac{1}{\nu - z_0} \right) d\rho(\nu)$$

for $z, z_0 \in \mathbb{C} \setminus \mathbb{R}$.

3.2 Proof (i) of Spectral Theory

Proof. Fix z s.t. $\text{Im} z \neq 0$, apply (3.2) to $\chi_b(x) = y_1(x, z) + m_b y_2(x, z)$, choose $m_b \in C_b$ to get

$$\int_0^b |\chi_b(x)|^2 dx = \int |\hat{\chi}_b(\lambda)|^2 d\rho_b(\lambda)$$

where

$$\begin{aligned} \hat{\chi}_b(\lambda) &= \int_0^b (y_1 + m_b y_2) y_2(x, \lambda) dx \\ &= \int_0^b \chi_b(x, z) y_2(x, \lambda) dx \\ &= \frac{1}{z - \lambda} ([\chi_b y_2](b) - [\chi_b y_2](0)) \end{aligned}$$

Now for $\lambda = \mu_k^b$, both $\chi_b(x, z)$ and $y_2(x, \mu_k^b)$ satisfy the boundary condition at $x = b$ by (3.1) so $[\chi_b y_2](b) = 0$. On the other hand, $[\chi_b y_2](0) = \chi_b y_2' - \chi_b' y_2 = 1$. Thus

$$\int_0^b |\chi_b(x)|^2 dx = \int_{-\infty}^\infty \frac{d\rho_b(\lambda)}{|z - \lambda|^2}, \quad \text{Im} z \neq 0 \quad (3.6)$$

Now fix $z = i$. In particular $C_b(i) \subset C_1(i)$ for $b \geq 1$ and hence $\exists K < \infty$ s.t.

$$\int \frac{d\rho_b(\lambda)}{1+\lambda^2} \leq K \quad \forall b \geq 1$$

i.e. the measure $\frac{d\rho_b(\lambda)}{1+\lambda^2}$ are uniformly bounded. It follows by weak compactness (the *Helly's selection principle* in this case), that $\exists b_n \rightarrow \infty$ and a finite measure $\frac{d\rho(\lambda)}{1+\lambda^2}$ such that $\int \frac{d\rho(\lambda)}{1+\lambda^2} \leq K$ and

$$\int s(\lambda) \frac{d\rho_{b_n}(\lambda)}{1+\lambda^2} \rightarrow \int s(\lambda) \frac{d\rho(\lambda)}{1+\lambda^2}$$

for all functions $s(\lambda)$ of compact support.

If $\lambda < \mu$ are points of continuity of $d\rho(\lambda)$, set

$$f_m(\nu) \equiv (1+\nu^2)s_m(\nu)$$

$$\tilde{f}_m(\nu) \equiv (1+\nu^2)\tilde{s}_m(\nu)$$

where

$$s_m = \begin{cases} 0 & x < \lambda - \frac{1}{m} \\ 1 & \lambda < x < \mu \\ 0 & x > \mu + \frac{1}{m} \end{cases}$$

and s_m is straight line connecting 0 and 1 for $\lambda - \frac{1}{m} < x < \lambda$, $\mu < x < \mu + \frac{1}{m}$.

$$\tilde{s}_m = \begin{cases} 0 & x < \lambda \\ 1 & \lambda + \frac{1}{m} < x < \mu - \frac{1}{m} \\ 0 & x > \mu \end{cases}$$

and \tilde{s}_m is straight line connecting 0 and 1 for $\lambda < x < \lambda + \frac{1}{m}$, $\mu - \frac{1}{m} < x < \mu$. Then for any m ,

$$\int \tilde{s}_m d\rho_{b_n}(\nu) \leq \rho_{b_n}(\mu) - \rho_{b_n}(\lambda) \leq \int s_m d\rho_{b_n}(\nu)$$

and so

$$\begin{aligned} \int \tilde{f}_m \frac{d\rho(\nu)}{1+\nu^2} &\leq \lim_n (\rho_{b_n}(\mu) - \rho_{b_n}(\lambda)) \\ &\leq \overline{\lim}_n (\rho_{b_n}(\mu) - \rho_{b_n}(\lambda)) \\ &\leq \int \tilde{f}_m \frac{d\rho(\nu)}{1+\nu^2} \end{aligned}$$

But if λ, μ are points of continuity of $d\rho$, then for any $\varepsilon > 0$,

$$\int \left(f_m - \tilde{f}_m \right) \frac{d\rho(\nu)}{1 + \nu^2} < \varepsilon$$

for m sufficiently large. It follows that

$$\lim_{n \rightarrow \infty} \rho_{b_n}(\mu) - \rho_{b_n}(\lambda)$$

exists, and it equals

$$\lim_{m \rightarrow \infty} \int s_m(\nu) d\rho(\nu) = \rho(\mu) - \rho(\lambda)$$

Also if $\text{Im} z \neq 0, z \neq i$

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$$\begin{aligned} I_n &\equiv \int \left(\frac{1}{|\lambda - i|^2} - \frac{1}{|\lambda - z|^2} \right) d\rho_{b_n}(\lambda) \\ &= \int \frac{\lambda^2 + |z|^2 - 2\lambda \text{Re} z - \lambda^2 - 1}{|\lambda - z|^2} \frac{d\rho_{b_n}(\lambda)}{1 + \lambda^2} \\ &= \int \frac{(|z|^2 - 1) - 2\lambda \text{Re} z}{|\lambda - z|^2} \frac{d\rho_{b_n}(\lambda)}{1 + \lambda^2} \\ &= \int h_m(\lambda) \frac{(|z|^2 - 1) - 2\lambda \text{Re} z}{|\lambda - z|^2} \frac{d\rho_{b_n}(\lambda)}{1 + \lambda^2} \\ &\quad + \int (1 - h_m(\lambda)) \frac{(|z|^2 - 1) - 2\lambda \text{Re} z}{|\lambda - z|^2} \frac{d\rho_{b_n}(\lambda)}{1 + \lambda^2} \end{aligned}$$

where h_m is any continuous function of compact support with $h_m(\lambda) = 1$ for $-m < \lambda < m$. As $\frac{(|z|^2 - 1) - 2\lambda \text{Re} z}{|\lambda - z|^2} \rightarrow 0$ as $\lambda \rightarrow \infty$. The second term can be made arbitrary small, uniformly in n by choosing m sufficiently large. On the other hand, the first term converges to

$$\int h_m(\lambda) \frac{(|z|^2 - 1) - 2\lambda \text{Re} z}{|\lambda - z|^2} \frac{d\rho(\lambda)}{1 + \lambda^2}$$

as $n \rightarrow \infty$. Thus

$$\begin{aligned} \int h_m(\lambda) \frac{(|z|^2 - 1) - 2\lambda \text{Re} z}{|\lambda - z|^2} \frac{d\rho(\lambda)}{1 + \lambda^2} - \varepsilon_m &\leq \liminf_n I_n \\ &\leq \overline{\lim}_n I_n \\ &\leq \int h_m(\lambda) \frac{(|z|^2 - 1) - 2\lambda \text{Re} z}{|\lambda - z|^2} \frac{d\rho(\lambda)}{1 + \lambda^2} + \varepsilon_m \end{aligned}$$

where $\varepsilon_m \rightarrow 0$ as $m \rightarrow \infty$. But then arguing as above

$$\int h_m \frac{(|z|^2 - 1) - 2\lambda \operatorname{Re} z}{|\lambda - z|^2} \frac{d\rho(\lambda)}{1 + \lambda^2} = \int \left(\frac{1}{|\lambda - i|^2} - \frac{1}{|\lambda - z|^2} \right) d\rho(\lambda) + \varepsilon'_m$$

where $\varepsilon'_m \rightarrow 0$ as $m \rightarrow \infty$. We conclude that $\lim_{n \rightarrow \infty} I_n$ exists and is equal to

$$\int \left(\frac{1}{|\lambda - i|^2} - \frac{1}{|\lambda - z|^2} \right) d\rho(\lambda) \quad (3.7)$$

But

$$\begin{aligned} I_n &= \int \left(\frac{1}{|\lambda - i|^2} - \frac{1}{|\lambda - z|^2} \right) d\rho_{b_n}(\lambda) \\ &= \int_0^{b_n} |\chi_{b_n}(x, i)|^2 dx - \int_0^{b_n} |\chi_{b_n}(x, z)|^2 dx \text{ by (3.6)} \\ &= \operatorname{Imm}_{b_n}(i) - \frac{\operatorname{Imm}_{b_n}(z)}{\operatorname{Im} z} \text{ by (2.18)} \\ &\rightarrow \operatorname{Imm}_\infty(i) - \frac{\operatorname{Imm}_\infty(z)}{\operatorname{Im} z} \text{ as } n \rightarrow \infty \end{aligned}$$

It follows from (3.7) that

$$\int \frac{1}{|\lambda - z|^2} d\rho(\lambda) = \frac{\operatorname{Imm}_\infty(z)}{\operatorname{Im} z} + c \quad (3.8)$$

where c is a real constant. (**Exercise**) A more detailed analysis shows that in fact $c = 0$.

Anyways, we see that equation (3.8) determines $d\rho(\lambda)$ uniquely, independent of the sequence $b_n \rightarrow \infty$. For if

$$\int \frac{1}{|\lambda - z|^2} d\tilde{\rho}(\lambda) = \frac{\operatorname{Imm}_\infty(z)}{\operatorname{Im} z} + \tilde{c}$$

for some other measure $d\tilde{\rho}(\lambda)$, $\int \frac{1}{|\lambda - z|^2} d\tilde{\rho}(\lambda) < \infty$, then

$$\int \frac{1}{|\lambda - z|^2} d\tilde{\rho}(\lambda) = \int \frac{1}{|\lambda - z|^2} d\rho(\lambda) + \tilde{c} - c$$

setting $z = i\gamma$ and letting $\gamma \rightarrow \infty$, γ real, we see by *dominated convergence* that $0 = 0 + \tilde{c} - c$. i.e. $\tilde{c} = c$.

This establishes (i) □

3.3 Proof (v) of Spectral Theory

Before we prove part (v), we need the following claim.

Claim 97. $m_\infty(\lambda)$ is analytic in \mathbb{C}_+ and in \mathbb{C}_- .

Proof. (prove claim) To see this, note that for fixed x , $y_1(x, \lambda)$ and $y_2(x, \lambda)$ are entire functions of λ . Indeed y_1, y_2 satisfy

$$y_1(x, \lambda) = \cos \sqrt{\lambda}x + \int_0^x \frac{\sin \sqrt{\lambda}(x-t)}{\sqrt{\lambda}} V(t) y_1(t, \lambda) dt$$

$$y_2(x, \lambda) = \frac{\sin \sqrt{\lambda}x}{\sqrt{\lambda}} + \int_0^x \frac{\sin \sqrt{\lambda}(x-t)}{\sqrt{\lambda}} V(t) y_2(t, \lambda) dt$$

These equations are solved by iteration e.g.

$$y_1^{(0)} = \cos \sqrt{\lambda}x$$

$$y_1^{(k)} = \cos \sqrt{\lambda}x + \int_0^x \frac{\sin \sqrt{\lambda}(x-t)}{\sqrt{\lambda}} V(t) y_1^{(k-1)}(t, \lambda) dt, \quad k \geq 1$$

Each $y_1^{(k)}(x, \lambda)$ is easily seen to be analytic and $y_1^{(k)}(x, \lambda) \rightarrow y_1(x, \lambda)$ uniformly for λ in compact sets, x fixed etc.

Also for any $\beta \in [0, \pi)$, $\cos \beta y_2(b, \lambda) + \sin \beta y_2'(b, \lambda)$ cannot vanish in $\mathbb{C} \setminus \mathbb{R}$. Otherwise the s.adj operator $H_b = -d^2/dx^2 + V(x)$, $D(H_b) = \{u \in L^2(0, b) : u'(0) = 0, \cos \beta u(b) + \sin \beta u'(b) = 0\}$ would have a non-real eigenvalue. It follows from (2.8),

$$m_b(\lambda) = -\frac{\cot \beta y_1(b, \lambda) + y_1'(b, \lambda)}{\cot \beta y_2(b, \lambda) + y_2'(b, \lambda)}$$

is analytic in $\mathbb{C} \setminus \mathbb{R}$ for any $\beta \in [0, \pi)$. Now from (2.11), (2.12), the radius of the circle C_b is given by

$$r_b = \frac{1}{|[y_2 y_2](b)|}$$

where $[y_2 y_2] = 2 |\operatorname{Im} \lambda| \int_0^b |y_2|^2 dx$ for $\operatorname{Im} \lambda \neq 0$. Also (**Exercise**) the center \tilde{m}_b of the circle is given by

$$\tilde{m}_b = -\frac{[y_1 y_2](b)}{[y_2 y_2](b)}.$$

In particular $r_b = r_b(\lambda)$ and $\tilde{m}_b = \tilde{m}_b(\lambda)$ are continuous in \mathbb{C}_+ and \mathbb{C}_- and it follows then in particular for $b = 1$, that if λ lies in a compact subset K of \mathbb{C}_+ or \mathbb{C}_- , that

$$L = \bigcup_{\lambda \in K} \{m : m \in \text{closed disk with center } \tilde{m}_b(\lambda) \text{ and radius } r_b(\lambda)\}$$

is a compact set. As $C_b(\lambda) \subset C_1(\lambda)$ for any $b \geq 1$, $\lambda \in \mathbb{C} \setminus \mathbb{R}$. It follows that, for any fixed β , $m_b(\lambda)$ is bounded in K , uniformly for $b \geq 1$. By *Vitali's theorem*, it follows that $m_\infty(\lambda) = \lim_{b \rightarrow \infty} m_b(\lambda)$ is analytic in K . This proves the claim. \square

We now prove (v) of spectral theory.

Proof. From (3.8), as $\text{Im} \frac{1}{\lambda - z} = \frac{\text{Im} z}{|\lambda - z|^2}$, we have for $\text{Im} z \neq 0$,

$$c \text{Im} z + \text{Im} m_\infty(z) = \int \text{Im} \frac{1}{\lambda - z} d\rho(\lambda) \quad (3.9)$$

Now fix $z_0 \in \mathbb{C} \setminus \mathbb{R}$, then

$$\begin{aligned} c \text{Im}(z - z_0) + \text{Im}(m_\infty(z) - m_\infty(z_0)) &= \int \text{Im} \left(\frac{1}{\lambda - z} - \frac{1}{\lambda - z_0} \right) d\rho(\lambda) \\ &= \text{Im} \int \left(\frac{1}{\lambda - z} - \frac{1}{\lambda - z_0} \right) d\rho(\lambda) \end{aligned}$$

Hence by the analyticity of $m_\infty(z)$ in $\mathbb{C} \setminus \mathbb{R}$ we have

$$m_\infty(z) = m_\infty(z_0) + \int \left(\frac{1}{\lambda - z} - \frac{1}{\lambda - z_0} \right) d\rho(\lambda) - c(z - z_0) + c_\pm \quad (3.10)$$

for $z \in \mathbb{C}_+$ or \mathbb{C}_- . (**Exercise** check $\int \left(\frac{1}{\lambda - z} - \frac{1}{\lambda - z_0} \right) d\rho(\lambda)$ is integrable.)

Now for $z \in \mathbb{C}_+$, if z_0 is also in \mathbb{C}_+ , we may set $z = z_0$ in (3.10) and the corresponding constant $c_+ = 0$. On the other hand if $z_0 \in \mathbb{C}_-$, then from (3.9), we have

$$c \frac{z_0 - \bar{z}_0}{2i} + \frac{m_\infty(z_0) - \overline{m_\infty(z_0)}}{2i} = \frac{1}{2i} \int \left(\frac{1}{\lambda - z_0} - \frac{1}{\lambda - \bar{z}_0} \right) d\rho(\lambda)$$

and substituting this relation in to (3.10), we have for $z \in \mathbb{C}_+$

$$\begin{aligned} m_\infty(z) &= \overline{m_\infty(z_0)} - c(z_0 - \bar{z}_0) + \int \left(\frac{1}{\lambda - z_0} - \frac{1}{\lambda - \bar{z}_0} \right) d\rho(\nu) \\ &\quad + \int \left(\frac{1}{\lambda - z} - \frac{1}{\lambda - z_0} \right) d\rho(\lambda) - c(z_0 - z) + c_+ \end{aligned}$$

so that

$$m_\infty(z) = \overline{m_\infty(z_0)} - c(z - \bar{z}_0) + \int \left(\frac{1}{\lambda - z} - \frac{1}{\lambda - \bar{z}_0} \right) d\rho(\lambda) + c_+ \quad (3.11)$$

Now for $\lambda \in \mathbb{C} \setminus \mathbb{R}$

$$\chi(x, \lambda) = y_1(x, \lambda) + m_\infty(\lambda)y_2(x, \lambda)$$

so

$$\overline{\chi(x, \bar{\lambda})} = \overline{y_1(x, \bar{\lambda})} + \overline{m_\infty(\bar{\lambda})y_2(x, \bar{\lambda})}$$

But (**Exercise**)

$$\overline{y_j(x, \bar{\lambda})} = y_j(x, \lambda), \quad j = 1, 2$$

and so

$$\overline{\chi(x, \bar{\lambda})} = y_1(x, \lambda) + \overline{m_\infty(\bar{\lambda})}y_2(x, \lambda)$$

from which we see that $\overline{\chi(x, \bar{\lambda})}$ is a solution of $Hf = \lambda f$ such that $\overline{\chi(x, \bar{\lambda})} \in L^2(\infty)$. Hence

$$\overline{m_\infty(\bar{\lambda})} = m_\infty(\lambda)$$

Inserting this relation in (3.11), we find

$$m_\infty(z) = m_\infty(\bar{z}_0) - c(z - \bar{z}_0) + \int \left(\frac{1}{\lambda - z} - \frac{1}{\lambda - \bar{z}_0} \right) d\rho(\lambda) + c_+$$

Now $\bar{z}_0 \in \mathbb{C}_+$ and we may take $z = \bar{z}_0$ to conclude again that $c_+ = 0$. Thus interchanging $z \in \mathbb{C}_+$ with $z \in \mathbb{C}_-$, we then see that

$$m_\infty(z) = m_\infty(z_0) + \int \left(\frac{1}{\lambda - z} - \frac{1}{\lambda - z_0} \right) d\rho(\lambda) - c(z - z_0)$$

for all $z, z_0 \in \mathbb{C} \setminus \mathbb{R}$. This proves part of (v), (provided we show $c = 0$ as in the exercise in the proof of part (i))

Conversely for $\mu < \lambda$ points of continuity for $d\rho(\nu)$ by (3.9)

$$\begin{aligned} \lim_{\varepsilon \downarrow 0} \int_\mu^\lambda \operatorname{Im} m_\infty(\nu + i\varepsilon) d\nu &= \lim_{\varepsilon \downarrow 0} \int_\mu^\lambda d\nu \left(\int_{-\infty}^\infty \frac{\varepsilon}{(\sigma - \nu)^2 + \varepsilon^2} d\rho(\sigma) - c\varepsilon \right) \\ &= \lim_{\varepsilon \downarrow 0} \int_{-\infty}^\infty d\rho(\sigma) \left[\arctan \frac{\lambda - \sigma}{\varepsilon} - \arctan \frac{\mu - \sigma}{\varepsilon} \right] \\ &= \pi (\rho(\lambda) - \rho(\mu)) \end{aligned}$$

(**Exercise** check that we can take the $\lim_{\varepsilon \downarrow 0}$ inside the integral)

Thus (v) is established. \square

3.4 Proof (ii) of Spectral Theory

Proof. We now prove (ii). Suppose $f \in C_0^\infty(0, \infty)$. Then for b large enough s.t. $\text{supp} f \subset (0, b)$, and for any $\mu > 0$

$$\begin{aligned}
\int_{|\nu| \geq \mu} |\hat{f}(\nu)|^2 d\rho_b(\nu) &\leq \frac{1}{\mu^2} \int_{|\nu| \geq \mu} \nu^2 |\hat{f}(\nu)|^2 d\rho_b(\nu) \\
&= \frac{1}{\mu^2} \int_{|\nu| \geq \mu} |\widehat{Hf}(\nu)|^2 d\rho_b(\nu) \\
&\leq \frac{1}{\mu^2} \int_{-\infty}^{\infty} |\widehat{Hf}(\nu)|^2 d\rho_b(\nu) \\
&= \frac{1}{\mu^2} \int_0^b |Hf|^2 dx \text{ by (3.2)} \\
&= \frac{1}{\mu^2} \int_0^\infty |Hf|^2 dx
\end{aligned}$$

Thus

$$\begin{aligned}
\left| \int_0^\infty |f(t)|^2 dt - \int_{-\mu}^\mu |\hat{f}(\lambda)|^2 d\rho_b(\lambda) \right| &\leq \int_{|\nu| \geq \mu} |\hat{f}(\nu)|^2 d\rho_b(\nu) \\
&\leq \frac{1}{\mu^2} \int_0^\infty |Hf|^2 dx
\end{aligned}$$

Letting $b \rightarrow \infty$, if $-\mu, \mu$ are points of continuity of $d\rho(\lambda)$, we get

$$\left| \int_0^\infty |f(t)|^2 dt - \int_{-\mu}^\mu |\hat{f}(\lambda)|^2 d\rho(\lambda) \right| \leq \frac{1}{\mu^2} \int_0^\infty |Hf|^2 dx$$

letting $\mu \rightarrow \infty$ s.t. $-\mu, \mu$ are points of continuity of $d\rho$, we obtain for any $f \in C_0^\infty(0, \infty)$,

$$\int_0^\infty |f(t)|^2 dt = \int_{-\infty}^\infty |\hat{f}(\lambda)|^2 d\rho(\lambda) \quad (3.12)$$

Now we use a standard argument to show that (3.12) holds for any $f \in L^2(0, \infty)$, where $\hat{f}(\lambda) = \text{l.i.m.} \int f(x)y_2(x, \lambda)dx$. We first suppose $f \in L^2(0, \infty)$ and vanishes for large t . Then we can approximate $f \in L^2(0, \infty)$ by $C_0^\infty(0, \infty)$ functions and (3.12) follows. But then for any $f \in L^2(0, \infty)$, set $f_a(t) = f(t)$ for $0 \leq t < a$, and $f_a(t) = 0$ for $t > a$. Then (3.12) holds for f_a and in fact for $a < d$

$$\int_a^d |f(t)|^2 dt = \int_{-\infty}^\infty |f_d(t) - f_a(t)|^2 dt = \int |\hat{f}_d(t) - \hat{f}_a(t)|^2 d\rho(\lambda)$$

and as $\int_a^d |f(t)|^2 dt \rightarrow 0$ as $d > a \rightarrow \infty$, it follows that $\{\hat{f}_a\}$ coverages l.i.m. to $\hat{f}(\lambda)$ on $d\rho(\lambda)$ and norms are preserved. Thus (ii) is proved. \square

3.5 Proof (iv) of Spectral Theory

Proof. To prove (iv), suppose $f \in C_0^\infty[0, \infty) \cap \{f(0) = 0\}$. As noted earlier, this is a domain of s.adjointness for H . Then for such f ,

$$\widehat{Hf}(\lambda) = \int_0^\infty y_2(x, \lambda) Hf = \int_0^\infty (Hy_2)f = \lambda \hat{f}(\lambda) \quad (3.13)$$

Now if $f \in D(H)$, $\exists f_n \in C_0^\infty[0, \infty) \cap \{f(0) = 0\}$ s.t.

$$f_n \rightarrow f \text{ in } L^2(0, \infty)$$

$$Hf_n \rightarrow Hf \text{ in } L^2(0, a)$$

In particular, as $f \rightarrow \hat{f}$ is an isometry by (ii)

$$\hat{f}_n \rightarrow \hat{f} \text{ in } L^2(0, \infty)$$

$$\widehat{Hf}_n \rightarrow \widehat{Hf} \text{ in } L^2(0, a)$$

but $\widehat{Hf}_n(\lambda) = \lambda \hat{f}_n(\lambda)$ by (3.13). Choosing a subsequence, we conclude that

$$\widehat{Hf}(\lambda) = \lim_{n \rightarrow \infty} \lambda \hat{f}_n(\lambda) \quad d\rho(\lambda) \text{ a.e.}$$

choosing a further subsequence if necessary, we then have

$$\hat{f}_n(\lambda) \rightarrow \hat{f}(\lambda)$$

and so $\widehat{Hf}(\lambda) = \lambda \hat{f}(\lambda) \quad d\rho(\lambda) \text{ a.e.}$

This proves (iv). □

3.6 Proof (iii) of Spectral Theory

As a preliminary to proving (iii), we prove the *expansion theorem*.

Theorem 98. (*expansion thm*)

$$f(x) = l.i.m. \int \hat{f}(\lambda) y_2(x, \lambda) d\rho(\lambda)$$

for any $f(x) \in L^2(0, \infty)$.

Proof. For $\Delta = (\mu, \lambda]$, set

$$f_{\Delta}(x) \equiv \int_{\Delta} \hat{f}(\lambda) y_2(x, \nu) d\rho(\nu)$$

which exists as $y_2(x, \cdot) \in L^2(\Delta, d\rho)$ for fixed x . By polarization

$$\int f_1 \bar{f}_2 dt = \int \hat{f}_1 \bar{\hat{f}}_2 d\rho(\lambda), \quad f_1, f_2 \in L^2(0, \infty) \quad (3.14)$$

Also for $p \in L^2(0, \infty)$, $p(t) \equiv 0$ for $t \geq a > 0$.

$$\begin{aligned} \int_0^a f_{\Delta}(t) \bar{p}(t) dt &= \int_{\Delta} d\rho(\lambda) \hat{f}(\lambda) \left(\int_0^a \bar{p}(t) y_2(t, \lambda) dt \right) \\ &= \int_{\Delta} \hat{f}(\lambda) \bar{\hat{p}}(\lambda) d\rho(\lambda) \end{aligned} \quad (3.15)$$

Setting $f_1 = f$, $f_2 = p$ in (3.14) and using (3.16), we obtain

$$\int (f - f_{\Delta})(t) \bar{p}(t) dt = \int_{\lambda \notin \Delta} \hat{f}(\lambda) \bar{\hat{p}}(\lambda) d\rho(\lambda)$$

and so by the Schwartz inequality

$$\left| \int (f - f_{\Delta})(t) \bar{p}(t) dt \right|^2 \leq \int_{\lambda \notin \Delta} |\hat{f}(\lambda)|^2 d\rho(\lambda) \cdot \int_{\lambda \notin \Delta} |\hat{p}(\lambda)|^2 d\rho(\lambda)$$

setting $p(t) = \begin{cases} (f - f_{\Delta})(t) & t < a \\ 0 & t \geq a \end{cases}$, we have

$$\begin{aligned} \left(\int_0^a |f - f_{\Delta}|^2 dt \right)^2 &\leq \left(\int_{\lambda \notin \Delta} |\hat{f}(\lambda)|^2 d\rho(\lambda) \right) \int |\widehat{f - f_{\Delta}}|^2(\lambda) d\rho(\lambda) \\ &= \int_{\lambda \notin \Delta} |\hat{f}(\lambda)|^2 d\rho(\lambda) \int_0^a |f - f_{\Delta}|^2 dt \end{aligned}$$

and so

$$\int_0^a |f - f_{\Delta}|^2 dt \leq \int_{\lambda \notin \Delta} |\hat{f}(\lambda)|^2 d\rho(\lambda)$$

As RHS is independent of a , we obtain

$$\int_0^{\infty} |f - f_{\Delta}|^2 dt \leq \int_{\lambda \notin \Delta} |\hat{f}(\lambda)|^2 d\rho(\lambda)$$

Letting $\Delta \rightarrow (-\infty, \infty)$, we have proved the expansion theorem □

Note 99. that en route we have proved that $f_\Delta \in L^2(0, \infty)$ for any Δ .

We also need the following fact.

Fact 100. Suppose $g \in L^2(d\rho)$, then

$$\check{g}(x) = l.i.m \int \hat{g}(\lambda) y_2(x, \lambda) d\rho(\lambda)$$

exists and the map $\hat{g} \mapsto \check{g}$ is bounded from $L^2(d\rho)$ to $L^2((0, \infty), dx)$.

Proof. Consider $\Delta_1 \supset \Delta_2$ and $p(x) \in L^2(0, \infty)$ with compact support. Interchanging the order of integration, we get as before in (3.16)

$$\int_0^\infty (f_{\Delta_1} - f_{\Delta_2}) \bar{p} = \int_{\Delta_1 \setminus \Delta_2} \hat{g}(\lambda) \bar{\hat{p}}(\lambda) d\rho(\lambda)$$

where $f_{\Delta_i}(t) = \int_{\Delta_i} \hat{g}(\lambda) y_2(t, \lambda) d\rho(\lambda)$.

Letting $p(t) = \begin{cases} (f_{\Delta_1} - f_{\Delta_2})(t) & t < a \\ 0 & t \geq a \end{cases}$, we obtain

$$\begin{aligned} \int_0^a |f_{\Delta_1} - f_{\Delta_2}|^2 dt &\leq \left(\int_{\Delta_1 \setminus \Delta_2} |\hat{g}(\lambda)|^2 d\rho(\lambda) \right)^{1/2} \left(\int |\hat{p}(\lambda)|^2 d\rho(\lambda) \right)^{1/2} \\ &= \left(\int_{\Delta_1 \setminus \Delta_2} |\hat{g}(\lambda)|^2 d\rho(\lambda) \right)^{1/2} \left(\int_0^a |f_{\Delta_1} - f_{\Delta_2}|^2 dt \right)^{1/2} \end{aligned}$$

i.e.

$$\left(\int_0^a |f_{\Delta_1} - f_{\Delta_2}|^2 dt \right)^{1/2} \leq \left(\int_{\mathbb{R} \setminus \Delta_2} |\hat{g}(\lambda)|^2 d\rho(\lambda) \right)^{1/2} \quad (3.16)$$

letting $a \rightarrow \infty$, we obtain

$$\int_0^\infty |f_{\Delta_1} - f_{\Delta_2}|^2 dt \leq \int_{\mathbb{R} \setminus \Delta_2} |\hat{g}(\lambda)|^2 d\rho(\lambda) \rightarrow 0$$

as $\Delta_1 \supset \Delta_2 \rightarrow (-\infty, \infty)$.

Setting $\Delta_2 = 0$ in (3.16) we have

$$\int_0^\infty |f_{\Delta_1}|^2 dt \leq \int_{\mathbb{R}} |\hat{g}(\lambda)|^2 d\rho(\lambda)$$

In particular $f_{\Delta_1} \in L^2(0, \infty)$, $\forall \Delta_1$ and letting $\Delta_1 \rightarrow (-\infty, \infty)$ and using the Cauchy property (3.15) we see that $\check{g}(x)$ exists as a l.i.m. and

$$\int_0^\infty |\check{g}(x)|^2 dx \leq \int |\hat{g}(\lambda)|^2$$

and $\hat{g} \mapsto \check{g}$ has norm ≤ 1 .

On the other hand, from the expansion theorem

$$(\hat{f})^\vee = f$$

i.e. $^\vee$ is the inverse of $^\wedge$ on the range of $^\wedge$. □

Now we are ready to prove (iii).

Proof. To prove that

$$(\check{g})^\wedge = g \tag{3.17}$$

and so complete the proof of (iii), we want to apply $^\vee$ to both sides of (3.17). it is clear that LHS is OK, because $(\check{g})^\wedge$ is in the range of $^\wedge$, so after applying $^\vee$, we got \check{g} .

Since $^\vee$ is 1-1 a.e., we only need to show RHS, g , is in the range of $^\wedge$, then we are done. So it is enough to show that $f \mapsto \hat{f}$ is onto. So suppose $f \mapsto \hat{f}$ is not onto. Then as $f \mapsto \hat{f}$ is an isometry, there must exist $\hat{g} \in L^2(d\rho)$ that has no corresponding g , then we have

$$\int \bar{\hat{g}}(\lambda) \hat{f}(\lambda) d\rho(\lambda) = 0 \quad \forall f \in L^2(0, \infty) \tag{3.18}$$

We want to show that $\hat{g}(\lambda) = 0$ on $d\rho$ a.e.

Fix $h(x) \in L^2(0, \infty)$ and set

$$f_z(x) = \frac{1}{\bar{H} - z} h \quad \text{Im} z \neq 0$$

Then $f_z \in D(\bar{H}) \subset L^2(0, \infty)$. As $(\bar{H} - z)f_z(x) = h$, we have by (iv)

$$(\lambda - z)\hat{f}_z(\lambda) = \hat{h}(\lambda)$$

i.e. $\hat{f}_z(\lambda) = \frac{\hat{h}(\lambda)}{\lambda - z}$. From 3.18, for such $\hat{f}_z(\lambda)$,

$$\int \bar{\hat{g}}(\lambda) \frac{\hat{h}(\lambda)}{\lambda - z} d\rho(\lambda) = 0, \quad \forall z \in \mathbb{C} \setminus \mathbb{R}.$$

It follows (**Exercise**) that

$$\bar{g}(\lambda)\hat{h}(\lambda) = 0 \quad \text{on } d\rho \text{ a.e.}$$

To conclude that $\hat{g}(\lambda) = 0$ on $d\rho$ a.e, set

$$h_n(x) = \begin{cases} n^2 & 0 < x < 1/n \\ 0 & x > 1/n \end{cases}$$

for $n = 1, 2, \dots$. Then as $y_2(x, \lambda) = x + O(x^2)$, as $x \rightarrow 0$.

$$\begin{aligned} \hat{h}_n(\lambda) &= n^2 \int_0^{1/n} y_2(x, \lambda) dx \\ &= n^2 \left(\frac{1}{2} \frac{1}{n^2} + O\left(\frac{1}{n^3}\right) \right) \\ &= \frac{1}{2} + O\left(\frac{1}{n}\right) \end{aligned}$$

Thus for each λ , $\hat{h}_n(\lambda) \rightarrow \frac{1}{2} \neq 0$. As $\bar{g}(\lambda)\hat{h}_n(\lambda) = 0$ for all n , this shows that $\hat{g}(\lambda) = 0$ as desired.

Hence (iii) is proved. This completes the proof of spectral theory. \square

Exercise 101. For $z \in \mathbb{C} \setminus \mathbb{R}$, show that

$$\hat{\chi}_z(\lambda) = \frac{1}{\lambda - z}$$

where $\chi_z(x) = \chi(x, z)$.

3.7 An Alternative Proof to Spectral Theory

For an alternative approach to the spectral theory of \bar{H} (theorem 96), see E.Titchmarsh, *Eigenfunction Expansions: Associated with Second-Order Differential Equations, Part I*.

Titchmarsh obtains eigenfunction expansions by integrating the

$$(\bar{H} - z)^{-1} f, \quad f \in L^2(\mathbb{R}_+)$$

where $(\bar{H} - z)^{-1}(x, y) = \begin{cases} y_2(x, z)\chi(y, z) & 0 \leq x < y \\ y_2(y, z)\chi(x, z) & y \leq x \end{cases}$ for $z \in \mathbb{C} \setminus \mathbb{R}$,

around upper and lower semi-circles in z plane. And letting $R \rightarrow \infty$, $\varepsilon \rightarrow 0$, where R is the radius of the semi-circles and ε is the vertical distance between the one straight edge of the semi-circles and the real axis.

Exercise 102. Follow through Titchmarsh approach for $V = 0$.

4 Spectral Theory (continued)

We now consider the case where $V(x)$ is a real valued continuous function on $[0, \infty)$ that is limit-circle at ∞ .

Example 103. An explicit example of such a $V(x)$ is given by

$$V(x) = -e^{2x}$$

One may check directly that for $\lambda \neq 0$ two independent solutions of $-y'' - e^{2x}y = \lambda y$ are given by $J_{is}(e^x)$ and $J_{-is}(e^x)$ where $s = \sqrt{\lambda}$ and $J_\nu(t)$ is a solution of Bessel's equation:

$$t^2 J_\nu''(t) + t J_\nu'(t) + (t^2 - \nu^2) J_\nu(t) = 0$$

As $t \rightarrow \infty$, we have (Abramowitz, Stegun, *Handbook of Mathematical Functions*, equation 9.2.1, page 364)

$$J_\nu(t) = \sqrt{\frac{2}{\pi t}} \cos\left(t - \frac{\nu\pi}{2} - \frac{\pi}{4}\right) + O\left(\frac{1}{t}\right)$$

and hence $J_{is}(e^x)$, $J_{-is}(e^x) = O(e^{-x/2}) \in L^2(0, \infty)$. Thus $V = -e^{2x}$ is limit-circle at ∞ .

4.1 Spectral Theory (Limit-Circle Case)

Suppose V is in the limit-circle case at ∞ . Again H denotes $-d^2/dx^2 + V(x)$ acting on $D(H) = C_0^\infty[0, \infty) \cap \{f(0) = 0\}$ (recall $C_0^\infty[0, \infty)$ means ∞ differentiable, compact support in $[0, \infty)$.) H is symmetric and $H^* = -d^2/dx^2 + V(x)$ with $D(H^*) = \{f \in L^2(0, \infty) : f, f \text{ abs cont, } -f'' + Vf \in L^2(0, \infty), f(0) = 0\}$.

Note that if $f, g \in D(H^*)$, then

$$[f, g](\infty) = \lim_{b \rightarrow \infty} (f\bar{g}' - f'\bar{g})(b)$$

exists and is finite. Indeed

$$\begin{aligned} 0 = (f, H^*g) - (H^*f, g) &= \lim_{b \rightarrow \infty} \int_0^b \bar{f} H^*g - \int_0^b \overline{H^*f} g \\ &= \lim_{b \rightarrow \infty} (\bar{f}'g - \bar{f}g')(b) - (\bar{f}'g - \bar{f}g')(0) \\ &= [gf](\infty) - [gf](0) \\ &= [gf](\infty) \end{aligned}$$

In particular $[u\chi_m](\infty) = 0$, $\chi_m = y_1 + my_2$, $m \in C_\infty$, $u \in D(H^*)$, as $g\chi_m \in D(H^*)$ for any $g \in C_0^\infty(0, \infty)$, $g(x) = 0$ for $0 < x < 1$; $g(x) = 1$ for $x > 2$.

Also if \tilde{H} is a s.adj extension of H , then $H \subset \tilde{H} \subset H^*$, so \tilde{H} is necessarily a restriction of H^* .

Theorem 104. *Fix $\lambda_0 \in \mathbb{C} \setminus \mathbb{R}$. The s.adj extension of H are in 1-1 correspondence with the points $m = m(\lambda_0)$ on the limit circle C_∞ . More precisely, if $m \in C_\infty = C_\infty(\lambda_0)$,*

$$H_m \equiv H^* \quad (4.1)$$

restricted on $D_m = D(H^) \cap \{u : [u\chi_m](\infty) = 0\}$, is a s.adj extension of H , where $\chi_m = \chi_m(x, \lambda_0) = y_1 + my_2$.*

Conversely, every self-adjoint extension of H is of the form H_m as in (4.1) for some unique $m \in C_\infty$.

4.2 Sketch of Proof of Spectral Theory

Reference of this proof see Coddington, Levinson P244-246.

Proof. Suppose $m \in C_\infty(\lambda_0)$. Construct the Green's function

$$G_{\lambda_0}(t, \tau) = \begin{cases} y_2(t, \lambda_0)\chi_m(\tau, \lambda_0) & 0 \leq t < \tau \\ \chi_m(t, \lambda_0)y_2(\tau, \lambda_0) & t > \tau \geq 0 \end{cases}$$

then $G_{\lambda_0}(t, \tau)$ is the kernel of a bounded map from $L^2(0, \infty)$ to $L^2(0, \infty)$. Indeed for $f \in L^2(0, \infty)$

$$(G_{\lambda_0}f)(t) = y_2(t) \int_t^\infty \chi_m(\tau) f(\tau) d\tau + \chi_m(t) \int_0^t y_2(\tau) f(\tau) d\tau$$

Hence by Minkowski inequality,

$$\begin{aligned} \int_0^\infty |(G_{\lambda_0}f)(t)|^2 dt &\leq 2 \int_0^\infty |y_2(t)|^2 \left(\int_0^\infty |\chi_m f| \right)^2 + 2 \int_0^\infty |\chi_m(t)|^2 \left| \int_0^\infty y_2 f \right|^2 \\ &\leq 4 \left(\int_0^\infty |y_2(t)|^2 \int_0^\infty |\chi_m(t)|^2 \right) \|f\|_{L^2}^2 \end{aligned} \quad (4.2)$$

Then a straight forward computation (see the reference) shows that if $f \in L^2(0, \infty)$, then $G_{\lambda_0}f \in D_m$ and $(H_m - \lambda_0)G_{\lambda_0}f = f$.

Conversely if $u \in D_m$, then $f \in (H_m - \lambda_0)u \in L^2(0, \infty)$ and $u = G_{\lambda_0}f$. Thus

$$(H_m - \lambda_0)G_{\lambda_0} = 1_{L^2(0, \infty)} \quad G_{\lambda_0}(H_m - \lambda_0) = 1_{D_m} \quad (4.3)$$

A further calculation using (4.3) shows that H_m is symmetric on D_m .

Also (4.3) shows that H_m is a closed operator on D_m . Indeed if $D_m \ni f_n \rightarrow f$, $Hf_n \rightarrow g$ then

$$f_n = G_{\lambda_0}(H_m - \lambda_0)f_n \implies f = G_{\lambda_0}(g - \lambda_0 f)$$

implies $f \in D_m$ and

$$(H_m - \lambda_0)f = (H_m - \lambda_0)G_{\lambda_0}(g - \lambda_0 f) = g - \lambda_0 f$$

and so $H_m f = g$. This shows H_m is closed. But from (4.3) for any $g \in L^2(0, \infty)$,

$$(H_m - \lambda_0)G_{\lambda_0}g = g$$

i.e. $(H_m - \lambda_0)h = g$, where $h = G_{\lambda_0}g$ and so $H_m - \lambda_0$ is surjective.

We now show that if $u \in D_m$, then $\bar{u} \in D_m$. Hence if $g \in L^2(0, \infty)$, $\exists h \in D_m$ s.t. $(H_m - \lambda_0)h = \bar{g}$. But then $\bar{h} \in D_m$ and as V is real, $(H_m - \bar{\lambda}_0)\bar{h} = g$, which shows that $H_m - \bar{\lambda}_0$ is also surjective. By general theory it follows that H_m is s.adj on D_m . Suppose $h \in D_m$, then $h = G_{\lambda_0}g$, where $g = (H_m - \lambda_0)f \in L^2$. Thus

$$h(t) = y_2(t) \int_t^\infty \chi(\tau)g(\tau) + \chi_m(t) \int_0^t y_2(\tau)g(\tau)$$

and

$$h'(t) = y_2'(t) \int_t^\infty \chi(\tau)g(\tau) + \chi_m'(t) \int_0^t y_2(\tau)g(\tau)$$

Now as $h \in D_m$, \bar{h}, \bar{h}' are absolute continuous $\bar{h}(0) = 0$ and $-\bar{h}'' + V\bar{h} = \overline{-h'' + Vh} \in L^2(0, \infty)$.

We now show that $[\bar{h}\chi_m](\infty)$ and hence $\bar{h} \in D_m$. But

$$\begin{aligned} [\bar{h}\chi_m](t) &= [\bar{y}_2\chi_m](t) \int_t^\infty \overline{\chi_m} \bar{g} d\tau + [\bar{\chi}_m\chi_m](t) \int_0^t \bar{y}_2 \bar{g} d\tau \\ &= [\bar{y}_2\chi_m](t) \int_t^\infty \overline{\chi_m} \bar{g} d\tau \end{aligned}$$

as $[\bar{\chi}_m\chi_m](t)$ is trivially zero. But as $\bar{y}_2 \in D(H^*)$, $[\bar{y}_2\chi_m](\infty)$ exists and is finite. It follows that $[\bar{h}\chi_m](\infty) = 0$ as desired.

Conversely, let \tilde{H} be a s.adj extension of H . Then $\exists g \in L^2(0, \infty)$, $g(x) = 0$ for $x > 1$, s.t.

$$h \equiv (\tilde{H} - \lambda_0)^{-1}g$$

is a non-zero solution $h(x) \not\equiv 0$ for $x > 1$ of $(\tilde{H} - \lambda_0)h = -h'' + (V - \lambda_0)h = 0$ for $x > 1$. Hence for $x > 1$

$$h(x) = c(y_1(x, \lambda_0) + my_2(x, \lambda_0)) = c\chi_m(x)$$

for some $c, m, c \neq 0$. A priori, m may not lie on C_∞ . However, as \tilde{H} is s.adj and $h \in D(\tilde{H})$. We have

$$\begin{aligned} 0 &= (\tilde{H}h, h) - (h, \tilde{H}h) \\ &= \lim_{b \rightarrow \infty} \int_0^b \overline{-h'' + Vh}h - \int_0^b \bar{h}(-h'' + Vh) \\ &= [hh](0) - \lim_{b \rightarrow \infty} [hh](b) \end{aligned}$$

But as $h \in D(\tilde{H}) \subset D(H^*)$, $[hh](0) = (h\bar{h}' - h'\bar{h})(0) = 0$ and so

$$0 = \lim_{b \rightarrow \infty} [hh](b) = |c|^2[\chi_m\chi_m](\infty).$$

i.e.

$$[\chi_m\chi_m](\infty) = 0 \tag{4.4}$$

which is equivalent, by previous calculation to the condition $m \in C_\infty$.

Now suppose $u \in D(\tilde{H})$, then again

$$0 = (u, \tilde{H}h) - (\tilde{H}u, h) \implies 0 = [uh](\infty) = \bar{c}[u\chi_m](\infty)$$

$$\text{i.e. } [u\chi_m](\infty) = 0$$

Hence $D(\tilde{H}) \subset D(H^*) \cap \{[u\chi_m](\infty) = 0\} = D_m$. Thus $\tilde{H} \subset H_m$, which implies $\tilde{H} = H_m$.

Finally if m, m' are distinct points on C_∞ , the above calculations show that if $H_m = H_{m'}$, then necessarily

$$[\chi_m\chi_{m'}](\infty) = 0 \tag{4.5}$$

but the center \hat{m} of the circle C_∞ is given by

$$[y_1y_2](\infty) + \hat{m}[y_2y_2](\infty) = 0$$

and the reciprocal of the radius of C_∞ is given by

$$|[y_2 y_2](\infty)| > 0$$

Now as $\chi_m = y_1 + m y_2$, by (4.4)

$$\begin{aligned} [y_2 \chi_m](\infty) &= [y_2 y_1](\infty) + \bar{m} [y_2 y_2](\infty) \\ &= (\bar{m} - \overline{\bar{m}}) [y_2 y_2](\infty) \end{aligned}$$

so that

$$[y_2 \chi_m](\infty) \neq 0$$

Now $\chi_m - \chi_{m'} = (m - m') y_2 \implies [\chi_m \chi_{m'}](\infty) = (m - m') [y_2 \chi_m](\infty) \neq 0$, which contradicts (4.5), (4.4). Hence

$$H_m \neq H_{m'}$$

This completes the sketch of the proof. \square

The proof of (4.2) actually show that

$$\int_0^\infty \int_0^\infty |G(t, \tau)|^2 dt d\tau < \infty$$

so that H_m has a resolvent which is Hilbert-Schmidt. So we have proved the following very interesting fact.

Fact 105. *If V is limit-circle at ∞ , then all s.adj extension of H have pure point spectrum with complete orthonormal set of eigenvectors.*

In the course of the above proof we showed that following fact.

Fact 106.

$$u \in D_m \iff \bar{u} \in D_m$$

This is a subtle fact.

Remark 107. In the course of the above proof we showed that H_m is closed on D_m , and then $\text{Ran}(H_m - \lambda_0) = \text{Ran}(H_m - \bar{\lambda}_0) = L^2(0, \infty)$ and so H_m is s.adj on D_m . It is not necessary for this conclusion to show that H_m is closed on D_m : the surjectivity of $H_m - \lambda_0$ is sufficient, then H_m is closed a posteriori.

4.3 Spectral Theory on \mathbb{R}

Now what happens $V(x)$ is on the whole line \mathbb{R} , as opposed to the half line \mathbb{R}_+ ? (We follow Coddington, Levinson pp246-).

Suppose $V(x)$ is continuous and real valued on \mathbb{R} . Let $H = -d^2/dx^2 + V(x)$ with domain $D(H) = C_0^\infty(\mathbb{R})$, then H is symmetric. As V is real-valued, H has s.adj extension. As before, we find $H^* = -d^2/dx^2 + V(x)$ with domain $D(H^*) = \{u \in L^2(\mathbb{R}) : u, u' \text{ abs cont. } -u'' + Vu \in L^2(\mathbb{R})\}$.

From the proof of theorem 72, H is e.s.a on $C_0^\infty(\mathbb{R}) \iff H$ is limit point at both ∞ and $-\infty$. Thus H is e.s.a on $C_0^\infty(\mathbb{R})$ iff for any $\lambda \in \mathbb{C} \setminus \mathbb{R}$, $(H - \lambda)\chi = 0$ has precisely one solution

$$\chi = \chi_+ = y_1 + m_\infty y_2 \in L^2(+\infty)$$

and precisely one solution

$$\chi = \chi_- = y_1 + m_{-\infty} y_2 \in L^2(-\infty)$$

Here, as before, $(H^* - \lambda)y_j = 0$, $y_1(0, \lambda) = y_2'(0, \lambda) = 1$, $y_1'(0, \lambda) = y_2(0, \lambda) = 0$. Generally χ_+ , χ_- are independent, but we will show later they may be dependent for some $\lambda = \lambda_0 \in \mathbb{C} \setminus \mathbb{R}$. Then $\exists \chi \in D(H^*) \subset L^2(\mathbb{R})$ s.t. $(H^* - \lambda)\chi = 0$.

4.4 Spectral Theory on an Interval

Now for any $a < 0$ and $b > 0$ consider the s.adj operator $H_{ab} = -d^2/dx^2 + V(x)$ with domain $D_{ab} = \{f \in L^2(a, b) : f, f' \text{ abs cont, } f'' \in L^2(a, b), \cos \alpha f(a) + \sin \alpha f'(a) = 0, \cos \beta f(b) + \sin \beta f'(b) = 0\}$ for some $0 \leq \alpha, \beta < \pi$. Then the spectrum of H_{ab} consists of real simple eigenvalues $\{\lambda_n^{(a,b)}\}_{n=1}^\infty$. (**Exercise** why?).

$\lambda_n \rightarrow \infty$ as $n \rightarrow \infty$, with an associated complete orthonormal set of eigenvectors $\{h_n^{(a,b)}\}$, $(H_{ab} - \lambda_n^{(a,b)})h_n^{(a,b)} = 0$. Parseval's equality holds (note that the eigenvectors are real) in the form

$$\int_a^b |f(x)|^2 = \sum_{n=1}^\infty \left| \int_a^b f(t) h_n^{(a,b)}(t) dt \right|^2 \quad (4.6)$$

for any $f \in L^2(a, b)$.

Now there exist real constants $r_{n_1}^{(a,b)}$, $r_{n_2}^{(a,b)}$ such that

$$h_n^{(a,b)}(t) = r_{n_1}^{(a,b)} y_1(t, \lambda_n^{(a,b)}) + r_{n_2}^{(a,b)} y_2(t, \lambda_n^{(a,b)})$$

Inserting this relation into (4.6), we find

$$\begin{aligned} \int_a^b |f(x)|^2 &= \sum_{n=1}^{\infty} \left(r_{n_1}^{(a,b)} \int_a^b f y_1(\lambda_n^{(a,b)}) + r_{n_2}^{(a,b)} \int_a^b f y_2(t, \lambda_n^{(a,b)}) \right) \\ &\quad \cdot \left(r_{n_1}^{(a,b)} \int_a^b \bar{f} \bar{y}_1(\lambda_n^{(a,b)}) + r_{n_2}^{(a,b)} \int_a^b \bar{f} \bar{y}_2(t, \lambda_n^{(a,b)}) \right) \end{aligned}$$

Set

$$g_j^{(a,b)}(\lambda) \equiv \int_a^b f(t) y_j(t, \lambda) dt, \quad \lambda \in \mathbb{R} \quad (4.7)$$

Then we have

$$\begin{aligned} \int_a^b |f(x)|^2 &= \sum_{n=1}^{\infty} \left(r_{n_1}^{(a,b)} g_1^{(a,b)}(\lambda_n^{(a,b)}) + r_{n_2}^{(a,b)} g_2^{(a,b)}(\lambda_n^{(a,b)}) \right) \\ &\quad \cdot \left(r_{n_1}^{(a,b)} \overline{g_1^{(a,b)}(\lambda_n^{(a,b)})} + r_{n_2}^{(a,b)} \overline{g_2^{(a,b)}(\lambda_n^{(a,b)})} \right) \\ &= \sum_{n=1}^{\infty} \left(\overline{g_1^{(a,b)}(\lambda_n^{(a,b)})}, \overline{g_2^{(a,b)}(\lambda_n^{(a,b)})} \right) \begin{pmatrix} r_{n_1}^2 & r_{n_1} r_{n_2} \\ r_{n_1} r_{n_2} & r_{n_2}^2 \end{pmatrix} \begin{pmatrix} g_1^{(a,b)}(\lambda_n^{(a,b)}) \\ g_2^{(a,b)}(\lambda_n^{(a,b)}) \end{pmatrix} \\ &= \int_{-\infty}^{\infty} \left(\overline{g_1^{(a,b)}(\lambda_n^{(a,b)})}, \overline{g_2^{(a,b)}(\lambda_n^{(a,b)})} \right) d\rho^{(a,b)}(\lambda) \begin{pmatrix} g_1^{(a,b)}(\lambda_n^{(a,b)}) \\ g_2^{(a,b)}(\lambda_n^{(a,b)}) \end{pmatrix} \quad (4.8) \end{aligned}$$

where $\rho^{(a,b)}(\lambda) = \left(\rho_{jk}^{(a,b)}(\lambda) \right)_{j,k=1,2}$ is a 2×2 real symmetric (hence Hermitian) valued function which is piecewise constant with jumps at the $\lambda_n^{(a,b)}$'s,

$$\rho^{(a,b)} \left(\lambda_n^{(a,b)} + 0^+ \right) - \rho^{(a,b)} \left(\lambda_n^{(a,b)} + 0^- \right) = \begin{pmatrix} r_{n_1}^{(a,b)^2} & r_{n_1}^{(a,b)} r_{n_2}^{(a,b)} \\ r_{n_1}^{(a,b)} r_{n_2}^{(a,b)} & r_{n_2}^{(a,b)^2} \end{pmatrix}$$

which is clearly positive definite. It follows that

Proposition 108. (i) $\rho^{(a,b)}(\lambda)$ is real, symmetric for any λ ; (ii) $\rho^{(a,b)}(\Delta) = \rho^{(a,b)}(\lambda) - \rho^{(a,b)}(\mu)$ is positive definite, if $\lambda > \mu$, $\Delta = (\mu, \lambda]$; (iii) the total variation of $\rho_{jk}^{(a,b)}(\lambda)$ is finite on every finite interval.

(Recall that *total variation* is finite means $\rho_{jk}^{(a,b)}(\lambda)$ has only a finite number of jumps in each finite interval.)

If $\chi_a = \chi_a(x, \lambda) = y_1 + m_a y_2$, $\lambda \in \mathbb{C} \setminus \mathbb{R}$ is chosen s.t. χ_a satisfies the boundary condition $\cos \alpha \chi_a(a) + \sin \alpha \chi'_a(a) = 0$, and $\chi_b = \chi_b(x, \lambda) =$

$y_1 + m_b y_2$, $\lambda \in \mathbb{C} \setminus \mathbb{R}$ is chosen s.t. χ_b satisfies the boundary condition $\cos \beta \chi_b(b) + \sin \beta \chi_b'(b) = 0$, then as before $m_a = m_a(\lambda)$ and $m_b = m_b(\lambda)$ lie on circles in the complex m -plane whose equations are, respectively,

$$[\chi_a \chi_a](a) = 0 \quad [\chi_b \chi_b](b) = 0$$

or equivalently, as before (cf. (2.10))

$$\int_a^0 |\chi_a(t, \lambda)|^2 dt = -\frac{\operatorname{Im} m_a(\lambda)}{\operatorname{Im} \lambda}$$

$$\int_0^b |\chi_b(t, \lambda)|^2 dt = \frac{\operatorname{Im} m_b(\lambda)}{\operatorname{Im} \lambda}$$

for $\lambda \in \mathbb{C} \setminus \mathbb{R}$. In particular $m_a(\lambda)$ and $m_b(\lambda)$ lie in opposite half-planes and one finds again as before (cf. (3.6)) that for $\lambda \in \mathbb{C} \setminus \mathbb{R}$

$$\int_{-\infty}^{\infty} \frac{d\rho_{jk}^{(a,b)}(\lambda)}{|\mu - \lambda|^2} = \frac{\operatorname{Im} M_{jk}^{(a,b)}(\lambda)}{\operatorname{Im} \lambda}, \quad 1 \leq j, k \leq 2$$

where $M_{jk}^{(a,b)}(\lambda)$ is analytic in $\mathbb{C} \setminus \mathbb{R}$ and moreover (for derivation see Coddington and Levinson pp246-250)

$$M_{12}^{(a,b)}(\lambda) = M_{21}^{(a,b)}(\lambda) = \frac{1}{2} \frac{m_a(\lambda) + m_b(\lambda)}{m_a(\lambda) - m_b(\lambda)}$$

$$M_{11}^{(a,b)}(\lambda) = \frac{1}{m_a(\lambda) - m_b(\lambda)} \tag{4.9}$$

$$M_{22}^{(a,b)}(\lambda) = \frac{m_a(\lambda)m_b(\lambda)}{m_a(\lambda) - m_b(\lambda)} \tag{4.10}$$

Note that the functions $\rho_{11}^{(a,b)}(\lambda)$ and $\rho_{22}^{(a,b)}(\lambda)$ are non-decreasing and for any fixed $\lambda \in \mathbb{C} \setminus \mathbb{R}$,

$$\frac{\operatorname{Im} M_{11}^{(a,b)}(\lambda)}{\operatorname{Im} \lambda} \text{ and } \frac{\operatorname{Im} M_{22}^{(a,b)}(\lambda)}{\operatorname{Im} \lambda}$$

are bounded for all $-\infty < a < b < \infty$, by our previous estimates for $m_a(\lambda)$, $m_b(\lambda)$, using (4.9), (4.10), it follows then by the *Helly Selection Theorem* that $\rho_{11}^{(a,b)}(\lambda)$ and $\rho_{22}^{(a,b)}(\lambda)$ converge along a sequence $(a_k, b_k) \rightarrow (-\infty, \infty)$ to non-decreasing functions $\rho_{11}^{(a,b)}(\lambda)$ and $\rho_{22}^{(a,b)}(\lambda)$ at all continuity points, where

$$\int \frac{d\rho_{jj}(\lambda)}{\lambda^2 + 1} \leq c < \infty, \quad j = 1, 2$$

However, $\rho_{12}^{(a,b)}(\lambda)$ is not monotone and so we cannot apply the Helly Selection Theorem to $\rho_{12}^{(a,b)}(\lambda)$ directly. Instead we consider the *Jordan Type Decomposition* of

$$\rho_{12}^{(a,b)}(\lambda) = \rho_{12+}^{(a,b)}(\lambda) - \rho_{12-}^{(a,b)}(\lambda)$$

where $\rho_{12\pm}^{(a,b)}(\lambda)$ are non-decreasing and for $\mu < \lambda$,

$$\rho_{12+}^{(a,b)}(\lambda) - \rho_{12+}^{(a,b)}(\mu) = \sum_{\substack{(a,b) \\ \mu < \lambda_n \leq \lambda \\ r_{n_1}, r_{n_2} > 0}} r_{n_1}^{(a,b)} r_{n_2}^{(a,b)}$$

$$\rho_{12-}^{(a,b)}(\lambda) - \rho_{12-}^{(a,b)}(\mu) = \sum_{\substack{(a,b) \\ \mu < \lambda_n \leq \lambda \\ r_{n_1}, r_{n_2} < 0}} \left| r_{n_1}^{(a,b)} r_{n_2}^{(a,b)} \right|$$

As $2 \left| r_{n_1}^{(a,b)} r_{n_2}^{(a,b)} \right| \leq r_{n_1}^{(a,b)^2} + r_{n_2}^{(a,b)^2}$, it is clear that $\left| \rho_{12}^{(a,b)} \right|(\lambda) \equiv \rho_{12+}^{(a,b)}(\lambda) + \rho_{12-}^{(a,b)}(\lambda)$ and

$$\int \frac{d \left| \rho_{12}^{(a,b)} \right|(\lambda)}{\lambda^2 + 1} \leq \int \frac{d \rho_{11}^{(a,b)}(\lambda)}{\lambda^2 + 1} + \frac{d \rho_{22}^{(a,b)}(\lambda)}{\lambda^2 + 1}$$

which is bounded for $a < b$. Hence $\rho_{12+}^{(a,b)}(\lambda) \rightarrow \rho_{12+}(\lambda)$, $\rho_{12-}^{(a,b)}(\lambda) \rightarrow \rho_{12-}(\lambda)$ along a sequence $(a_k, b_k) \rightarrow (-\infty, \infty)$ and

$$\int \frac{d \rho_{12\pm}(\lambda)}{\lambda^2 + 1} \leq c < \infty \quad (4.11)$$

Thus $\rho_{12}^{(a,b)}(\lambda) \rightarrow \rho_{12+}(\lambda) - \rho_{12-}(\lambda)$ as $(a, b) = (a_k, b_k) \rightarrow (-\infty, \infty)$, Thus $\rho^{(a,b)}(\lambda)$ converges to a limit along a sequence $(a_k, b_k) \rightarrow (-\infty, \infty)$.

Moreover $\rho(\lambda)$ satisfies the properties Proposition 108 (i)-(iii). If H is e.s.a, i.e. H is in the limit-point case at ∞ and $-\infty$, then $\rho(\lambda)$ is unique, since in this situation both m_a and m_b tend to points $m_{-\infty}$, m_{∞} respectively and as in (3.5),

$$\rho_{jk}(\lambda) - \rho_{jk}(\mu) = \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_{\mu}^{\lambda} \text{Im} M_{jk}(\nu + i\varepsilon) d\nu$$

where $M_{jk}(\lambda) = \lim_{(a,b) \rightarrow (-\infty, \infty)} M_{jk}^{(a,b)}(\lambda)$. In particular, $M_{11}(\lambda) = 1/(m_{-\infty}(\lambda) - m_{\infty}(\lambda))$ etc.

Exercise 109. One can also get expansion and completeness results as in Theorem 96. As a exercise, prove them.

Exercise 110. There are analogous results in the limit circle case at either or both points, ∞ or $-\infty$. Exercise prove them.

4.5 Diagonalizing Unitary Map

Let $\rho(\lambda)$ be any limit matrix of the set $\{\rho^{(a,b)}\}$ as $(a, b) \rightarrow (-\infty, \infty)$ as above (limit point case or otherwise). The analog of the unitary map which diagonalize $-d^2/dx^2 + V(x)$ in Theorem 96 is the following.

Let $f \in L^2(\mathbb{R})$, then

$$\begin{aligned} g(\lambda) &= (g_1(\lambda), g_2(\lambda)) \\ &\equiv \lim_{(a,b) \rightarrow (-\infty, \infty)} \left(\int_a^b f(t) y_1(t, \lambda) dt, \int_a^b f(t) y_2(t, \lambda) dt \right) \end{aligned}$$

exists in $L^2(d\rho)$, i.e.

$$\|g - g_{ab}\|^2 = \int (\bar{g} - \bar{g}_{ab})(\lambda) d\rho(\lambda) (g - g_{ab})^T \rightarrow 0$$

as $(a, b) \rightarrow (-\infty, \infty)$, where (cf. (4.7))

$$g_{ab}(\lambda) = \left(\int_a^b f(t) y_1(t, \lambda) dt, \int_a^b f(t) y_2(t, \lambda) dt \right)$$

Note 111. That as $\rho(\lambda)$ satisfies Proposition 108 (ii), $\|\cdot\|$ defines a *bona fide norm*.

Moreover the map

$$V : L^2(\mathbb{R}) \rightarrow L^2(d\rho)$$

$$f \mapsto g = (g_1, g_2)$$

is a surjective isometry, i.e. a unitary map. (cf. (4.8))

$$\|f\|_{L^2(\mathbb{R})}^2 = \int_{\mathbb{R}} \overline{g(\lambda)} d\rho(\lambda) g(\lambda)^T \quad (4.12)$$

The inverse

$$V^{-1} : L^2(d\rho) \rightarrow L^2(\mathbb{R})$$

$$g = (g_1, g_2) \mapsto f$$

is given by

$$f(x) = \int (y_1(x, \lambda), y_2(x, \lambda)) d\rho(\lambda) g(\lambda)^T \quad (4.13)$$

where again the integral is a limit in the sense

$$f(x) = \lim_{n \rightarrow \infty} \int_{-n}^n (y_1(x, \lambda), y_2(x, \lambda)) d\rho(\lambda) g(\lambda)^T$$

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

Most importantly V diagonalizes \tilde{H} , where \tilde{H} is the s.adj extension of H corresponding to $d\rho$, i.e. if $f \in D(\tilde{H})$, then

$$(V\tilde{H}f)(\lambda) = \lambda g(\lambda) = (\lambda g_1(\lambda), \lambda g_2(\lambda)) \quad (4.14)$$

where $Vf(\lambda) = g(\lambda) = (g_1(\lambda), g_2(\lambda))$.

However V is still not diagonalizing map U we desire. By general s.adjointness theory we know there exists

$$\begin{aligned} U : L^2(\mathbb{R}) &\rightarrow \bigoplus_{n=1}^M L^2(\mathbb{R}, d\mu_n) \\ f &\rightarrow (f_1(x), f_2(x), \dots, f_n(x)) \\ \|f\|_{L^2(\mathbb{R})}^2 &= \sum_{j=1}^M \|f_j\|_{L^2(d\mu_i)}^2 \end{aligned}$$

The problem is that $d\rho(\lambda)$ is not diagonal. We proceed as follows.

We know that for $\mu < \lambda$, $\Delta = (\mu, \lambda]$, $\rho(\Delta)$ is positive definite, i.e.

$$\bar{v}\rho(\Delta)v^T \geq 0 \quad \forall v = (v_1, v_2) \in \mathbb{C}^2$$

In particular $\rho_{11}(\Delta)$ and $\rho_{22}(\Delta)$ are ≥ 0 and

$$\det \rho(\Delta) = \rho_{11}(\Delta)\rho_{22}(\Delta) - \rho_{12}^2(\Delta) \geq 0$$

i.e.

$$|\rho_{12}(\Delta)| \leq (\rho_{11}(\Delta)\rho_{22}(\Delta))^{1/2} \leq \rho_{11}(\Delta) + \rho_{22}(\Delta) \quad (4.15)$$

Now by virtue of Proposition 108 (ii) and (4.11), each of the functions $\rho_{ij}(\lambda)$ induces an indefinite Borel measure $d\mu_{ij}(\lambda)$ on \mathbb{R} , i.e. for continuous functions h of compact support,

$$\int h(\lambda) d\rho_{ij}(\lambda) = \int h(\lambda) d\mu_{ij}(\lambda)$$

where the integral on the left is a Lebesgue-Stieltjes integral and integral on the right is an indefinite Lebesgue integral. Now it follows from (4.15) (**Exercise**) that the measures $d\mu_{ij}(\lambda)$ are absolutely continuous w.r.t. the measure

$$d\nu(\lambda) \equiv d\mu_{11}(\lambda) + d\mu_{12}(\lambda)$$

Thus

$$d\mu_{ij}(\lambda) = f_{ij}d\nu(\lambda)$$

where $f_{ij}(\lambda)$ is a real $L^1_{loc}(d\nu)$ function, $f_{12}(\lambda) = f_{21}(\lambda)$. We then have in (4.12)

$$\|f\|_{L^2(\mathbb{R})}^2 = \int \overline{g(\lambda)} F(\lambda) g(\lambda)^T d\nu(\lambda) \quad (4.16)$$

where $F(\lambda) = \begin{pmatrix} f_{11}(\lambda) & f_{12}(\lambda) \\ f_{21}(\lambda) & f_{22}(\lambda) \end{pmatrix}$.

As $F(\lambda)$ is real and positive definite, we can diagonalize it

$$F(\lambda) = Q(\lambda) \begin{pmatrix} s_+(\lambda) & 0 \\ 0 & s_-(\lambda) \end{pmatrix} Q(\lambda)^T \quad (4.17)$$

and $Q(\lambda)Q(\lambda)^T = I$, $s_+(\lambda) \geq s_-(\lambda) \geq 0$. Moreover the maps $\lambda \mapsto s_{\pm}(\lambda)$, $\lambda \mapsto Q(\lambda)$ can be chosen in a measurable way. Indeed on the set $\{f_{12}(\lambda) \neq 0\}$

$$s_{\pm}(\lambda) \equiv \frac{f_{11}(\lambda) + f_{22}(\lambda) \pm \sqrt{(f_{11} - f_{22})^2 + 4f_{12}^2(\lambda)}}{2}$$

$$Q(\lambda) = (q_+(\lambda), q_-(\lambda))$$

where

$$q_{\pm}(\lambda) = \frac{1}{\sqrt{f_{12}^2(\lambda) + (s_{\pm}(\lambda) - f_{11}(\lambda))^2}} \begin{pmatrix} f_{12}(\lambda) \\ s_{\pm}(\lambda) - f_{11}(\lambda) \end{pmatrix}$$

and on the set $f_{12}(\lambda) = 0$,

$$s_+(\lambda) = f_{11}(\lambda) \quad s_-(\lambda) = f_{22}(\lambda)$$

and

$$Q(\lambda) = I$$

Inserting (4.17) into (4.16) we obtain

$$\|f\|_{L^2(\mathbb{R})}^2 = \int \overline{g(\lambda)} Q(\lambda) \begin{pmatrix} s_+ & 0 \\ 0 & s_- \end{pmatrix} Q(\lambda)^T g(\lambda)^T d\nu(\lambda)$$

i.e.

$$\|f\|_{L^2(\mathbb{R})}^2 = \int |\tilde{g}_+(\lambda)|^2 s_+(\lambda) d\nu(\lambda) + |\tilde{g}_-(\lambda)|^2 s_-(\lambda) d\nu(\lambda)$$

where $\tilde{g} = (\tilde{g}_+, \tilde{g}_-) = g(\lambda)Q(\lambda)$.

In (4.13) we obtain

$$\begin{aligned} f(x) &= \int (y_1, y_2) Q(\lambda) \begin{pmatrix} s_+ & 0 \\ 0 & s_- \end{pmatrix} Q(\lambda)^T g(\lambda)^T d\nu(\lambda) \\ &= \int (\tilde{y}_+(x, \lambda) \tilde{g}_+(x, \lambda) s_+(\lambda) + \tilde{y}_-(x, \lambda) \tilde{g}_-(x, \lambda) s_-(\lambda)) d\nu(\lambda) \end{aligned}$$

where \tilde{g} is as above and

$$\tilde{y}(x, \lambda) = (\tilde{y}_+, \tilde{y}_-) = (y_1(x, \lambda), y_2(x, \lambda))Q(\lambda)$$

Thus

$$Uf(\lambda) \equiv (Vf(\lambda))Q(\lambda)$$

is the desired map.

For $f \in D(\tilde{H})$ by (4.14),

$$U\tilde{H}f(\lambda) = (V\tilde{H}f)(\lambda)Q(\lambda) = \lambda g(\lambda)Q(\lambda) = \lambda \tilde{g}(\lambda)$$

where $\tilde{g} = Uf$.

Finally we note that for $f_1, f_2 \in L^2(\mathbb{R})$, we have the above by polarization that

$$(f_1, f_2)_{L^2(\mathbb{R})} = \int (\tilde{g}_+^1(x, \lambda) \tilde{g}_+^2(x, \lambda) s_+(\lambda) + \tilde{g}_-^1(x, \lambda) \tilde{g}_-^2(x, \lambda) s_-(\lambda)) d\nu(\lambda)$$

with $f_j \mapsto \tilde{g}^j = (\tilde{g}_+^j, \tilde{g}_-^j)$, $j = 1, 2$.

In particular if $\tilde{g} = (\tilde{g}_+, \tilde{g}_-) \in L^2(s_+(\lambda)d\nu(\lambda), s_-(\lambda)d\nu(\lambda))$ and we set

$$f_{\pm}(x) = \int \tilde{y}_{\pm}(x, \lambda) \tilde{g}_{\pm}(\lambda) s_{\pm}(\lambda) d\nu(\lambda)$$

so that

$$f_+ \longleftrightarrow (\tilde{g}_+, 0) \quad f_- \longleftrightarrow (0, \tilde{g}_-)$$

and we conclude from that $(f_+, f_-)_{L^2(\mathbb{R})} = 0$.

This implies that U maps $L^2(\mathbb{R})$ onto the direct orthogonal sum

$$L^2(s_+(\lambda)d\nu(\lambda)) \oplus L^2(s_-(\lambda)d\nu(\lambda))$$

as desired.

Remark 112. The idea of using the *majorizing measure* $d\mu_{11} + d\mu_{22}$ which enabled us to diagonalize the map V , is a very useful and fundamental trick, that goes back in various circumstances to von Neumann's proof of the *Radon-Nikodym Theorem*. (see Reed Simon Vol I pp344-346)

5 Applications to Spectral Theory

5.1 Quadratic Form Revisit

Lecture 10
(11/15/13)

We now consider some explicit examples of the spectral theorem.

First consider $V(x)$ is a continuous function on $[0, \infty)$ such that

$$V(x) \rightarrow \infty$$

as $x \rightarrow \infty$.

We will strengthen the condition for V above successively as we proceed. In section 5.2, we will look at $V(x) \rightarrow 0$ as $x \rightarrow \infty$. In section 5.3, we take $V(x) \in L^1(0, \infty)$.

Claim 113. $H = -d^2/dx^2 + V(x)$, where V is above, with domain $D(H) = \{f \in C_0^\infty[0, \infty) : f(0) = 0\}$ is e.s.a.

Proof. It is enough to show that $Hf = 0$ has a solution that is not in L^2 at ∞ . Now for some $x_0 \geq 0$, $V(x) \geq 0$ for $x \geq x_0$. Let $-f'' + Vf = 0$ be a solution with $f(x_0) = 0$, $f'(x_0) = 1$. Then $f(x) > 0$ for all $x > x_0$.

Otherwise there is a smallest value $x_1 > x_0$ s.t. $f(x) > 0$ for $x_0 < x < x_1$ but $f(x_1) = 0$. But for all $x_0 < x < x_1$, $f''(x) = Vf \geq 0$. Hence $f'(x) \uparrow$ and so $f'(x) \geq 1 \forall x_1 > x > x_0$, thus

$$f(x) = f(x_0) + \int_{x_0}^x f'(t) dt \geq x - x_0 > 0$$

for $x_0 < x < x_1$. In particular $f(x_1) > 0$ which is a contradiction. Thus $f(x) > 0 \forall x > x_0$ and so as above $f(x) \geq x - x_0 \forall x > x_0$ and so $f \notin L^2(\infty)$. \square

Claim 114. The spectrum of \bar{H} is purely discrete. $\sigma(\bar{H}) = \{\lambda_j\}$, $\lambda_i \rightarrow \infty$, as $j \rightarrow \infty$.

Exercise 115. One can also show spectrum of \bar{H} is simple.

Proof. (Claim 114) Let L be any fixed number. Then there exists $x_L \geq 0$ such that $V(x) \geq L \forall x \geq x_L$. Let H_- denote the operator $-d^2/dx^2 + V(x)$ acting on smooth functions on $[0, x_L]$ and let H_+ denote the operator $-d^2/dx^2 + V(x)$ acting on smooth functions on $[x_L, \infty)$ with compact support.

Let H_N ($_N$ means Neumann boundary condition) denote the operator $H_- \oplus H_+$ acting on $L^2(0, x_L) \oplus L^2(x_L, \infty)$. Then in the sense of quadratic forms (cf. Example 54)

$$H_N = H_- \oplus H_+ \leq H \quad (5.1)$$

i.e. if $u \in Q(H) = \{f \in C_0^\infty[0, \infty), f(0) = 0\}$, then $u \in Q(H_- \oplus H_+) = \{f \in C_0^\infty[0, x_L], f(0) = 0\} \oplus \{f \in C_0^\infty[x_L, \infty)\}$ and

$$\int_0^{x_L} f'^2 + V f^2 dx + \int_{x_L}^\infty f'^2 + V f^2 dx \leq \int_0^\infty f'^2 + V f^2$$

As $V(x)$ is clearly bounded below, both quadratic forms are closeable and associated with their closures, we obtain the Friedrichs extension H_N^F and H^F of H_N and H respectively. As H_N and H are e.s.a. (**Exercise** why?) we must have

$$H_N^F = \bar{H}_- \oplus \bar{H}_+$$

and

$$H^F = \bar{H}$$

It follows from (5.1) that

$$\bar{H}_- \oplus \bar{H}_+ \leq \bar{H} \quad (5.2)$$

in the sense of quadratic forms, i.e. $Q(\bar{H}) \subset Q(\bar{H}_- \oplus \bar{H}_+)$ and if $u \in Q(\bar{H})$, $(u, \bar{H}_- \oplus \bar{H}_+ u) \leq (u, \bar{H} u)$

It follows by Min-Max theorem, then

$$\mu_n(\bar{H}_- \oplus \bar{H}_+) \leq \mu_n(\bar{H}), \quad n \geq 1 \quad (5.3)$$

where

$$\mu_n(A) = \sup_{\psi_1, \dots, \psi_{n-1}} \inf_{\substack{\psi \perp \langle \psi_1, \dots, \psi_{n-1} \rangle \\ \|\psi\| = 1, \psi \in Q(A)}} q_A(\psi, \psi)$$

Now as $V(x) \geq L$ for $x \geq x_L$, it follows that $\sigma(\bar{H}_+) \subset [L, \infty)$. On the other hand, the spectrum of \bar{H}_- is discrete and goes to infinity. Thus the operator $\bar{H}_- \oplus \bar{H}_+$ can only have a finite number of eigenvalues below L . Hence by the min-max theorem, $\exists n_0 < \infty$ s.t.

$$\mu_n(\bar{H}_- \oplus \bar{H}_+) \geq L, \quad \forall n \geq n_0$$

But then by (5.3), $\mu_n(\bar{H}) \geq L$ for $n \geq n_0$. Again by min-max theorem, \bar{H} can only have discrete spectrum below L , and as L is arbitrary, this proves the claim (114). \square

Remark 116. (5.1) is decidedly *not* true in the sense of operators: in particular if $u \in D(\bar{H})$, it does not belong in general to $D(\bar{H}_- \oplus \bar{H}_+)$, this is the great advantage of quadratic form methods!

Remark 117. In any dimension n , if $V \in L^2_{loc}(\mathbb{R}^n)$ and $V(x) \geq 0$, then $H = -\Delta + V(x)$ is e.s.a. on $C_0^\infty(\mathbb{R}^n)$. (see Reed Simon Vol II Thm X.28 p184)

Remark 118. We noted in Fact 105 that if V is limit circle at ∞ , then any s.adj extension of H has pure point spectrum. The above example shows that this situation can also occur in the limit point case.

Here is another proof of Claim 114.

Proof. Again consider the quadratic form

$$q(f) = (f, Hf) = \int_0^\infty |f'|^2 + V|f|^2$$

with domain $Q(H) = \{f \in C_0^\infty[0, \infty), f(0) = 0\}$, it is easy to see that the domain of the closure \bar{q} of q is given by

$$\bar{Q} = \{f \in L^2 : f \text{ abs cont, } f' \in L^2(0, \infty), |V|^{1/2} f \in L^2(0, \infty), f(0) = 0\}$$

As noted above, associated with Q , we have the Friedrichs extension H^F of H with $D(H^F) \subset \bar{Q}$ and $u \in D(H^F) \iff u \in \bar{Q}$ and for some $v \in L^2(0, \infty)$, $\bar{q}(f, u) = (f, v) \forall f \in \bar{Q}$. By definition, $H^F u = v$,

Moreover, as H is e.s.a, $H^F = \bar{H}$. Now let $b > M$ and so $-b \notin \sigma(\bar{H})$ and $(\bar{H} + b)^{-1}$ exists as a bounded operator. We obtain that $(\bar{H} + b)^{-1}$ is compact. Hence $(\bar{H} + b)^{-1}$ has purely discrete spectrum $\gamma_n \rightarrow 0$, i.e. \bar{H} has purely discrete spectrum $\lambda_n = \gamma_n^{-1} \rightarrow \infty$.

So suppose $g_n \in L^2(0, \infty)$, $\|g_n\| \leq c < \infty$ and let $f_n = (\bar{H} + b)^{-1} g_n$. We must show that f_n has a convergent subsequence in $L^2(0, \infty)$.

As $f_n \in D(\bar{H}) = D(H^F)$, we must have $f_n \in \bar{Q}$ and

$$\begin{aligned} \bar{q}(f_n) &= \int |f_n'|^2 + V|f_n|^2 \\ &= (f_n, H^F f_n) \\ &= (f_n, \bar{H} f_n) \\ &= (f_n, (\bar{H} + b)f_n) - \|f_n\|^2 b \\ &= (f_n, g_n) - b\|f_n\|^2 \end{aligned}$$

As $\|g_n\| \leq c$ and $(\bar{H} + b)^{-1}$ is bounded, we have $\|f_n\| \leq \|(\bar{H} + b)^{-1}\| c$, and so

$$\int |f'_n|^2 + V |f_n|^2 \leq c$$

It now follows from above (note that $V(x) \rightarrow \infty$ as $x \rightarrow \infty$) by the *Rellich compactness Theorem* that f_n has a convergent subsequence in $L^2(0, \infty)$. This completes the proof. \square

For proof of the Rellich compactness Theorem, see Reed Simon Vol IV Thm XIII 65 p247.

5.2 Essential Spectrum Theorem

Read proof of *Weyl's Essential Spectrum Theorem* and proof of corollary 122 below, Reed Simon Vol IV pp 111-114.

Theorem 119. (essential spectrum theorem) *Let A be s.adj operator, let B be a closed operator so that:*

(a) *For some (hence all) $z \in \rho(B) \cap \rho(A)$, $(A - z)^{-1} - (B - z)^{-1}$ is compact. And either (b1) $\sigma(A) \neq \mathbb{R}$ and $\rho(B) \neq \emptyset$, or (b2) there are points of $\rho(B)$ in both the upper and lower half-planes. Then*

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

Definition 120. Let A be s.adj in \mathcal{H} . An operator C with $D(A) \subset D(C)$ is called *relatively compact* with respect to A iff $C(A + i)^{-1}$ is compact.

Note 121. $C(A + i)^{-1}$ is compact $\iff C(A - z)^{-1}$ is compact for any $z \in \rho(A)$.

Recall that the discrete spectrum, σ_{disc} , of a s.adj operator A is the set of isolated eigenvalues of A of finite multiplicity. Thus $\lambda \in \sigma_{disc}(A)$, if

$$\{z : 0 < |z - \lambda| < \varepsilon\} \cap \sigma(A) = \emptyset,$$

for some $\varepsilon > 0$ and $0 < \dim[N(A - \lambda)] < \infty$.

The essential spectrum of A , $\sigma_{ess}(A)$, is defined to be $\sigma(A) \setminus \sigma_{disc}(A)$. Thus $\lambda \in \sigma_{ess}(A)$ if either λ is an isolated eigenvalue of A of ∞ multiplicity, or every deleted neighborhood of λ contains a point in the spectrum of A .

We will need the following corollary to the essential spectrum theorem.

Corollary 122. *Let A be a s.adj operator and let C be relatively compact perturbation of A . Then if C is symmetric, $B = A + C$ is s.adj on $D(A)$ and $\sigma_{ess}(B) = \sigma_{ess}(A)$.*

We now consider the operator $H = -d^2/dx^2 + V(x)$ acting on $D(H) = \{f \in L^2(0, \infty) : f \in C_0^\infty[0, \infty), f(0) = 0\}$ where V is real valued and continuous and converges to 0 as $x \rightarrow \infty$, i.e. $\lim_{x \rightarrow \infty} V(x) = 0$.

Theorem 123. *Assume V is real valued and continuous and converges to zero as $x \rightarrow \infty$, then H is e.s.a on $D(H)$ and*

$$\sigma(\bar{H}) = \sigma_{disc}(\bar{H}) \cup \sigma_{ess}(\bar{H})$$

where $\sigma_{disc}(\bar{H})$ is an at most countable set $\{\lambda_n\}$, $\lambda_n < 0$, $\lambda_n \rightarrow 0$ as $n \rightarrow \infty$, $\dim N(\bar{H} - \lambda_n) = 1$, and $\sigma_{ess}(\bar{H}) = [0, \infty)$.

Next lecture we will show \bar{H} may have imbedded L^2 eigenvalues in $[0, \infty)$.

Proof. The function $u \equiv 1$ solves $-u'' = 0$ and as $u \notin L^2(\infty)$, $H_0 = -d^2/dx^2$ on $C_0^\infty[0, \infty) \cap \{f(0) = 0\}$ is e.s.a. $D(\bar{H}_0) = \{f \in L^2(0, \infty) : f, f' \text{ abs cont, } f'' \in L^2, f(0) = 0\}$. As $V(x) \rightarrow 0$ as $x \rightarrow \infty$, V is relatively compact w.r.t. \bar{H}_0 .

Indeed note first that as $V \in L^\infty(\mathbb{R}_+)$, $D(\bar{H}_0) \subset D(V)$. Now if $\|f_n\| \leq c$, then by Rellich's compactness criterion $\{g_n = (\bar{H}_0 + i)^{-1}f_n\}$ has a subsequence $\{g_{n'}\}$ which is Cauchy in $L^2(K)$ for each compact subset K on $[0, \infty)$.

Let $\varepsilon > 0$ be given. Choose $L > 0$ s.t. $|V(x)| < \varepsilon$ for $x \geq L$, then for any $n' > m'$

$$\begin{aligned} V(\bar{H}_0 + i)^{-1}f_{n'} - V(\bar{H}_0 + i)^{-1}f_{m'} &= \underbrace{V\chi_{|x|>L}(\bar{H}_0 + i)^{-1}(f_{n'} - f_{m'})}_{\equiv I} \\ &\quad + \underbrace{V\chi_{|x|\leq L}(g_{n'} - g_{m'})}_{\equiv II} \end{aligned}$$

$$\text{where } \chi_{|x|>L} = \begin{cases} 1 & |x| > L \\ 0 & |x| < L \end{cases}.$$

Now $\|I\| \leq \varepsilon \|(\bar{H}_0 + i)^{-1}\| 2c = 2\varepsilon c$ and $\|II\| \leq \|V\|_\infty \|g_{n'} - g_{m'}\|_{L^2(0,L)}$. So we can make $\|II\|$ as small as we want because $|x| \leq L$ is a compact set, hence $g_{n'}$ is Cauchy. Hence $\exists N$ s.t. $n' > m' \geq N \implies$

$\|Vg_{n'} - Vg_{m'}\| < (2c + 1)\varepsilon$. As $\varepsilon > 0$ is arbitrary, this shows V is relatively compact w.r.t. \bar{H}_0 .

Now for $f \in D(H_N)$, $(f, H_0 f) = \int_0^\infty |f'|^2 \geq 0$, we see that $\sigma(H_0) \subset [0, \infty)$. If $\lambda > 0$, let $y(x, \lambda) = \sin \sqrt{\lambda}x$, then $-y'' = \lambda y$. Let $\chi \in C_0^\infty(\mathbb{R})$, $0 \leq \chi(x) \leq 1$, $\chi \not\equiv 0$, and let $\chi_n(x) = \chi(\frac{x}{n})$, $x > 0$. Then clearly $y_n(x) = \chi_n(x)y(x) \in \bar{H}_0$. We define

$$\begin{aligned} (\bar{H}_0 - \lambda)y_n &\equiv \chi_n(-y'' - \lambda y) - 2\chi'_n y' - \chi''_n y \\ &= -2\chi'_n y' - \chi''_n y \end{aligned}$$

Now

$$\begin{aligned} \|\chi'_n y'\|^2 &= \frac{1}{n^2} \int_0^\infty \left| \chi'(\frac{x}{n}) y'(x) \right|^2 dx \\ &\leq \lambda \frac{1}{n^2} \int_0^\infty \chi'(\frac{x}{n})^2 dx \\ &= \lambda \frac{1}{n} \int_0^\infty \chi'(x)^2 dx \end{aligned}$$

$$\begin{aligned} \|\chi''_n y\|^2 &= \frac{1}{n^4} \int_0^\infty \left| \chi''(\frac{x}{n}) y(x) \right|^2 dx \\ &\leq \frac{1}{n^3} \int_0^\infty \chi''(x)^2 dx \end{aligned}$$

Thus $\|(\bar{H}_0 - \lambda)y_n\| = O(\frac{1}{\sqrt{n}})$. Finally

$$\begin{aligned} \|y_n\|^2 &= \int_0^\infty \chi^2(\frac{x}{n}) y^2(x) dx \\ &= n \int_0^\infty \chi^2(x) \sin^2 \sqrt{\lambda} n x dx \\ &= n \int_0^\infty \chi^2(x) \frac{1 - \cos 2\sqrt{\lambda} n x}{2} dx \\ &= \underbrace{\frac{n}{2} \int_0^\infty \chi^2(x) dx}_{\neq 0} + O(1) \end{aligned}$$

Thus for $\hat{y}_n = y_n / \|y_n\|$, $\|\hat{y}_n\| = 1$.

$$\|(\bar{H}_0 - \lambda)\hat{y}_n\| = O(\frac{1}{n}) \rightarrow 0$$

as $n \rightarrow \infty$.

Thus any $\lambda > 0$ lies in $\sigma(\bar{H}_0)$. Thus $\sigma_{ess}(\bar{H}_0) = [0, \infty)$.

By corollary to Weyl's Essential Spectrum Theorem, $\sigma_{ess}(\bar{H}) = \sigma_{ess}(\bar{H}_0) = [0, \infty)$. Necessarily $\sigma_{disc}(\bar{H}) \subset (-\infty, 0)$. The only possible accumulation point of the λ_n 's in $\sigma_{disc}(\bar{H})$ is 0, for if $\lambda_{k_n} \rightarrow \lambda < 0$, then λ would be a point in $\sigma_{ess}(\bar{H})$ which is not in $[0, \infty)$. \square

The above proof of theorem 123 is operator theoretic. We can also proceed using the limit point / limit circle theory we have developed in theorem 96.

Proof. (Alternative Proof) We have for $V = 0$,

$$y_1(x, \lambda) = \cos \sqrt{\lambda}x, \quad y_2(x, \lambda) = \frac{\sin \sqrt{\lambda}x}{\sqrt{\lambda}}$$

then

$$\chi = y_1 + m_\infty y_2 = \frac{e^{i\sqrt{\lambda}x}}{2} \left(1 + \frac{m_\infty}{i\sqrt{\lambda}}\right) + \frac{e^{-i\sqrt{\lambda}x}}{2} \left(1 - \frac{m_\infty}{i\sqrt{\lambda}}\right)$$

Now suppose $\lambda \in \mathbb{C}_+$, $\sqrt{\lambda}$ in the 1st quadrant. Then $e^{i\sqrt{\lambda}x}$ decays exponentially as $x \rightarrow \infty$ and $e^{-i\sqrt{\lambda}x}$ grows exponentially $x \rightarrow \infty$. As $\chi \in L^2(\infty)$, we must have $m_\infty(\lambda) = i\sqrt{\lambda}$.

(note that $\text{Im}m_\infty(\lambda) = \text{Re}\sqrt{\lambda} > 0$ so that $\frac{\text{Im}m_\infty(\lambda)}{\text{Im}\lambda} > 0$, as it should.)

Then by (3.5),

$$\begin{aligned} \rho(\lambda) - \rho(\mu) &= \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_\mu^\lambda \text{Im}m_\infty(\nu + i\varepsilon) d\nu \\ &= \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_\mu^\lambda \text{Re}\sqrt{\nu + i\varepsilon} d\nu \end{aligned}$$

Now $\text{Re}\sqrt{\nu + i\varepsilon} \rightarrow \begin{cases} \sqrt{\nu} & \nu > 0 \\ 0 & \nu \leq 0 \end{cases}$, so

$$\rho(\lambda) - \rho(\mu) = \frac{1}{\pi} \int_\mu^\lambda \sqrt{\nu} d\nu = \begin{cases} \frac{2}{3\pi} (\lambda^{3/2} - \mu^{3/2}) & 0 \leq \mu < \lambda \\ \frac{2}{3\pi} \lambda^{3/2} & \mu \leq 0 < \lambda \\ 0 & \mu < \lambda \leq 0 \end{cases}$$

Thus we have

$$\rho(\lambda) = \frac{2}{3\pi} \lambda^{3/2} \chi_{>0}(\lambda)$$

$$d\rho(\lambda) = \frac{1}{\pi} \lambda^{1/2} d\lambda \chi_{>0}(\lambda) \quad (5.4)$$

thus \bar{H}_0 is \cong to multiple by λ on $L^2\left(\frac{1}{\pi}\lambda^{1/2}d\lambda, (0, \infty)\right)$, and so any point $\lambda > 0$ lies in $\sigma_{ess}(\bar{H}_0)$. \square

Note 124. By Parseval's relation we have

$$\|f\|^2 = \frac{1}{\pi} \int_0^\infty \lambda^{1/2} \left| \hat{f}(\lambda) \right|^2 d\lambda$$

where

$$\hat{f}(\lambda) = \int_0^\infty y_2(x, \lambda) f(x) dx = \frac{1}{\sqrt{\lambda}} \int_0^\infty \sin \sqrt{\lambda} x f(x) dx$$

Thus

$$\begin{aligned} \|f\|^2 &= \frac{1}{\pi} \int_0^\infty \frac{1}{\sqrt{\lambda}} \left| \int_0^\infty \sin \sqrt{\lambda} x f(x) dx \right|^2 d\lambda \\ &= \frac{2}{\pi} \int_0^\infty \left| \int_0^\infty \sin kx f(x) dx \right|^2 dk \end{aligned} \quad (5.5)$$

This is the well-known property for the sine-transform.

Observe that

$$\begin{aligned} \int_0^\infty \sin kx f(x) dx &= \frac{1}{2i} \left(\int_0^\infty e^{ikx} f(x) dx - \int_0^\infty e^{-ikx} f(x) dx \right) \\ &= \frac{1}{2i} \left(\int_0^\infty e^{ikx} f(x) dx - \int_{-\infty}^0 e^{ikx} f(-x) dx \right) \\ &= \frac{1}{2i} \int_{-\infty}^\infty e^{ikx} \tilde{f}(x) dx \end{aligned}$$

if we set $\tilde{f}(x) = \begin{cases} f(x) & x > 0 \\ -f(-x) & x < 0 \end{cases}$, and clearly

$$\begin{aligned} \left\| \tilde{f} \right\|_{L^2(\mathbb{R})}^2 &= 2 \|f\|_{L^2(\mathbb{R}_+)}^2 \\ &= \frac{2}{\pi} \int_{-\infty}^\infty \left| \int_0^\infty \sin kx f(x) dx \right|^2 dk \text{ by (5.5)} \\ &= \frac{2}{\pi} \int_{-\infty}^\infty \frac{1}{4} \left| \int_{-\infty}^\infty e^{ikx} \tilde{f}(x) dx \right|^2 dk \\ &= \int_{-\infty}^\infty \left| \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty e^{ikx} \tilde{f}(x) dx \right|^2 dk \end{aligned}$$

verifying again that $\tilde{f} \rightarrow \hat{\tilde{f}} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^\infty e^{ikx} \tilde{f}(x) dx$ is an isometry from $L^2(\mathbb{R}, dx)$ to $L^2(\mathbb{R}, dx)$.

5.3 Commutation Technique

We now show that it is possible for a real potential $V(x)$, $V(x) \rightarrow 0$ as $x \rightarrow \infty$ to have an L^2 eigenvalue $\lambda > 0$ imbedded in the essential spectrum, i.e. λ is not isolated, $\lambda \notin \sigma_{disc}(\bar{H})$.

We use a very old trick called *commutation*. (See P. Deift, *Applications of a Commutation Formula* (1978))

Suppose ψ is a solution of $H\psi = -\psi'' + V\psi = 0$, i.e. $V = \psi''/\psi$. Then

$$H = A^*A$$

where $A = \psi \frac{d}{dx} \frac{1}{\psi}$. Indeed for any f ,

$$\begin{aligned} A^*Af &= -\frac{1}{\psi} \frac{d}{dx} \psi^2 \frac{d}{dx} \frac{f}{\psi} \\ &= -\frac{1}{\psi} \frac{d}{dx} \psi^2 \frac{f'\psi - f\psi'}{\psi^2} \\ &= -\frac{1}{\psi} \frac{d}{dx} (f'\psi - f\psi') \\ &= -f'' + f \frac{\psi''}{\psi} \\ &= -f'' + Vf \\ &= Hf \end{aligned} \tag{5.6}$$

(we neglect for now points x , s.t. $\psi(x) = 0$)

We note from this representation that if $H\psi = 0$, then $H\phi = 0$ where $\phi = \psi \int^x \frac{dt}{\psi^2}$. Indeed

$$H\phi = \left(-\frac{1}{\psi} \frac{d}{dx} \psi^2 \frac{d}{dx} \frac{1}{\psi} \right) \psi \int^x \frac{dt}{\psi^2} = -\frac{1}{\psi} \frac{d}{dx} \psi^2 \frac{1}{\psi^2} = 0$$

Thus if we have 1 solution we can use it to construct the other.

Set

$$H_1 = AA^* = -\psi \frac{d}{dx} \frac{1}{\psi^2} \frac{d}{dx} \psi$$

From the preceding calculation (5.6), we must have

$$H_1 = -\frac{d^2}{dx^2} + V_1$$

where

$$\begin{aligned}
V_1 &= \psi(\psi^{-1})'' \\
&= \psi(-\psi^{-2}\psi')' \\
&= \psi(2\psi^{-3}\psi'^2 - \psi^{-2}\psi'') \\
&= 2\left(\frac{\psi'}{\psi}\right)^2 - \frac{\psi''}{\psi}
\end{aligned}$$

now $2\frac{d^2}{dx^2}\ln\psi = 2\frac{d}{dx}\frac{\psi'}{\psi} = 2\frac{\psi''}{\psi} - 2\left(\frac{\psi'}{\psi}\right)^2$, hence

$$V_1 = \frac{\psi''}{\psi} - 2\frac{d^2}{dx^2}\ln\psi = V - 2\frac{d^2}{dx^2}\ln\psi$$

Thus the result of a commutation is to deform a Schrodinger H to a new Schrodinger operator H_1 ,

$$V \rightarrow V_1 = V - 2\frac{d^2}{dx^2}\ln\psi$$

Now as $H_1 = -\psi\frac{d}{dx}\psi^{-2}\frac{d}{dx}\psi$, we see that ψ^{-1} is 1 solution of $H_1\psi^{-1} = 0$. By our previous considerations $\psi^{-1}\int_0^x \psi^2(t)dt$ is a 2nd solution, thus any combination $\psi_c = \psi^{-1} + c\psi^{-1}\int_0^x \psi^2(t)dt$ is also a solution. Here we have fixed the lower limit of the integration.

We can now perform a commutation on H_1 using ψ_c (if we take $c = 0$, this commutation would take us back to H .) We have

$$H_1 = -\psi_c^{-1}\frac{d}{dx}\psi_c^2\frac{d}{dx}\psi_c^{-1} = A_c^*A_c$$

and then after commutator

$$\begin{aligned}
H_c &= A_cA_c^{-1} \\
&= -\psi_c\frac{d}{dx}\psi_c^{-2}\frac{d}{dx}\psi_c \\
&= -\frac{d^2}{dx^2} + V_1 - 2\frac{d^2}{dx^2}\ln\psi_c \\
&= -\frac{d^2}{dx^2} + V - 2\frac{d^2}{dx^2}\ln\psi\psi_c
\end{aligned}$$

i.e.

$$H_c = -\frac{d^2}{dx^2} + V - 2\frac{d^2}{dx^2}\ln\left(1 + c\int_0^x \psi(t)^2 dt\right)$$

From these calculations, we see that whatever singularities were introduced by the zero's of ψ in the first commutation, they are canceled out in the second commutation, provided we take $c > 0$ and choose a real solution ψ of $H\psi = -\psi'' + V\psi = 0$. Furthermore $H_c\psi_c^{-1} = 0$, where

$$\psi_c^{-1} = \frac{\psi}{1 + c \int_0^x \psi(t)^2 dt}$$

Now for any $\lambda > 0$, take $V = -\lambda$ and let $\psi = \sin \sqrt{\lambda}x$, then $H\psi = -\psi'' + V\psi = 0$.

$$\begin{aligned} H_c &= -\frac{d^2}{dx^2} - \lambda - 2\frac{d}{dx} \frac{\psi}{1 + c \int_0^x \psi^2} \\ &= -\frac{d^2}{dx^2} - \lambda - 2\left(\underbrace{\frac{\psi'}{1 + c \int_0^x \psi^2} - \frac{c\psi^3}{(1 + c \int_0^x \psi^2)^2}}_{\sim \frac{1}{x} \text{ as } x \rightarrow \infty} \right) \end{aligned}$$

Also $\psi_c^{-1}(0) = 0$ and $\psi_c^{-1}(x) \sim \frac{1}{x} \in L^2(\infty)$, thus

$$\hat{H} = -\frac{d^2}{dx^2} + \hat{V}, \quad \hat{V} = -\frac{d^2}{dx^2} \ln \left(1 + c \int_0^x \psi(t)^2 dt \right)$$

is a Schrodinger operator with a smooth potential, $\hat{V}(x) \rightarrow 0$ as $x \rightarrow \infty$. $D(\hat{H}) = \{f \in L^2(0, \infty) : f, f' \text{ abs cont, } f'' \in L^2, f(0) = 0\}$ has an L^2 -eigenvalue imbedded in the essential spectrum at $\lambda > 0$.

5.4 L^1 Potentials

We now consider $H = -d^2/dx^2 + V(x)$ with $V(x)$ real valued and continuous and instead of requiring $V(x) \rightarrow 0$ as $x \rightarrow \infty$ as in Theorem (123), we assume that

$$\int_0^\infty |V(x)| dx < \infty \tag{5.7}$$

Note 125. That if in addition $V(x)$ is uniformly continuous on $(0, \infty)$, then (5.7) $\implies V(x) \rightarrow 0$ as $x \rightarrow \infty$.

Exercise 126. Suppose $V(x)$ is not uniformly continuous on $(0, \infty)$, and construct an example for which (5.7) holds but not $V(x) \rightarrow 0$ as $x \rightarrow \infty$.

We will show below that H is e.s.a. on the standard domain

$$D(H) = C_0^\infty[0, \infty) \cap \{u(0) = 0\}$$

Hence by previous argument

$$\bar{H} = H^* = -d^2/dx^2 + V(x)$$

$$D(\bar{H}) = D(H^*) = \{u \in L^2(0, \infty) : u, u' \text{ abs cont, } -u'' + Vu \in L^2(0, \infty), u(0) = 0\}$$

Note that in general $D(\bar{H}) \neq D(\bar{H}_0) = \{u \in L^2 : u, u' \text{ abs cont, } u'' \in L^2, u(0) = 0\}$.

Remark 127. Indeed if $D(\bar{H}) = D(\bar{H}_0)$, then $D(\bar{H}_0) \subset D(V) = \{u \in L^2 : Vu \in L^2\}$.

Consider $T = V(H_0 + 1)^{-1}$, then T is an everywhere defined closed operator. Indeed, let $u_n \rightarrow u$ and $Tu_n \rightarrow v$. As T is everywhere defined, we just need to show that $Tu = v$. But as $(H_0 + 1)^{-1}$ is bounded, $w_n = (H_0 + 1)^{-1}u_n$ converges to $w = (H_0 + 1)^{-1}u \in D(V)$. Thus we have

$$D(V) \ni w_n \rightarrow w$$

$$Vw_n = Tu_n \rightarrow v$$

As V is clearly closed on $D(V)$, this implies $w \in D(V)$ and $Vw = v$, thus $Tu = V(H_0 + 1)^{-1}u = Vw = v$, as desired.

It follow that

$$\|Vf\|_{L^2(0, \infty)}^2 \leq a\|f\|_{L^2(0, \infty)}^2 + b\|f''\|_{L^2(0, \infty)}^2, \quad \forall f \in D(\bar{H}_0) \quad (5.8)$$

for some $a, b > 0$. (**Exercise** why?)

In particular, let $f_0 \in C_0^\infty(\mathbb{R})$ where $f_0(x) = \begin{cases} 1 & |x| < 1/2 \\ 0 & |x| > 1 \end{cases}$. For $x \geq 0$, set

$$f_n(x) = f_0\left(\frac{x-n}{n}\right) \in D(\bar{H}_0)$$

Then

$$\begin{aligned} \|f\|^2 &= \int_0^\infty f_0^2\left(\frac{x-n}{n}\right) = \int f_0^2\left(\frac{y}{n}\right)dn = c_0n \\ \|f''\| &= \frac{1}{n^2} \int_0^\infty f_0''^2\left(\frac{x-n}{n}\right) = \frac{1}{n} \int_0^\infty f_0''^2(n)dn = \frac{c_1}{n} \end{aligned}$$

but

$$\|Vf\|^2 = \int_0^\infty V^2(x)f_0^2\left(\frac{x-n}{n}\right) \geq \int_{\frac{n}{2}}^{\frac{3n}{2}} V^2(x)dx$$

Together with (5.8), this implies

$$\int_{\frac{n}{2}}^{\frac{3n}{2}} V^2(x) dx \leq ac_0 n + \frac{bc_1}{n}. \quad (5.9)$$

Now it is easy to construct examples where $\int_0^\infty |V(x)| dx < \infty$ but (5.9) fails. E.g let

$$V(x) = \sum_{k=1}^{\infty} k^{2-\delta} \chi_{[k, k+\frac{1}{k^3}]}, \quad 0 < \delta < \frac{1}{2}.$$

Theorem 128. *We now give a fundamental analytic proof that*

$$\sigma_{ess}(\bar{H}) \subset [0, \infty).$$

we will give an ode proof later.

Proof. As $\int_0^\infty |V(x)| dx < \infty$, we have for any $f \in Q(\bar{H}_0) = \{f \in L^2(0, \infty) : f \text{ abs cont, } f' \in L^2(0, \infty), f(0) = 0\}$, and so for any ε , $\exists a_\varepsilon > 0$ st

$$\begin{aligned} \left| \int V |f|^2 \right| &\leq \int |V| |f|^2 \\ &\leq \left(\int |V| dx \right) \|f\|_{L^\infty}^2 \\ &\leq \left(\int |V| dx \right) \left(a_\varepsilon \|f\|_{L^2}^2 + \varepsilon \|f'\|_{L^2}^2 \right) \\ &= \|V\|_{L^1} a_\varepsilon \|f\|_{L^2}^2 + \|V\|_{L^1} \varepsilon (f, \bar{H}_0 f) \end{aligned} \quad (5.10)$$

Now let $1 > \delta > 0$ be given and choose $L > 0$ st

$$\int_{|x|>L} |V(x)| dx < \delta$$

Let $V_L(x) = V(x) \chi_{|x|>L}$. Applying (5.10) to V_L we obtain

$$\left| \int V_L |f|^2 \right| \leq \delta a_\varepsilon \|f\|^2 + \delta \varepsilon (f, \bar{H}_0 f)$$

And so for $f \in Q(\bar{H}_0) = \text{form domain}$

$$\begin{aligned} (f, \bar{H}_0 + V_L f) &= (f, \bar{H}_0 f) + (f, V_L f) \\ &\geq (f, \bar{H}_0 f) - \delta a_\varepsilon \|f\|^2 - \delta \varepsilon (f, \bar{H}_0 f) \\ &= (1 - \delta \varepsilon) (f, \bar{H}_0 f) - \delta a_\varepsilon \|f\|^2 \end{aligned}$$

or for any $0 < \varepsilon, \delta < 1$

$$(f, \bar{H}_0 f) \leq \frac{\delta a_\varepsilon}{1 - \delta \varepsilon} \|f\|^2 + \frac{1}{1 - \delta \varepsilon} (f, \bar{H}_0 + V_L f) \quad (5.11)$$

Using the fact that $H_0 + V_L$ is e.s.a. on $D(H)$ (**Exercise** why?), and so the Friedrichs extension of $H_0 + V_L$ is $\overline{H_0 + V_L}$. It follows from (5.11) by min-max that

$$\mu_n(\bar{H}_0) \leq \frac{\delta a_\varepsilon}{1 - \delta \varepsilon} + \frac{1}{1 - \delta \varepsilon} \mu_n(\overline{H_0 + V_L})$$

As $\mu_n(\bar{H}_0) \geq 0$ we conclude that

$$\mu_n(\overline{H_0 + V_L}) \geq -\delta a_\varepsilon \quad (5.12)$$

Now as $W_L = V(x)\chi_{|x| \leq L}$ ($V = V_L + W_L$) is bounded with compact support, it follows that W_L is relatively compact w.r.t. $\overline{H_0 + V_L}$. Indeed consider

$$S = W_L(\overline{H_0 + V_L} + i)^{-1}$$

let $\|u_n\| \leq c$, then $v_n = u_n/(\overline{H_0 + V_L} + i)$ has the property

$$\|(\overline{H_0 + V_L} + i)\sigma_n\|^2 = \|u_n\|^2 \leq c^2$$

i.e.

$$\|\overline{H_0 + V_L} v_n\|^2 + \|v_n\|^2 \leq c^2$$

from which it follows (**Exercise** why?) that

$$|(v_n, \overline{H_0 + V_L} v_n)| + \|v_n\|^2 \leq c'^2$$

but then by (5.11)

$$\|v'_n\|^2 = (v_n, H_0 v_n) \leq c''^2$$

and

$$\|v_n\|^2 \leq c''^2$$

and so by Rellich, v_n has a subsequence v'_n that converges locally. In particular $Su'_n = W_L v'_n$ converges in L^2 .

We conclude by Weyl's Essential Spectrum Theorem that

$$\begin{aligned} \sigma_{ess}(\bar{H}) &= \sigma_{ess}(\overline{H_0 + V_L + W_L}) \\ &= \sigma_{ess}(\overline{H_0 + V_L} + W_L) \\ &= \sigma_{ess}(\overline{H_0 + V_L}) \end{aligned}$$

But for any fixed $\varepsilon > 0$, we have from (5.12) and the min-max theorem that

$$\sigma_{ess}(\bar{H}) \subset [-\delta a_\varepsilon, \infty)$$

As $\delta > 0$ is arbitrary, we conclude that

$$\sigma_{ess}(\bar{H}) \subset [0, \infty).$$

□

We now apply ode/limit-point/limit-circle techniques to $H = H_0 + V$.

For any $z \in \bar{\mathbb{C}}_+ \setminus \{0\} = \{z \neq 0: \text{Im} z \geq 0\}$, we define the energy $\lambda = z^2$ and consider the integral equation

$$f(x, z) = e^{ixz} + \int_x^\infty \frac{\sin z(t-x)}{z} V(t) f(t, z) dt \quad (5.13)$$

We will show that for any $z \in \bar{\mathbb{C}}_+ \setminus \{0\}$, that equation has a unique solution which is bounded as $x \rightarrow \infty$. Note that if such a solution exists, then

$$f' = iz e^{ixz} - \int_x^\infty \cos z(t-x) V(t) f(t, z)$$

$$\begin{aligned} f'' &= -z^2 e^{ixz} + V(x) f(x, z) - z \int_x^\infty \sin z(t-x) V(t) f(t, z) \\ &= -z^2 \left(e^{ixz} + \int_x^\infty \frac{\sin z(t-x) V f}{z} \right) + V f \end{aligned}$$

i.e.

$$\lambda f = z^2 f = -f'' + V f$$

We solve (5.13) by iteration. First set

$$m(x, z) \equiv f(x, z) e^{-ixz} \quad (5.14)$$

then m solves the equation

$$m(x, z) = 1 + \int_x^\infty D_z(t-x) V(t) m(t, z)$$

where

$$D_z(y) = \frac{e^{2izy} - 1}{2iz}.$$

For $k = 0, 1, 2, \dots$, set

$$m_{k+1}(x, z) = 1 + \int_x^\infty D_z(t - x)V(t)m_k(t, z)dt \quad (5.15)$$

where $m_0(x, z) = 1$.

Note that

$$|D_z(y)| \leq c_z, \quad \forall y \geq 0$$

Note that

$$c_z \rightarrow 0 \text{ as } |z| \rightarrow \infty, y \geq 0. \quad (5.16)$$

From (5.15) we have for $k \geq 1$

$$|m_{k+1}(x, z) - m_k(x, z)| \leq c_z \int_x^\infty |V(t)| |m_k(t, z) - m_{k-1}(t, z)|$$

or

$$\delta_k(x, z) \leq c_z \int_x^\infty |V(t)| \delta_{k-1}(t, z)dt \quad (5.17)$$

where

$$\delta_k(x, z) = |m_{k+1}(x, z) - m_k(x, z)|, \quad k \geq 1$$

Claim 129. We assume by induction that

$$\delta_k \leq \frac{c_z^{k+1}}{(k+1)!} \left(\int_x^\infty |V(t)| dt \right)^{k+1}, \quad k \geq 0 \quad (5.18)$$

Proof. As

$$\begin{aligned} \delta_0 &= |m_1(x, z) - m_0(x, z)| \\ &= \left| \int_x^\infty D_z(t - x)V(t)m_0 \right| \leq c_z \int_x^\infty |V(t)| dt \end{aligned}$$

We see that (5.18) is true for $k \geq 0$. Assuming the proposition is true for k , we obtain from (5.17)

$$\begin{aligned} \delta_{k+1} &\leq c_z \int_x^\infty |V(t)| \frac{c_z^{k+1}}{(k+1)!} \left(\int_t^\infty |V(s)| ds \right)^{k+1} \\ &= -\frac{c_z^{k+2}}{(k+2)!} \int_x^\infty \frac{d}{dt} \left(\int_t^\infty |V(s)| ds \right)^{k+2} \\ &= \frac{c_z^{k+2}}{(k+2)!} \left(\int_x^\infty |V(s)| ds \right)^{k+2} \end{aligned}$$

which proves the induction. \square

Hence for $l > 0$, $k \geq 0$

$$\begin{aligned}
|m_{k+l} - m_k| &\leq \sum_{j=k}^{k+l-1} |m_{j+1} - m_j| \\
&\leq \sum_{j=k}^{k+l-1} \frac{c_z^{j+1}}{(j+1)!} \left(\int_x^\infty |V(s)| ds \right)^{j+1} \\
&\leq \sum_{j=k}^\infty \frac{(c_z \int_x^\infty |V(s)| ds)^{j+1}}{(j+1)!} \tag{5.19}
\end{aligned}$$

which goes to zero as $k \rightarrow \infty$. Moreover the convergence is uniform for $x \in \mathbb{R}$ and also for z in $\bar{\mathbb{C}}_+ \setminus \{0\}$ as long as z stays away from 0, it follow that $m_k(x, z) \rightarrow m(x, z)$ uniformly for $x \in \mathbb{R}$ and $z \in \bar{\mathbb{C}}_+$ away form 0.

This means that for any $z \in \bar{\mathbb{C}}_+ \setminus \{0\}$, we may take the limit in (5.14) to obtain

$$m(x, z) = 1 + \int_x^\infty D_z(t-x)V(t)m(t, z)dt$$

as desired. Note that letting $l \rightarrow \infty$ in (5.19) with $h = 0$, we obtain the bound

$$|m(x, z) - 1| \leq \sum_0^\infty \frac{(c_z \int_x^\infty |V| ds)^{j+1}}{(j+1)!} = e^{c_z \int_x^\infty |V(t)| dt} - 1 \tag{5.20}$$

In particular, that for $z \in \bar{\mathbb{C}}_+ \setminus \{0\}$, $m(x, z)$ is bounded on \mathbb{R} .

And $m(x, z) \rightarrow 1$ as $x \rightarrow \infty$.

In particular

$$f(x, z) = m(x, z)e^{izx}$$

is bounded as $x \rightarrow \infty$. In fact, it decays exponentially for $z \in \mathbb{C}_+$, in particular, it is L^2 at $+\infty$.

Moreover as $m(x, z) \sim 1$ as $x \rightarrow \infty$, we can construct as 2nd solution to $-y^2 + Vy = z^2y$ according to the commutation formula

$$\tilde{f} = f \int_x^\infty \frac{dt}{f^2} = m e^{izx} \int_x^\infty \frac{dt}{m^2 e^{izx^2}} \sim e^{izx} e^{-2izx} = e^{-izx} \rightarrow \infty$$

Hence $\tilde{f} \notin L^2$ at infinity, so we have proof here that V is in the limit point case at ∞ .

Alternatively for $z \in \mathbb{R} \setminus \{0\}$, $f(x, z)$ is oscillating at ∞ , and so V cannot be in the limit circle case. It follows that for $z \in \mathbb{C}_+$, $f(x, z)$ is the unique solution of $Hf = z^2f$ in L^2 at ∞ .

Observe that it follows by induction that for each k , $m_k(x, z)$ is analytic in \mathbb{C}_+ and as the convergence is uniform in compact subsets of \mathbb{C}_+ , it follows that for each x , $m(x, z)$ is analytic in \mathbb{C}_+ . Similar considerations imply that for each x , $m(x, z)$ is continuous in $\bar{\mathbb{C}}_+ \setminus \{0\}$.

The solutions $-y_j'' + Vy_j = z^2 y_j$ with $y_1(0, z) = y_2'(0, z) = 1$ and $y_1'(0, z) = y_2(0, z) = 0$ are obtained by solving the integral equations again by iteration

$$y_1(x, z) = \cos zx + \int_0^x \frac{\sin(x-t)z}{z} V(t) y_1(t, z) dt$$

$$y_2(x, z) = \frac{\sin zx}{z} + \int_0^x \frac{\sin(x-t)z}{z} V(t) y_2(t, z) dt$$

respectively. Now these equations may be solved for all z (set $\frac{\sin zx}{z} = x$ for $z = 0$) and one finds that $y_1(x, z)$ and $y_2(x, z)$ are analytic $\forall z \in \mathbb{C}$, for any fixed x .

Now we know that for $z^2 \notin \mathbb{R}$, i.e. $z \in \mathbb{C}_+ \setminus i\mathbb{R}$,

$$f(x, z) = f(0, z) (y_1(x, z) + m_\infty y_2(x, z))$$

Differentiate at $x = 0$, one obtains

$$m_\infty(z) = \frac{f'(0, z)}{f(0, z)}$$

Note 130. For $z^2 \in \mathbb{C} \setminus \mathbb{R}$. i.e. $z \notin i\mathbb{R}_+$ neither $f(0, z)$ nor $f'(0, z)$ can vanish. This is because $m_\infty(z)$ is analytic and non-zero in this region (recall $\frac{\text{Im} m_\infty(\lambda)}{\text{Im} \lambda} = \int_0^\infty |\chi|^2 dx \neq 0$) and so if $f(0, z) = 0$, then $f'(0, z) = 0$ and vice versa. But then $f(0, z) \equiv 0$, as f solves a 2nd order ode, but $f(x, z) = m(x, z)e^{izx} \sim e^{izx} \neq 0$ for $x \rightarrow \infty$.

Lecture 12
(12/6/13)

6 Applications to Spectral Theory (continued)

6.1 L^1 Potentials (continued)

Now from (3.5), at points $\mu < \lambda$ of continuity of ρ we have

$$\begin{aligned}\rho(\lambda - \mu) &= \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_{\mu}^{\lambda} \operatorname{Im} \frac{f'(0, \sqrt{v+i\varepsilon})}{f(0, \sqrt{v+i\varepsilon})} d\nu \\ &= \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_{\mu}^{\lambda} \left(\frac{f'(0, \sqrt{v+i\varepsilon})}{f(0, \sqrt{v+i\varepsilon})} - \overline{\frac{f'(0, \sqrt{v+i\varepsilon})}{f(0, \sqrt{v+i\varepsilon})}} \right) d\nu \\ &= \lim_{\varepsilon \downarrow 0} \frac{1}{2\pi i} \int_{\mu}^{\lambda} \frac{f'(0, \sqrt{v+i\varepsilon}) \overline{f(0, \sqrt{v+i\varepsilon})} - \overline{f'(0, \sqrt{v+i\varepsilon})} f(0, \sqrt{v+i\varepsilon})}{|f(0, \sqrt{v+i\varepsilon})|^2} d\nu\end{aligned}$$

Suppose $0 < \mu < \lambda$, then

$$\begin{aligned}\rho(\lambda - \mu) &= \frac{1}{2\pi i} \int_{\mu}^{\lambda} \frac{f'(0, \sqrt{v}) \overline{f(0, \sqrt{v})} - \overline{f'(0, \sqrt{v})} f(0, \sqrt{v})}{|f(0, \sqrt{v})|^2} d\nu \\ &= \frac{1}{\pi} \int_{\mu}^{\lambda} \frac{\sqrt{v}}{|f(0, \sqrt{v})|^2} d\nu\end{aligned}$$

and so for $\lambda > 0$ (see (5.4) when $V = 0$ and so $f(0, \sqrt{\lambda}) = 1$)

$$\frac{d\rho}{d\lambda} = \frac{\sqrt{\lambda}}{\pi |f(0, \sqrt{\lambda})|^2}. \quad (6.1)$$

use this result for $z > 0$,

$$y_2(x, z^2) = \frac{\overline{f(0, z)} f(x, z) - f(0, z) \overline{f(x, z)}}{2iz}$$

Indeed $\operatorname{RHS}(x=0) = 0$ and $\frac{d}{dx} \operatorname{RHS}|_{x=0} = \frac{\overline{f(0)} f'(0) - f(0) \overline{f'(0)}}{2iz} = 1$.

For $\lambda > 0$, writing $f(0, z) = |f(0, z)| e^{i\eta(z)}$, use the result above

$$\begin{aligned}y_2(x, \lambda) &= \frac{|f(0, \sqrt{\lambda})|}{2i\sqrt{\lambda}} (e^{-i\eta(\sqrt{\lambda})} f(x, \sqrt{\lambda}) - e^{i\eta(\sqrt{\lambda})} \overline{f(x, \sqrt{\lambda})}) \\ &\sim \frac{|f(0, \sqrt{\lambda})|}{2i\sqrt{\lambda}} (e^{i(x\sqrt{\lambda} - \eta(\sqrt{\lambda}))} - e^{-i(x\sqrt{\lambda} - \eta(\sqrt{\lambda}))})\end{aligned}$$

as $x \rightarrow \infty$.

$$y(x, \lambda) \sim \frac{f(0, \sqrt{\lambda})}{\sqrt{\lambda}} \sin \left(x\sqrt{\lambda} - \eta(\sqrt{\lambda}) \right)$$

$\eta(\sqrt{\lambda})$ is called the *phase shift*. (note $\eta = 0$ if $V = 0$.)

Now suppose $\mu < \lambda < 0$. Although $f(0, z) \neq 0$ in $\{\operatorname{Re} z > 0, \operatorname{Im} z > 0\}$, it is possible that $f(0, z) = 0$ for some $z \in i\mathbb{R}_+$. In fact if $f(0, i\gamma) = 0$, $\gamma > 0$ then $f(x, i\gamma) \sim e^{-\gamma x} \in L^2(0, \infty)$ and so $-\gamma^2 = (i\gamma)^2$ is an L^2 eigenvalue of \bar{H} .

Now as $f(0, z)$ is analytic in \mathbb{C}_+ and $f(0, z) \rightarrow 1$ as $z \rightarrow \infty$ (see (5.16), (5.20)) the zero's $f(0, z)$ on $i\mathbb{R}$, if any, are isolated and can only accumulate at 0. Suppose that $f(0, i\gamma) = 0$ for some $\gamma > 0$, we show that $\frac{df}{dz}(0, i\gamma) \neq 0$.

Recall that (see (2.18)) for $\lambda \in \mathbb{C} \setminus \mathbb{R}$

$$\int_0^\infty |\chi(x, \lambda)|^2 dx = \frac{\operatorname{Im} m_\infty(\lambda)}{\operatorname{Im} \lambda} > 0$$

Now as $f(0, i\gamma) = 0$, we must have $f'(0, i\gamma) \neq 0$. Suppose $f(0, z) = (z - i\gamma)^p \alpha(1 + O(z - i\gamma))$ for some integer $p \geq 1$. (As $f(0, z)$ is analytic at $z = i\gamma$, it must vanish at most at a power rate as $z \rightarrow i\gamma$.) and some $\alpha > 0$.

For $z = i\gamma + \delta + i\delta'$, $\delta^2 + \delta'^2$ small, $\delta > 0$, we have

$$\begin{aligned} m_\infty &= \frac{f'(0, z)}{f(0, z)} = \frac{f'(0, i\gamma)(1 + O(z - i\gamma))}{\alpha(\delta + i\delta')^p(1 + O(\delta + i\delta'))} \\ &= \frac{\beta}{(\delta + i\delta')^p}(1 + O(\delta + i\delta')) \end{aligned}$$

for some $\beta \neq 0$. On the other hand, $\operatorname{Im} \lambda > 0$ and hence we must have

$$\operatorname{Im} \frac{\beta}{(\delta + i\delta')^p}(1 + O(\delta + i\delta')) > 0$$

for all δ, δ' small $\delta > 0$ Now

$$\delta + i\delta' = \sqrt{\delta^2 + \delta'^2} e^{i\phi}$$

where $\cos \phi > 0$ i.e. $-\pi/2 < \phi < \pi/2$, we must have

$$\operatorname{Im} e^{-ip\phi} e^{i\theta}(1 + O(\delta + i\delta')) > 0$$

where $\beta = |\beta|e^{i\theta}$, i.e.

$$\sin(\theta - p\phi) + O(\sqrt{\delta + i\delta'}) > 0 \tag{6.2}$$

Now if $p \geq 2\pi$, $p\phi$ runs through an interval of sign $\geq 2\pi$ and so (6.2) fails for some $\phi \in (-\pi/2, \pi/2)$. Thus we must have $p = 1$ i.e. $\frac{df}{dz}(0, i\gamma) \neq 0$.

Now $f(0, i\gamma)$, $f'(0, i\gamma)$ are real and so in particular $\frac{df}{d\gamma}(0, i\gamma) = i\frac{df}{dz}(0, i\gamma)$ is real. We have for $z \sim i\gamma$ $\text{Re} z > 0$

$$\begin{aligned} m_\infty(z^2) &= \frac{f'(0, z)}{f(0, z)} = \frac{if'(0, i\gamma)(1 + O(z - i\gamma))}{(z - i\gamma)\frac{d}{d\gamma}f(0, i\gamma)(1 + O(z - i\gamma))} \\ &= i\frac{f'(0, i\gamma)}{\frac{d}{d\gamma}f(0, i\gamma)} \frac{1}{z - i\gamma} (1 + O(z - i\gamma)) \end{aligned}$$

consider $\mu < -\gamma^2 < \lambda < 0$, $\lambda - \mu$ small. i.e. $\sqrt{-\lambda} < \gamma < \sqrt{-\mu}$

$$\begin{aligned} \text{Imm}_\infty(z^2) &\sim \text{Im} i \frac{f'(0, i\gamma)}{\frac{d}{d\gamma}f(0, i\gamma)} \frac{\bar{z} + i\gamma}{(z - i\gamma)^2} \\ &= \frac{f'(0, i\gamma)}{\frac{d}{d\gamma}f(0, i\gamma)} \frac{\text{Re} z}{(\text{Re} z)^2 + (\text{Im} z - \gamma)^2} \end{aligned}$$

also $\sqrt{\nu + i\varepsilon} = \sqrt{-|\nu| + i\varepsilon} \sim i\sqrt{|\nu|}(1 - \frac{i\varepsilon}{2|\nu|}) = i\sqrt{|\nu|} + \frac{\varepsilon}{2\sqrt{|\nu|}}$.

Hence

$$\text{Imm}_\infty(z^2) \sim \frac{f'(0, i\gamma)}{\frac{d}{d\gamma}f(0, i\gamma)} \frac{\frac{\varepsilon}{2\sqrt{|\nu|}}}{(\frac{\varepsilon}{2\sqrt{|\nu|}})^2 + (\sqrt{|\nu|} - \gamma)^2}$$

Hence for $\varepsilon > \text{small}$

$$\begin{aligned} \frac{1}{\pi} \int_\mu^\lambda \text{Imm}_\infty(\nu + i\varepsilon) d\nu &\sim \frac{1}{\pi} \int_\mu^\lambda \frac{f'(0, i\gamma)}{\frac{d}{d\gamma}f(0, i\gamma)} \frac{\frac{\varepsilon}{2\sqrt{|\nu|}}}{(\frac{\varepsilon}{2\sqrt{|\nu|}})^2 + (\sqrt{|\nu|} - \gamma)^2} d\nu \\ &= \frac{1}{\pi} \int_{\sqrt{-\mu}}^{\sqrt{-\lambda}} \frac{f'(0, i\gamma)}{\frac{d}{d\gamma}f(0, i\gamma)} \frac{\frac{\varepsilon}{2s}}{(\frac{\varepsilon}{2s})^2 + (s - \gamma)^2} (-2s) ds \\ &= \frac{2}{\pi} \int_{\sqrt{-\mu}}^{\sqrt{-\lambda}} \frac{f'(0, i\gamma)}{\frac{d}{d\gamma}f(0, i\gamma)} \frac{\frac{\varepsilon}{2}s^2}{(\frac{\varepsilon}{2})^2 + s^2(s - \gamma)^2} ds \\ &= \frac{2}{\pi} \int_{(\sqrt{-\mu} - \gamma)2/\varepsilon}^{(\sqrt{-\lambda} - \gamma)2/\varepsilon} \frac{f'(0, i\gamma)}{\frac{d}{d\gamma}f(0, i\gamma)} \frac{(\gamma + \frac{\varepsilon}{2}t)^2}{1 + (\gamma + \frac{\varepsilon}{2}t)^2 t^2} dt \end{aligned}$$

Now $\frac{(\gamma + \frac{\varepsilon}{2}t)^2}{1 + (\gamma + \frac{\varepsilon}{2}t)^2 t^2} \leq \frac{A}{1 + t^2}$ for some $A < \infty$.

Hence by dominated convergence, as $\varepsilon \downarrow 0$

$$\begin{aligned} \frac{1}{\pi} \int_{\mu}^{\lambda} \operatorname{Im} m_{\infty}(\nu + i\varepsilon) d\nu &\rightarrow \frac{2}{\pi} \int_{-\infty}^{\infty} \frac{f'(0, i\gamma)}{\frac{d}{d\gamma} f(0, i\gamma)} \frac{\gamma^2}{1 + \gamma^2 t^2} dt \\ &= 2\gamma \frac{f'(0, i\gamma)}{\frac{d}{d\gamma} f(0, i\gamma)} \end{aligned}$$

As $f(0, z)$ and $f'(0, z)$ are real on $i\mathbb{R}_+$, and so $m_{\infty}(z^2)$ is real for $z \in i\mathbb{R}_+$, it follows that $\rho(\lambda) - \rho(\mu) = 0$ if there is no $z \in i\mathbb{R}_+$ with $f(0, z) = 0$ and $\lambda < z^2 < \mu < 0$. Thus $\rho(\lambda)$ is piecewise constant for $\lambda > 0$ with jumps $2\gamma \frac{f'(0, i\gamma)}{\frac{d}{d\gamma} f(0, i\gamma)}$ at points $\lambda = -\gamma^2$, where $f(0, i\gamma) = 0$, $\gamma > 0$.

Now at $z = i\gamma$, $f(x, i\gamma)$ is in $L^2(0, \infty)$ and $f(0, i\gamma) = 0$. Thus $y_2(x_1 - \gamma^2) = \frac{f(x, i\gamma)}{f'(0, i\gamma)}$.

If $g \in L^2(0, \infty)$, the contribution of $\lambda = -\gamma^2$ to Parseval's relation (3.4),

$$\int_0^{\infty} |g(x)|^2 dx = \int d\rho(\lambda) |\hat{g}(\lambda)|^2$$

is given by

$$\begin{aligned} 2\gamma \frac{f'(0, i\gamma)}{\frac{d}{d\gamma} f(0, i\gamma)} \left| \int_0^{\infty} y_2(x, -\gamma^2) g(x) dx \right|^2 & \quad (6.3) \\ &= \frac{2\gamma}{\frac{d}{d\gamma} f(0, i\gamma) f'(0, i\gamma)} \left| \int_0^{\infty} f(x, i\gamma) g(x) dx \right|^2 \end{aligned}$$

we have

$$\begin{aligned} -f'' + Vf &= -\gamma^2 f \\ -\dot{f}'' + V\dot{f} &= -\gamma^2 \dot{f} - 2\gamma f \end{aligned}$$

where $\dot{f} = \frac{d}{d\gamma} f(x, i\gamma)$.

$$\begin{aligned} \frac{d}{dx} \dot{f}' f - \dot{f} f' &= \dot{f}'' f - \dot{f} f'' \\ &= (V + \gamma^2) \dot{f} f - \dot{f} (V + \gamma^2) f + 2\gamma f^2 \end{aligned}$$

Integration 0 to ∞ , we obtain

$$\left[\dot{f}' f - \dot{f} f' \right]_0^{\infty} = 2\gamma \int_0^{\infty} f^2$$

LHS = $0 - \left[0 - \dot{f}(0, i\gamma)f'(0, i\gamma)\right]$. hence

$$2\gamma \int_0^\infty f(x, i\gamma)^2 dx = \dot{f}(0, i\gamma)f'(0, i\gamma) \quad (6.4)$$

Inserting (6.4) into (6.3), we obtain using (6.1), and assuming only one zero $f(0, i\gamma) = 0$,

$$\begin{aligned} \int_0^\infty |g(x)|^2 dx &= \left| \int_0^\infty \hat{f}(x, i\gamma)g(x)dx \right|^2 \\ &\quad + \frac{1}{\pi} \int_0^\infty |\hat{g}(x)|^2 \frac{\sqrt{\lambda}d\lambda}{\left|f(0, \sqrt{\lambda})\right|^2} \end{aligned}$$

where $\hat{f}(x, i\gamma) = \frac{f(x, i\gamma)}{\sqrt{\int_0^\infty |f(x, i\gamma)|^2 dx}}$ is the normalized eigenvector corresponding to $\lambda = -\gamma^2$.

If $f(0, i\gamma_j) = 0$, $\gamma_j > 0$, $1 \leq j \leq N \leq \infty$, then we have a contribution

$$\sum_{j=1}^N \left| \int_0^\infty \hat{f}(x, i\gamma_j)g(x)dx \right|^2$$

to the Plancherel formula.

We conclude that

Theorem 131. *$V(x)$ is continuous and real valued, and*

$$\int_0^\infty |V(x)| dx < \infty$$

then

$$\sigma(\bar{H}) = \sigma_{ess}(\bar{H}) \cup \sigma_{disc}(\bar{H})$$

where $\sigma_{ess}(\bar{H}) = \sigma_{ac}(\bar{H}) = [0, \infty)$ and $\sigma_{disc}(\bar{H}) = \{\lambda_j\}_{j=1}^N$, $N < \infty$, where each $\lambda_j \leq 0$ and is a simple eigenvalue.

The λ_j 's can only accumulate at 0.

6.2 Discrete Spectrum finite or infinite

Is the discrete spectrum finite or infinite? (see Reed-Simon Vol IV)

Theorem 132. Let $V(x)$ be continuous and real valued on $[0, \infty)$ such that $V(x) \rightarrow 0$ as $x \rightarrow \infty$. Let \bar{H} = closure of $-d^2/dx^2 + V$ on $C_0^\infty[0, \infty) \cap \{u(0) = 0\}$

(i) If $V(x) \leq -\frac{a}{x^{2-\varepsilon}}$ for some $a, \varepsilon > 0$, for $x > R_0$ for some R_0 , then $\sigma_{disc}(\bar{H})$ is infinite.

(ii) If $V(x) \geq -\frac{1}{4}bx^{-2}$ for $x > R_0$ for some R_0 , and $b < 1$, then $\sigma_{disc}(\bar{H})$ is finite.

Proof. (i) By previous result, $\sigma_{ess}(\bar{H}) = [0, \infty)$ in both cases (i) and (ii).

Let $\psi \in C_0^\infty(\mathbb{R})$ with support in $\{1 < x < 2\}$, $\|\psi\|_{L^2(0, \infty)} = 1$, $\psi \geq 0$. For $R > 0$, let $\psi_R = R^{-1/2}\psi(\frac{x}{R})$ so $\|\psi_R\|_{L^2(0, \infty)} = 1$ and $\text{supp}\psi_R \subset \{R < x < 2R\}$. If $R > R_0$ we conclude that

$$\begin{aligned} (\psi_R, H\psi_R) &= (\psi_R, -d^2/dx^2\psi_R) + (\psi_R, V\psi_R) \\ &\leq (\psi_R, -d^2/dx^2\psi_R) - a(\psi_R, x^{-2+\varepsilon}\psi_R) \\ &= \frac{1}{R^2}(\psi, -d^2/dx^2\psi) - \frac{a}{R^{2-\varepsilon}}(\psi, x^{-2+\varepsilon}\psi) \end{aligned}$$

Hence $\exists R_1 > R_0$ s.t. $(\psi_R, H\psi_R) < 0$ for $R < R_1$. Let $\psi_n = \psi_{2^n R_1}$, $n = 1, 2$. As $\text{supp}\psi_n \subset \{2^n R_1 < x < 2^{n+1} R_1\}$ the ψ_n 's are orthonormal and also $(\psi_n, H\psi_m) = 0$ if $n \neq m$.

Now let N be given. Let f_1, \dots, f_{N-1} be any given functions in $L^2(0, \infty)$. Then $\exists a_1, \dots, a_N$, $\sum_1^N |a_i|^2 = 1$, s.t.

$$\psi = a_1\psi_1 + \dots + a_N\psi_N \perp \langle f_1, \dots, f_{N-1} \rangle$$

and $\|\psi\|^2 = \sum_1^N |a_i|^2 = 1$, thus

$$\begin{aligned} \inf_{\substack{g \in Q(H) \\ g \perp \langle f_1, \dots, f_{N-1} \rangle \\ \|g\| = 1}} (g, Hg) &\leq (\psi, H\psi) \\ &= \left(\sum_1^N a_i \psi_i, H \sum_1^N a_i \psi_i \right) \\ &= \sum_1^N |a_i|^2 (\psi_i, H\psi_i) \\ &\leq \left(\max_{1 \leq i \leq N} (\psi_i, H\psi_i) \right) \sum_1^N |a_i|^2 \\ &= \max_{1 \leq i \leq N} (\psi_i, H\psi_i) \end{aligned}$$

Hence

$$\begin{aligned}\mu_N &= \sup_{f_1, \dots, f_{N-1}} \inf_{\substack{g \in Q(H) \\ g \perp \langle f_1, \dots, f_{N-1} \rangle \\ \|g\| = 1}} (f, Hf) \\ &\leq \max_{1 \leq i \leq N} (\psi_i, H\psi_i) \\ &< 0\end{aligned}$$

Thus $\mu_N < 0 \forall N$ and so by Min-Max, as $\sigma_{ess}(\bar{H}) = [0, \infty)$, $\sigma_{disc}(\bar{H})$ is infinite.

Proof of (ii).

Recall Hardy's inequality: if $f \in C_0^\infty(0, \infty)$, then

$$\int_0^\infty |f'|^2 dx \geq \frac{1}{4} \int_0^\infty \frac{|f|^2}{x^2} dx$$

To prove Hardy, it's enough to consider real f .

Now for $f \in C_0^\infty(0, \infty)$, by commutation

$$\begin{aligned}0 &\leq \int_0^\infty \left| \sqrt{x} \frac{d}{dx} \frac{f}{\sqrt{x}} \right|^2 dx \\ &= - \int_0^\infty f \left(\frac{1}{\sqrt{x}} \frac{d}{dx} x \frac{d}{dx} \frac{1}{\sqrt{x}} f \right) dx \\ &= \int_0^\infty -f f'' + f^2 \frac{1}{\sqrt{x}} (\sqrt{x})'' dx \\ &= \int_0^\infty f'^2 + f^2 \left(-\frac{1}{4x^2} \right) dx\end{aligned}$$

and Hardy is proved.

Let $W = V + \frac{1}{4}bx^{-2}$, then as quadratic forms on $C_0^\infty(0, \infty)$,

$$\begin{aligned}-\frac{d^2}{dx^2} + V &= -(1-b)\frac{d^2}{dx^2} + W + b\left(-\frac{d^2}{dx^2} - \frac{1}{4}\frac{1}{x^2}\right) \quad (6.5) \\ &\geq -(1-b)\frac{d^2}{dx^2} + W \\ &\geq -(1-b)\frac{d^2}{dx^2} + \tilde{W}\end{aligned}$$

where $\tilde{W} = \min(W(x), 0)$, as $W(x) \geq 0$ for $2 > R_0$, \tilde{W} has compact support.

By Min-Max, as the form inequalities (6.5) are preserved under closure of the forms

$$\mu_n(-\frac{d^2}{dx^2} + V) \geq (1-b)\mu_n(-\frac{d^2}{dx^2} + \frac{\tilde{W}}{1-b}) \quad (6.6)$$

but by the proof of claim 114 $-\frac{d^2}{dx^2} + \frac{\tilde{W}}{1-b}$ has only a finite number of bounded states below 0, and

$$\inf \sigma_{ess}(-\frac{d^2}{dx^2} + \frac{\tilde{W}}{1-b}) = 0$$

for $n \geq \tilde{N}$ for some \tilde{N} . But then by (6.6) and the fact that $\sigma_{ess}(-\frac{d^2}{dx^2} + V) = [0, \infty)$,

$$\mu_n(-\frac{d^2}{dx^2} + V) = 0$$

for $n \geq N$, and hence $-\frac{d^2}{dx^2} + V$ has only a finite number of eigenvalues below 0. This proves the theorem. \square

6.3 Zeros of eigenfunctions

A very important result for Schrodinger operator in 1 dim is the following *comparison theorem*.

Theorem 133. *Suppose ψ is a real solution on (a, b) of*

$$\psi'' + g_1\psi = 0$$

and ϕ is a real solution of

$$\phi'' + g_2\phi = 0$$

Let $g_2(x) > g_1(x)$ on (a, b) . If x_1 and x_2 are successive zeros of ψ on (a, b) , then ϕ must vanish at some point in (x_1, x_2) .

Proof. We have

$$\psi''\phi - \psi\phi'' + (g_1 - g_2)\psi\phi = 0 \quad (6.7)$$

Without loss of generality we can assume $\psi(t)$ and $\phi(t) > 0$ for t on (x_1, x_2) . Then integrating (6.7), we obtain

$$\int_{x_1}^{x_2} (\psi''\phi - \psi\phi'') dx > 0$$

i.e.

$$(\psi'\phi - \psi\phi')(x_2) > (\psi'\phi - \psi\phi'')(x_1)$$

but as $\psi(x_1) = \psi(x_2) = 0$ we must have

$$\psi'\phi(x_2) > \psi'\phi(x_1)$$

but clearly $\psi'(x_2) < 0$ and $\psi'(x_1) > 0$, but $LHS \leq 0$ and $RHS \geq 0$, which is impossible. Thus ϕ must vanish for some $x_1 < x < x_2$. \square

Now let V be a real valued and continuous function on $[0, \infty)$ with

$$\int_0^\infty |V(x)| dx < \infty$$

as above. Then we know that $H = -d^2/dx^2 + V(x)$ defined on $D(H) = C_0^\infty[0, \infty) \cap \{u(0) = 0\}$ is e.s.a. and $\bar{H} = H^* = H_F$ where H_F is the Friedrichs extension of H . Let $Q_0 = \{f \in L^2(0, \infty) : f \text{ abs cont, } f' \in L^2, f(0) = 0\}$ then $g \in D(\bar{H}) = D(H_F)$ iff $g \in Q_0$ and

$$Q(f, g) = \int_0^\infty \bar{f}'g' + V\bar{f}g = (f, H_F g) = (\bar{f}, -g'' + Vg) \quad (6.8)$$

$\forall f \in Q_0$.

In particular we see that if $f \in Q_0$ and $g \in D(\bar{H})$, then for $x > 0$,

$$\begin{aligned} \int_0^x f'g' + Vfg &= fg'|_0^x + \int_0^x fH_F g \\ &= fg'(x) + \int_0^x fH_F g \end{aligned}$$

Letting $x \rightarrow \infty$, we see from (6.8) that

$$\lim_{x \rightarrow \infty} fg'(x) = 0 \quad (6.9)$$

We also know from our previous results that

$$\sigma(\bar{H}) = \sigma_{ess}(\bar{H}) \cup \sigma_{disc}(\bar{H})$$

where $\sigma_{ess}(\bar{H}) = \sigma_{ac}(\bar{H}) = [0, \infty)$, and $\sigma_{disc}(\bar{H}) = \{\lambda_i\}_{i=0}^N$, $0 \leq N \leq \infty$, with $\lambda_0 < \lambda_1 < \dots < \lambda_i < \dots < 0$, and the λ_i 's can only accumulate at 0.

By Min-Max for $k \geq 0$

$$\lambda_k = \sup_{(\psi_1, \dots, \psi_k)} \inf_{\substack{\psi \perp \langle \psi_1, \dots, \psi_k \rangle \\ \psi \in Q(\bar{H}) = Q_0 \\ \|\psi\| = 1}} Q(\psi)$$

where $Q(\psi) = \int_0^\infty |\psi'|^2 + \int_0^\infty V|\psi|^2$.

Theorem 134. Let $u_k \neq 0$ be the eigenvalue (unique up to scalar multiples) corresponding to λ_k , $k \geq 0$, $\bar{H}u_k = \lambda_k u_k$. Then $u_k(x)$ has precisely k zero in $(0, \infty)$.

Proof. Suppose $u_k(x)$ has $\geq k+1$ zeros in $(0, \infty)$,

$$x_0 \equiv 0 < x_1 < x_2 < \dots < x_k < x_{k+1} < \dots$$

Note that $u_k(0) = 0$ as $u_k \in Q_0$ For $0 \leq j \leq k$ let

$$\chi_j(x) = u_k \chi_{[x_j, x_{j+1})}(x)$$

and let

$$\chi_{j+1}(x) = u_k \chi_{[x_{j+1}, \infty)}(x)$$

then the $k+2$ functions $\chi_0, \dots, \chi_{k+1}$ are independent and lie in Q_0 . If $\psi_1, \dots, \psi_{k+1}$ is any collection of $k+1$ functions, then $\exists a_0, a_1, \dots, a_{k+1}$ with $\sum_{j=0}^{k+1} |a_j|^2 = 0$ s.t. $\psi = \sum_{j=0}^{k+1} a_j \chi_j \perp \psi_l$, $l = 1, 2, \dots, k+1$. Then

$$\begin{aligned} \inf_{\substack{g \perp \langle \psi_1, \dots, \psi_{k+1} \rangle \\ g \in Q_0 \\ \|g\| = 1}} Q(g) &\leq \frac{Q(\psi)}{\|\psi\|^2} \\ &= \left(\sum_{j=0}^k |a_j|^2 \int_{x_j}^{x_{j+1}} |u'_k(x)|^2 + Q|u_k|^2 + |a_{k+1}|^2 \int_{x_{j+1}}^{\infty} |u'_k|^2 + Q|u_k|^2 \right) / \|\psi\|^2 \end{aligned}$$

As $u_k(x) = 0$ for $x = x_j$, $0 \leq j \leq k+1$, we have

$$\int_{x_j}^{x_{j+1}} |u'_k|^2 + |u_k|^2 V = \int_{x_j}^{x_{j+1}} \bar{u}_k \bar{H} u_k$$

for $0 \leq j \leq k$. Also for $y > x_{k+1}$,

$$\begin{aligned} \int_{x_{k+1}}^y |u'_k|^2 + |u_k|^2 V &= \bar{u}_k u'_k|_{x_{k+1}}^y + \int_{x_{j+1}}^y \bar{u}_k \bar{H} u_k \\ &= (\bar{u}_k u'_k)(y) + \int_{x_{j+1}}^y \bar{u}_k \bar{H} u_k \end{aligned}$$

But as $\bar{u}_k \in Q_0$ and $u_k \in D(\bar{H})$, $\lim_{y \rightarrow \infty} (\bar{u}_k u'_k)(y) = 0$ by (6.9), we conclude that

$$\begin{aligned} \inf_{\substack{g \perp \langle \psi_1, \dots, \psi_{k+1} \rangle \\ g \in Q_0 \\ \|g\| = 1}} Q(g) &\leq (\lambda_k \sum_{j=0}^k |a_j|^2 \int_{x_j}^{x_{j+1}} |u_k(x)|^2 + |a_{k+1}|^2 \int_{x_{j+1}}^{\infty} |u_k|^2) / \|\psi\|^2 \\ &= \lambda_k \end{aligned}$$

But then by Min-Max $\lambda_{k+1} \leq \lambda_k$, which is a contradiction.

Hence $u_k(x)$ has at most k zero's. In order to prove that $u_k(x)$ has precisely k zero's in $(0, \infty)$, it is clearly sufficient to show that $u_{k+1}(x)$ has more zeros in $(0, \infty)$ than $u_k(x)$, $k \geq 0$, so fix $k \geq 0$ and suppose $u_k(x)$ has j zeros, $j \leq k$ in $(0, \infty)$

$$x_1 < x_2 < \dots < x_j$$

Now by theorem 133, as $\lambda_{k+1} > \lambda_k$, u_{k+1} has at least 1 zero in each of the intervals (x_i, x_{i+1}) , $0 \leq i < j-1$. Suppose that $u_{k+1}(x)$ has no zeros in (x_j, ∞) , wlog we can assume $u_{k+1}(x)$ and $u_k(x) > 0$ in (x_i, ∞) . Then for $y > x_j$, we obtain as in the proof of theorem 133,

$$(u'_k u_{k+1} - u_k u'_{k+1})(y) - (u'_k u_{k+1} - u_k u'_{k+1})(x_j) = (\lambda_2 - \lambda_1) \int_{x_j}^y u_k u_{k+1}$$

But as $u_k, u_{k+1} \in D(\bar{H}) \subset Q_0$ we have from (6.9), $\lim_{u \rightarrow \infty} (u'_k u_{k+1} - u_k u'_{k+1})(y) = 0$, then

$$0 - (u'_k u_{k+1} - u_k u'_{k+1})(x_j) = (\lambda_2 - \lambda_1) \int_{x_j}^y u_k u_{k+1}$$

i.e.

$$-u'_k u_{k+1}(x_j) = (\lambda_2 - \lambda_1) \int_{x_j}^y u_k u_{k+1} > 0 \quad (6.10)$$

But $u'_k(x_j) > 0$ and $u_{k+1}(x_j) \geq 0$, thus $LHS \leq 0$, and we obtain a contradiction. Thus $u_{k+1}(x)$ also has a zero in (x_j, ∞) . Hence $u_{k+1}(x)$ has at least $j+1$ zero's in $(0, \infty)$, which is what we wanted to show. \square

Remark 135. Similar argument show that on a finite interval $[a, b]$, $H = -d^2/dx^2 + V(x)$ with boundary conditions

$$\cos \alpha u(a) + \sin \alpha u'(a) = 0$$

$$\cos \beta u(b) + \sin \beta u'(b) = 0$$

α, β given, has eigenvalues $\lambda_0 < \lambda_1 < \dots < \lambda_k < \dots$, $\lambda_k \rightarrow \infty$ with associated eigenfunctions $u_k(x)$ with the property that $u_k(x)$ has precisely k zeros in (a, b) .

For an ode proof of this fact, see Coddington, Levinson chapter 8.

Question 136. *How much of the theory goes through for pdes? For example, does the "nth" eigenfunction $u(x)$ of Laplacian with Dirichlet boundary conditions in a region Ω in \mathbb{R}^d have the property that $\{x \in \Omega : u(x) \neq 0\}$ have n components? (see Courant, Hilbert II)*

Theorem 137. Let V and $\bar{H} = -d^2/dx^2 + V$ be as above and assume in addition that

$$\int_0^\infty x |V(x)| dx < \infty$$

then

$$\#\{\lambda_k < 0 : \lambda_k \text{ is an } L^2 \text{ eigenvalue of } \bar{H}\} \leq \int_0^\infty x |V(x)| dx < \infty \quad (6.11)$$

Proof. (See Coddington, Levinson p255 problem 3)

Let $h(x) = |V(x)|$. Suppose that α and β are successive zero's of a real solution ψ of

$$\psi'' + h\psi = 0$$

$0 \leq \alpha < \beta < \infty$. Then claim:

$$\psi(x) = a(x - \alpha) - \int_\alpha^x (x - s)h(s)\psi(s)ds \quad (6.12)$$

for some a . Indeed if ψ solves (6.12), then

$$\psi'(x) = a - \int_a^x h\psi$$

gives

$$\psi'' = -h\psi$$

but $\psi(\alpha) = 0$ and $\psi'(\alpha) = a$, so if we choose a appropriately, the claim is established.

Now wlog we have $\psi(x) > 0$ for $\alpha < x < \beta$ and $u = \psi'(\alpha) > 0$ thus from (6.12),

$$0 \leq \psi(x) \leq a(x - \alpha)$$

gives

$$|\psi(x)| \leq |a|(x - \alpha)$$

$\alpha \leq x \leq \beta$. Now as $\psi(\beta) = 0$, we obtain from (6.12),

$$\begin{aligned} a(\beta - a) &= \int_\alpha^\beta (\beta - s)h(s)\psi(s)ds \\ &\leq \int_\alpha^\beta (\beta - s)h(s)a(s - \alpha) \\ &\leq \int_\alpha^\beta (\beta - \alpha)h(s)a(s - \alpha) \end{aligned}$$

thus

$$1 \leq \int_{\alpha}^{\beta} (s - \alpha) h(s) ds$$

Now suppose that ψ has n zeros in $(0, \infty)$

$$x_0 = 0 < x_1 < x_2 < \dots < \infty$$

and suppose $\psi(0) = 0$, $\psi'' + h\psi = 0$ then

$$\begin{aligned} n &< \sum_{j=0}^{n-1} \int_{x_j}^{x_{j+1}} (s - x_j) h(s) ds \\ &= \sum_{j=0}^{n-1} \int_{x_j}^{x_{j+1}} s h(s) ds \\ &\leq \int_0^{\infty} s |V(s)| ds \end{aligned} \tag{6.13}$$

Now consider the operator $\bar{K} = -d^2/dx^2 - |V|$ with V replaced by $-|V|$. Suppose $\mu < 0$ is an $L^2(0, \infty)$ eigenvalue for \bar{K} whose associated eigenfunction $u(x)$ has n zeros in $(0, \infty)$

$$x_0 = 0 < x_1 < \dots < x_n$$

then by theorem 133 as $\mu < 0$ the solution ψ of $\bar{K}\psi = 0$, $\psi(0) = 0$, has at least 1 zero in each of the n intervals (x_{i-1}, x_i) , $1 \leq i \leq n$ but ψ must also have a zero in (x_n, ∞) !

To see this we note that as $\int_0^{\infty} x |V(x)| dx < \infty$, we can take $\lambda \downarrow 0$ in the equation 5.13 with $V \rightarrow -|V|$ for $f(x, z)$ to obtain the equation

$$f(x, 0) = 1 + \int_x^{\infty} (t - x)(-|V(t)|)f$$

which we can integrate as before to obtain a solution of $f'' + hf = 0$ with $f(x, 0) \rightarrow 1$ as $x \rightarrow \infty$. Also $f'(x) \rightarrow 0$ as $x \rightarrow \infty$ But then

$$g = f \int^x \frac{ax}{f^2} \sim x$$

as $x \rightarrow \infty$ is a second solution. It follows that the solution y of $y'' + hy = 0$ with $y(0) = 0$, $y'(0) = 1$ is a linear combination of f and g and hence $y(x)$ and $y'(x)$ grow at most linearly as $x \rightarrow \infty$. But as $\mu < 0$, $u(x)$ and

$u'(x)$ as exponentially decreasing as $x \rightarrow \infty$. hence arguing as in the proof of Theorem 134, we obtain the analog of (6.10)

$$-u'y(x_n) = (0 - \mu) \int_{x_n}^{\infty} u y dx$$

which again shows that y must have a zero in (x_n, ∞) . Thus y has $n+1$ zeros in $(0, \infty)$. Thus by (6.13)

$$n+1 < \int_0^{\infty} x |V(x)| dx$$

Thus $\#\{\text{eigenvalues } \mu < 0 \text{ of } K\} < \int_0^{\infty} x |V(x)| dx$, but then as

$$\bar{H} = -d^2/dx^2 + V \geq -d^2/dx^2 - |V| = \bar{K}$$

(6.11) follows by Min-Max. □

6.4 Things to Do During the Winter Break

Because we don't have time to finish them, we will leave the proof for the break.

Theorem 138. *Suppose $V(x)$ is continuous and real valued on \mathbb{R} such that*

$$\int_{-\infty}^{\infty} |V(x)| dx < \infty$$

then (i) $H = -d^2/dx^2 + V(x)$ is e.s.a.

(ii) $\sigma(\bar{H}) = \sigma_{ess}(\bar{H}) \cup \sigma_{disc}(\bar{H})$ where $\sigma_{ess}(\bar{H}) = \sigma_{ac}(\bar{H}) = [0, \infty)$ and has multiplicity 2, $\sigma_{disc}(\bar{H}) = \{\lambda_k < 0\}$ where the λ_k 's can only accumulate at 0.

(iii) if $\int_{-\infty}^{\infty} |x| |V(x)| dx < \infty$, then

$$\#\sigma_{ess}(\bar{H}) \leq 1 + \int_{-\infty}^{\infty} |x| |V(x)| dx \quad (6.14)$$

(iv) if $\int V(x) dx < \infty$, (by Min-Max) that

$$\sigma_{ess}(\bar{H}) \neq \emptyset.$$

(hence the '1' in (6.14) is necessary.)

Theorem 139. Suppose $V(x)$ is continuous, real valued and periodic on \mathbb{R} , $V(x+p) = V(x)$, for some $p > 1$.

then (i)

$$H = -d^2/dx^2 + V(x)$$

with $D(H) = C_0^\infty(\mathbb{R})$ is e.s.a

(ii)

$$\sigma(\bar{H}) = \sigma_{ess}(\bar{H}) = \sigma_{ac}(\bar{H})$$

where $\sigma_{ac}(\bar{H})$ is a countable union of intervals, i.e.

$$\sigma_{ac}(\bar{H}) = \sum_{i \in I} (\lambda_i, \lambda_{i+1})$$

$\lambda_i < \lambda_{i+1}$ for all $i \in I$. The spectrum is uniformly of multiplicity 2.

The spectral theory of $H = -d^2/dx^2 + V(x)$ with $V(x)$ periodic is often referred to as *Floquet Theory*.