

Lecture Notes and Background Materials on Linear Operators in Hilbert Space

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Comment These lecture notes assume familiarity with basic properties of Hilbert spaces and Lebesgue theory, as presented in my online document “Lecture Notes and Background Materials on Lebesgue Theory from a Hilbert and Banach Space Perspective, Including an Application to Fractal Image Compression.” A major reference for the material on Sturm-Liouville operators is the book “Differential Operators of Mathematical Physics. An Introduction” by Günter Hellwig, Addison-Wesley, Reading, Massachusetts, 1967.

Chapter 1

Sturm-Liouville Operators

In the following we assume that \mathcal{H} is a separable Hilbert space with inner product (\cdot, \cdot) .

1.1 Definitions from operator theory

Definition 1 *We say that A is a **linear operator** on \mathcal{H} if there is a subspace $\mathcal{D}_A \subseteq \mathcal{H}$ such that for every $u \in \mathcal{D}_A$ there is a unique vector $Au \in \mathcal{H}$. Furthermore,*

$$A(\alpha u + \beta v) = \alpha Au + \beta Av$$

*for all scalars α, β and all $u, v \in \mathcal{D}_A$. We say that \mathcal{D}_A is the **domain** of A . The set*

$$\mathcal{R}_A = \{Au : u \in \mathcal{D}_A\}$$

*is called the **range** of A . The set*

$$\mathcal{N}_A = \{u \in \mathcal{D}_A : Au = \theta\}$$

*is called the **null space** of A .*

Lemma 1 \mathcal{R}_A and \mathcal{N}_A are subspaces of \mathcal{H} .

Note that the domain of A may be a strict subspace of \mathcal{H} so that Au won't make sense for all $v \in \mathcal{H}$, just for $v \in \mathcal{D}_A$.

Definition 2 *Let A and B be linear operators on \mathcal{H} .*

- We say A **equals** B ($A = B$) provided $\mathcal{D}_A = \mathcal{D}_B$ and $Au = Bu$ for all $u \in \mathcal{D}_A$.
- We say A is an **extension** of B ($A \supseteq B$) if $\mathcal{D}_A \supseteq \mathcal{D}_B$ and $Au = Bu$ for all $u \in \mathcal{D}_B$.

We can construct sums, scalar multiples, and products of linear operators, but we have to be careful about their precise domains of definition:

Definition 3 Let A and B be linear operators on \mathcal{H} . The following are also linear operators.

- $A + B$:

$$(A + B)u = Au + Bu, \quad \mathcal{D}_{A+B} = \mathcal{D}_A \cap \mathcal{D}_B$$

- αA :

$$(\alpha A)u = \alpha(Au), \quad \mathcal{D}_{\alpha A} = \mathcal{D}_A$$

- AB :

$$(AB)u = A(Bu), \quad \mathcal{D}_{AB} = \{u \in \mathcal{D}_B : Bu \in \mathcal{D}_A\}$$

- O :

$$Ou = \theta, \quad \text{for all } u \in \mathcal{H}, \quad \text{the zero operator}$$

- I :

$$Iu = u, \quad \text{for all } u \in \mathcal{H}, \quad \text{the identity operator.}$$

If $AB = BA$, the operators are said to **commute**.

We say that A is **one-to-one** (1-1) provided whenever $Au = Av$ with $u, v \in \mathcal{D}_A$ we have $u = v$, i.e., provided $\mathcal{N}_A = \{\theta\}$. If A is 1-1 it is **invertible**, that is there exists an operator A^{-1} on \mathcal{H} such that $\mathcal{D}_{A^{-1}} = \mathcal{R}_A$, $\mathcal{R}_{A^{-1}} = \mathcal{D}_A$ and defined as follows:

$$A^{-1}u = v \longleftrightarrow Av = u.$$

If A is 1-1 then

$$AA^{-1}u = u, \quad \text{for all } u \in \mathcal{R}_A = \mathcal{D}_{A^{-1}},$$

$$A^{-1}Av = v, \quad \text{for all } v \in \mathcal{D}_A = \mathcal{R}_{A^{-1}}.$$

Thus

$$AA^{-1} = I_{\mathcal{R}_A}, \quad A^{-1}A = I_{\mathcal{D}_A}.$$

Definition 4 We say that A is a **symmetric operator** on \mathcal{H} if

1. $\overline{\mathcal{D}_A} = \mathcal{H}$, i.e., every $u \in \mathcal{H}$ is the limit of some Cauchy sequence of vectors in \mathcal{D}_A , so \mathcal{D}_A is **dense** in \mathcal{H} .
2. $(au, v) = (u, Av)$ for all $u, v \in \mathcal{D}_A$.

Definition 5 The complex number λ is an **eigenvalue** of the linear operator A if there is a nonzero $u \in \mathcal{D}_A$ such that $Au = \lambda u$. Here u is called an **eigenvector**. The set

$$S_p = \{\lambda : \lambda \text{ is an eigenvalue of } A\}$$

is the **point spectrum** of A .

Lemma 2 A linear operator A has an inverse if and only if 0 is not an eigenvalue of A .

PROOF: A^{-1} exists $\longleftrightarrow A$ is 1-1 $\longleftrightarrow \mathcal{N}_A = \{\theta\} \longleftrightarrow 0$ is not an eigenvalue of A . Q.E.D.

Definition 6 An operator B on \mathcal{H} is **bounded** if there exists a finite number $M > 0$ such that $\|Bu\| < M\|u\|$ for all $u \in \mathcal{D}_B$. (Recall that $\|u\|^2 = (u, u)$.) We say the B is **bounded below** if there exists a real number α such that $(Au, u) \geq \alpha\|u\|^2$ for all $u \in \mathcal{D}_B$.

1.2 Regular Sturm-Liouville operators on an interval

The ingredients of the **regular Sturm-Liouville eigenvalue problem** on a finite interval $[\ell, m]$, $\ell < m$ of the real line are the following. The equation to be solved is of the form

$$(p(x)u')' + (\lambda k(x) - q(x))u = 0, \quad x \in [\ell, m] \quad (1.1)$$

subject to the conditions

1. p, p', q, k real valued and continuous in $[\ell, m]$. (In some cases we drop the continuity requirement.)

2. $p > 0, k > 0$ in $[\ell, m]$. (If only $p \geq 0, k \geq 0$ we have the **singular** S-L problem).
3. λ a complex number.
4. The matrix of real numbers

$$\begin{pmatrix} \alpha_{11}, & \alpha_{12}, & \alpha_{13}, & \alpha_{14} \\ \alpha_{21}, & \alpha_{22}, & \alpha_{23}, & \alpha_{24} \end{pmatrix}$$

is of rank 2.

5. The boundary conditions are

$$\begin{aligned} \alpha_{11}u(\ell) + \alpha_{12}u'(\ell) + \alpha_{13}u(m) + \alpha_{14}u'(m) &\equiv B_1u = 0, \\ \alpha_{21}u(\ell) + \alpha_{22}u'(\ell) + \alpha_{23}u(m) + \alpha_{24}u'(m) &\equiv B_2u = 0. \end{aligned} \quad (1.2)$$

The S-L problem is to find all values of λ such that equation (1.1) has a nonzero solution u satisfying the boundary conditions (1.2).

NOTE: The motivation for this problem is the equations that arise from applying the method of separation of variables to the partial differential equations of mathematical physics.

Now we will formulate the S-L problem in terms of operator theory. let $\mathcal{H} = L_c^2([\ell, m], k)$, the space of complex-valued Lebesgue square-integrable functions on the bounded interval $[\ell, m]$, with weight function k . Here the complex inner product is

$$(u, v) = \int_{\ell}^m u(x) \overline{v(x)} k(x) dx, \quad u, v \in L_c^2([\ell, m], k).$$

The **generalized Sturm-Liouville operator** A is defined by

$$Au = \frac{1}{k(x)} [-(p(x)u')' + q(x)u], \quad u \in \mathcal{D}_A \quad (1.3)$$

where

$$\mathcal{D}_A = \{u \in C^2[\ell, m] : B_1u = B_2u = 0\} \quad (1.4)$$

and $C^2[\ell, m]$ is the space of complex functions with 2 continuous derivatives on the closed interval $[\ell, m]$.

NOTE:

- \mathcal{D}_A is dense in \mathcal{H} .
- If the boundary conditions take the separated form

$$B_1 u = \alpha_{11} u(\ell) + \alpha_{12} u'(\ell), \quad B_2 u = \alpha_{21} u(m) + \alpha_{22} u'(m), \quad (1.5)$$

then A is an **ordinary Sturm-Liouville operator**.

Definition 7 An operator B in L_c^2 is **real** if $u \in \mathcal{D}_B \longrightarrow \bar{u} \in \mathcal{D}_B$ and $B\bar{u} = \overline{Bu}$.

We see that the S-L operator A is real.

Now we write equation (1.1) in the form

$$u'' + \frac{p'}{p} u' + \frac{\lambda k - q}{p} u \equiv Du = 0, \quad \ell \leq x \leq m. \quad (1.6)$$

By the standard theory of second order ordinary differential equations we know the following:

- Given 2 complex numbers a, b and any $x_0 \in [\ell, m]$ there is a unique solution $u(x, \lambda)$ of (1.6) with $u(x_0, \lambda) = a, u'(x_0, \lambda) = b$.
- The solutions u of $Du = 0$ form a 2-dimensional complex vector space. There exist 2 linearly independent solutions $u_1(x, \lambda), u_2(x, \lambda)$ that form a basis for the solution space, and u_1, u_2 are entire functions of the complex variable λ .
- The determinant

$$\begin{vmatrix} u_1(x) & u_2(x) \\ u_1'(x) & u_2'(x) \end{vmatrix} = W(x)$$

is called the **Wronskian** of the 2 solutions u_1, u_2 . It has the property that $p(x)W(x)$ is constant on $[\ell, m]$. Here the solutions u_1, u_2 are linearly independent if and only if this constant is nonzero.

Theorem 1 Let A be an S-L operator and $\{u_1, u_2\}$ a basis for the solution space of $Du = 0$. Then

1. λ is an eigenvalue of A in \mathcal{H} if and only if $\Delta(\lambda) = 0$, where

$$\Delta(\lambda) = \begin{vmatrix} B_1 u_1 & B_2 u_2 \\ B_2 u_1 & B_2 u_2 \end{vmatrix}$$

PROOF: λ is an eigenvalue of A with eigenfunction u if and only if there exist complex constants c_1, c_2 , not both zero, such that $u = c_1 u_1 + c_2 u_2$ and

$$B_1 u = c_1 B_1 u_1 + c_2 B_1 u_2 = 0,$$

$$B_2 u = c_1 B_2 u_1 + c_2 B_2 u_2 = 0,$$

and these equations can hold if and only if $\Delta(\lambda) = 0$. *Q.E.D.*

2. The eigenvalues of A are either a) all complex numbers, or b) a countable number of eigenvalues with no finite accumulation point.

PROOF: This follows from a standard result in complex variable theory. Indeed, $\Delta(\lambda)$ is an entire function of λ . If it had an uncountable number of zeros or a finite accumulation point, then this analytic function would be identically zero. *Q.E.D.*

Theorem 2 Let A be an S - L operator, μ a complex number, and set $\tilde{A} = A - \mu I$. Then

1. \tilde{A}^{-1} exists if and only if μ is not an eigenvalue of A .
2. If $\tilde{A}^{-1} = (A - \mu I)^{-1}$ exists then

$$\mathcal{D}_{\tilde{A}^{-1}} = \mathcal{R}_{\tilde{A}} = \{f(x) : f \in C^0([\ell, m])\}$$

(where $C^0([\ell, m])$ is the space of continuous functions on the interval) and there exists a function $g(x, y, \mu)$, the **Green's function**, such that

$$(A - \mu I)^{-1} f(x) = \int_{\ell}^m g(x, y, \mu) f(y) k(y) dy$$

PROOF: We start by trying to solve the equation $(A - \mu I)u(x) = f(x)$ for some continuous function f , subject to the boundary conditions $R_1 u = R_2 u = 0$. Thus the differential equation to be solved is

$$u'' + \frac{p'}{p} u' + \frac{\mu k - q}{p} u = -\frac{k}{p} f. \quad (1.7)$$

Now let $u_1(x, \mu), u_2(x, \mu)$ be a basis for the solution space of the homogeneous equation $(A - \mu I)u = 0$, (without the boundary conditions). Then using the standard method of variation of parameters we can derive the solution $h(x)$ of (1.7) given by

$$\begin{aligned} h(x) &= \int_{\ell}^m \frac{u_1(x, \mu)u_2(y, \mu) - u_2(x, \mu)u_1(y, \mu)}{W(y, \mu)} \left(\frac{k(y)f(y)}{p(y)} \right) dy \\ &= \int_{\ell}^m h(x, y, \mu) k(y) f(y) dy, \end{aligned}$$

where

$$h(x, y, \mu) = \begin{cases} 0 & \text{if } y > x \\ \frac{u_1(x, \mu)u_2(y, \mu) - u_2(x, \mu)u_1(y, \mu)}{W(y, \mu)p(y)} & \text{if } x \geq y. \end{cases}$$

Note that $h(\ell) = h'(\ell) = 0$.

REMARKS:

1. $h(x, y, \mu)$ satisfies the homogeneous equation (1.6) in the variable x , if $x \neq y$.
2. Let

$$\begin{aligned} \frac{\partial h}{\partial x}(y^+, y, \mu) &= \lim_{t \rightarrow 0, t > 0} \frac{\partial h}{\partial x}(y + t, y, \mu), \\ \frac{\partial h}{\partial x}(y^-, y, \mu) &= \lim_{t \rightarrow 0, t > 0} \frac{\partial h}{\partial x}(y - t, y, \mu). \end{aligned}$$

Then

$$\frac{\partial h}{\partial x}(y^+, y, \mu) - \frac{\partial h}{\partial x}(y^-, y, \mu) = -\frac{1}{p(y)}, \quad \ell < y < m,$$

i.e., there is a discontinuity in $\frac{\partial h}{\partial x}(x, y, \mu)$ at $x = y$.

3. $h(x, y, \mu)$ is continuous in x and y .

Now set $u(x) = c_1 u_1(x, \mu) + c_2 u_2(x, \mu) + h(x, \mu)$ for constants c_1, c_2 . Then we have our desired solution u if and only if c_1, c_2 can be chosen so that

$$B_1 u = c_1 B_1 u_1 + c_2 B_1 u_2 + B_1 h = 0,$$

$$B_2 u = c_1 B_2 u_1 + c_2 B_2 u_2 + B_2 h = 0,$$

and this is possible if and only if $\Delta(\mu) \neq 0$. Thus, either μ is not an eigenvalue and there is a unique solution u to $(A - \mu I)u = f$, $u \in \mathcal{D}_A$, or μ is an eigenvalue and the inverse operator doesn't exist.

Now, for μ not an eigenvalue we set

$$g(x, y, \mu) = h(x, y, \mu) + b_1(y)u_1(x, \mu) + b_2(y)u_2(x, \mu)$$

and determine b_1, b_2 such that, in the variable x , $B_1g = B_2g = 0$. This leads to the equations

$$-B_1h = b_1B_1u_1 + b_2B_1u_2, \quad -B_2h = b_1B_2u_1 + b_2B_2u_2$$

that, since $\Delta(\mu) \neq 0$ have the unique solution

$$\Delta(\mu)b_1 = \begin{vmatrix} -B_1h & B_1u_2 \\ -B_2h & B_2u_2 \end{vmatrix}, \quad \Delta(\mu)b_2 = \begin{vmatrix} B_1u_1 & -B_1h \\ B_2u_1 & -B_2h \end{vmatrix}.$$

Therefore

$$g(x, y, \mu) = \frac{1}{\Delta(\mu)} \begin{vmatrix} u_1(x, \mu) & u_2(x, \mu) & h(x, y, \mu) \\ B_1u_1 & B_1u_2 & B_1h \\ B_2u_1 & B_2u_2 & B_2h \end{vmatrix}.$$

Note that

1. g satisfies the homogeneous equation (1.6) in variable x , if $x \neq y$.
2. $\frac{\partial h}{\partial x}(y^+, y, \mu) - \frac{\partial h}{\partial x}(y^-, y, \mu) = -\frac{1}{p(y)}$, $\ell < y < m$.
3. g is continuous in x and y .
4. g is the unique function with these properties.

Thus

$$\begin{aligned} u(x) &= \int_{\ell}^m g(x, y, \mu) f(y) k(y) dy \\ &= \int_{\ell}^m h(x, y, \mu) k f dy + u_1(x, \mu) \int_{\ell}^m b_1(y) k f dy + u_2(x, \mu) \int_{\ell}^m b_2(y) k f dy \end{aligned} \tag{1.8}$$

if and only if $(A - \mu I)u = f$ for $u \in \mathcal{D}_A$. Q.E.D.

These results simplify considerably for the ordinary Sturm-Liouville problem. In that case the boundary conditions separate, so that

$$B_1u = \alpha_1u(\ell) + \alpha_2u'(\ell), \quad B_2u = \beta_1u(m) + \beta_2u'(m).$$

To take advantage of this fact we choose our basis functions u_1, u_2 such that $u_1(x, \mu)$ satisfies $Du_1 = 0$ and the left-hand boundary condition $B_1u_1 = 0$, and $u_2(x, \mu)$ satisfies $Du_2 = 0$ and the right-hand boundary condition $B_2u_2 = 0$. (Exercise: Show that this works if μ is not an eigenvalue.) Then

$$h(x, y, \mu) = \begin{cases} 0 & \text{if } y > x \\ \frac{u_1(x, \mu)u_2(y, \mu) - u_2(x, \mu)u_1(y, \mu)}{W(y, \mu)p(y)} & \text{if } x \geq y, \end{cases}$$

and

$$B_1h = 0, \quad B_2h = \frac{(B_2u_1)u_2(y, \mu)}{W(y, \mu)p(y)}.$$

Now $\Delta(\mu) = -(B_1u_2)(B_2u_1)$ and the Green's function takes the simple form

$$\begin{aligned} g(x, y, \mu) &= \frac{1}{\Delta(\mu)} \begin{vmatrix} u_1(x, \mu) & u_2(x, \mu) & h(x, y, \mu) \\ 0 & B_1u_2 & 0 \\ B_2u_1 & 0 & \frac{(B_2u_1)u_2(y, \mu)}{W(y, \mu)p(y)} \end{vmatrix} \\ &= \begin{cases} -\frac{u_1(x, \mu)u_2(y, \mu)}{W(y, \mu)p(y)} & y > x \\ -\frac{u_2(x, \mu)u_1(y, \mu)}{W(y, \mu)p(y)} & x \geq y. \end{cases} \end{aligned} \quad (1.9)$$

1.3 Symmetric and self-adjoint operators on Hilbert space

Let A be a linear operator on the separable Hilbert space \mathcal{H} , with domain \mathcal{D}_A .

Definition 8 A is a **symmetric operator** if $\overline{\mathcal{D}_A} = \mathcal{H}$ and

$$(Au, v) = (u, Av) \text{ for all } u, v \in \mathcal{D}_A.$$

Recall that real symmetric matrices and complex hermitian matrices have very nice spectral properties and, if \mathcal{H} is finite dimensional, the matrix of A with respect to an ON basis would be either real symmetric or complex hermitian. Each such matrix has an associated ON eigenbasis. However, if \mathcal{H} is infinite dimensional then things become much more complicated. The best analogy to these diagonalizable matrices is the self-adjoint operator, an extension of a symmetric operator. For appropriate choices of boundary conditions and domains, S-L operators provide examples of these abstract objects. We begin this exploration, by presenting a few nice properties of symmetric operators.

Theorem 3 *let A be a symmetric operator on \mathcal{H} . Then the following hold:*

1. $\overline{(Au, u)} = (Au, u)$ for all $u \in \mathcal{D}_A$, i.e., (Au, u) is real.
2. If λ is an eigenvalue of A , then λ is real.
3. If μ, λ are distinct eigenvalues of A with corresponding eigenvectors u, v , respectively, then $(u, v) = 0$.

PROOF: 1) $\overline{(Au, u)} = (u, Au) = (Au, u)$. 2) If λ is an eigenvalue of A with eigenvector u , then $Au = \lambda u$ and

$$\lambda(u, u) = (Au, u) = (u, Au) = \overline{\lambda}(u, u)$$

so $\lambda = \overline{\lambda}$. 3) If u, v are eigenvectors corresponding to distinct eigenvalues λ, μ then

$$\lambda(u, v) = (Au, v) = (u, Av) = \mu(u, v)$$

so $(\lambda - \mu)(u, v) = 0$ which implies $(u, v) = 0$. Q.E.D.

Theorem 4 *Suppose \mathcal{H} is a complex Hilbert space and A is a linear operator with $\overline{\mathcal{D}_A} = \mathcal{H}$. Then A is symmetric if and only if (Au, u) is real for all $u \in \mathcal{D}_A$. (Note that this result holds only for complex Hilbert spaces.)*

PROOF: \implies : Follows from the preceding theorem.

\impliedby : It is straightforward to verify the following identities for all $u, v \in \mathcal{D}_A$:

$$4(Au, v) =$$

$$(A(u+v), u+v) - (A(u-v), u-v) + i(A(u+iv), u+iv) - i(A(u-iv), u-iv),$$

$$4(u, Av) =$$

$$(u+v, A(u+v)) - (u-v, A(u-v)) + i(u+iv, A(u+iv)) - i(u-iv, A(u-iv)).$$

Since (Aw, w) is real for all $w \in \mathcal{D}_A$ we have $(Aw, w) = \overline{(Aw, w)} = (w, Aw)$, so, by the identities, $(Au, v) = (u, Av)$. Q.E.D.

We have already defined the adjoint of a bounded operator. The definition of the adjoint of a general linear operator is more delicate. Suppose A is an operator with $\overline{\mathcal{D}_A} = \mathcal{H}$.

Definition 9 Denote by \mathcal{D}_{A^*} the set of all $v \in \mathcal{H}$ such that the linear functional $f_v(u) = (Au, v)$ is bounded on \mathcal{D}_A . For $v \in \mathcal{D}_{A^*}$ let \tilde{f}_v be the unique bounded extension of f_v to \mathcal{H} . By the Riesz representation theorem there exists a unique vector $v^* \in \mathcal{H}$ such that $\tilde{f}_v(u) = (u, v^*)$, for all $u \in \mathcal{H}$. This mapping $v \rightarrow v^*$ of \mathcal{D}_{A^*} to \mathcal{H} defines A^* . We write $A^*v = v^*$. Then

$$(Au, v) = (u, A^*v), \quad \text{for all } u \in \mathcal{D}_A, v \in \mathcal{D}_{A^*}.$$

Lemma 3 \mathcal{D}_{A^*} is a subspace of \mathcal{H} and A^* is a linear operator on \mathcal{D}_{A^*} .

PROOF: Let $u, v \in \mathcal{D}_{A^*}$ and α, β complex scalars. Then for every $w \in \mathcal{D}_A$ we have

$$\begin{aligned} (Aw, \alpha u + \beta v) &= \overline{\alpha}(Aw, u) + \overline{\beta}(Aw, v) \\ &= \overline{\alpha}(w, A^*u) + \overline{\beta}(w, A^*v) = (w, \alpha A^*u + \beta A^*v), \end{aligned}$$

so by the Cauchy-Schwarz inequality

$$|(Aw, \alpha u + \beta v)| \leq \|w\| \cdot \|\alpha u + \beta v\|, \quad \text{for all } w \in \mathcal{D}_A.$$

Thus $\alpha u + \beta v \in \mathcal{D}_{A^*}$ and $A^*(\alpha u + \beta v) = \alpha A^*u + \beta A^*v$. Q.E.D.

In general the domain of A^* need not be dense in \mathcal{H} . However, if A is symmetric then \mathcal{D}_{A^*} is dense. Indeed it is easy to show the following.

Theorem 5 Let A be a linear operator with $\overline{\mathcal{D}_A} = \mathcal{H}$. Then A is symmetric if and only if $A \subseteq A^*$.

Definition 10 Let A be a linear operator with $\overline{\mathcal{D}_A} = \mathcal{H}$. A is said to be **self-adjoint** if $A = A^*$.

Clearly, every self-adjoint operator is symmetric. However, we will see that not every symmetric operator is self-adjoint. In general all we can say is that a symmetric operator A is contained in its adjoint, i.e., that A^* is an extension of A . The following, however, is easy to prove.

Lemma 4 If A is a bounded symmetric operator with $\mathcal{D}_A = \mathcal{H}$ then A is self-adjoint.

To understand in more detail the relation between A and A^* we need the concept of closure of an operator. As usual, we assume that A has dense domain.

Definition 11 The operator A is **closed** if whenever $\{u_n\}$ is a Cauchy sequence in \mathcal{D}_A converging to u , ($u_n \rightarrow u$) such that $\{Au_n\}$ is also a Cauchy sequence with $Au_n \rightarrow v$, then $u \in \mathcal{D}_A$ and $Au = v$.

Definition 12 An operator \bar{A} in \mathcal{H} is called the **closure** of A if

$$\mathcal{D}_{\bar{A}} = \left\{ v \in \mathcal{H} : \text{there is } \{u_n\} \in \mathcal{D}_A \text{ such that } u_n \rightarrow v, Au_n \rightarrow w \text{ and } \bar{A}v = w \right\}$$

Definition 13 An operator A is **closable** if it has a closure \bar{A} .

NOTE: A is closable if and only if whenever $\{u_n\}$ and $\{v_n\}$ are sequences in \mathcal{D}_A with $Au_n \rightarrow w$ and $Av_n \rightarrow z$ then $w = z$. Setting $u_n - v_n = y_n$, we see finally that A is closable if and only if whenever there is a sequence $\{y_n\}$ in \mathcal{D}_A with $y_n \rightarrow \theta$ and $Ay_n \rightarrow x$ we always have $x = \theta$.

Lemma 5 A bounded operator is closable.

PROOF: Let A be a bounded operator with bound M . Suppose $\{u_n\}$ is a sequence in \mathcal{D}_A with $u_n \rightarrow \theta$ and $Au_n \rightarrow v$. But, $\|Au_n\| \leq M\|u_n\| \rightarrow 0$ so $\|v\| = 0$ and $v = \theta$. Thus A is closable. Q.E.D.

The following is straightforward to verify.

Lemma 6 If A is bounded and $\overline{\mathcal{D}_A} = \mathcal{H}$, then \bar{A} is bounded and $\mathcal{D}_{\bar{A}} = \mathcal{H}$.

The next result is deeper and uses the axiom of choice; its proof can be found in .

Theorem 6 A closed operator A with closed domain \mathcal{D}_A is bounded on its domain.

Theorem 7 Let A be an operator with $\overline{\mathcal{D}_A} = \mathcal{H}$. Then A^* is closed.

PROOF: Let $\{u_n\}$ be a sequence in \mathcal{D}_{A^*} such that $u_n \rightarrow u$ and $A^*u_n \rightarrow v$. Then for all $w \in \mathcal{D}_A$ we have

$$(w, A^*u_n) = (Aw, u_n)$$

so in the limit as $n \rightarrow \infty$ we have $(w, v) = (Aw, u)$. This shows that $u \in \mathcal{D}_{A^*}$ and $A^*u = v$. Q.E.D.

Corollary 1 *If A is symmetric then it is closable.*

PROOF: If A is symmetric then $A \subseteq A^*$. Since A^* is closed, A must be closable. Q.E.D.

Lemma 7 *If $A \subset B$ then $B^* \subset A^*$.*

PROOF: Let $w \in \mathcal{D}_{B^*}$. Then for all $u \in \mathcal{D}_A$ we have

$$(Au, w) = (Bu, w) = (u, B^*w).$$

The right-hand side is a bounded linear functional of u , so $w \in \mathcal{D}_{A^*}$ and $A^*w = B^*w$. Q.E.D.

1.3.1 The graph of an operator

We digress to discuss the concept of the graph of an operator, a very useful tool in the study of extensions of symmetric operators.

Suppose $\mathcal{H}_1, \mathcal{H}_2$ are Hilbert spaces with inner products $(\cdot, \cdot)_1, (\cdot, \cdot)_2$, respectively.

Definition 14 *The **direct sum** $\mathcal{H}_1 \oplus \mathcal{H}_2$ of two Hilbert spaces is the set of all ordered pairs $[v_1, v_2]$, $v_j \in \mathcal{H}_j$, with inner product*

$$([u_1, u_2], [v_1, v_2]) = (u_1, v_1)_1 + (u_2, v_2)_2,$$

and norm

$$||[v_1, v_2]||^2 = ||v_1||_1^2 + ||v_2||_2^2.$$

It is straightforward to verify that $\mathcal{H}_1 \oplus \mathcal{H}_2$ is itself a Hilbert space.

Definition 15 *Let T be a linear operator on the Hilbert space \mathcal{H} , with dense domain. The **graph** $\Gamma(T)$ of T is the set of all ordered pairs $[u, Tu] \in \mathcal{H} \oplus \mathcal{H}$ with $u \in \mathcal{D}_T$*

Note the following important properties of the graph:

1. $\Gamma(T)$ is a subspace of $\mathcal{H} \oplus \mathcal{H}$.

2. T is a closed operator in \mathcal{H} if and only if $\Gamma(T)$ is a closed subspace of $\mathcal{H} \oplus \mathcal{H}$.

PROOF: This follows immediately from the identity

$$||[u_i, Tu_i] - [u_j, Tu_j]||^2 = ||u_i - u_j||^2 + ||Tu_i - Tu_j||^2.$$

The primary utility of the graph of T is in property 2. The awkward definition of a closed operator is replaced by the simple concept of a closed subspace.

Lemma 8 *The inverse of a closed operator is closed.*

PROOF: Let T be an invertible operator on \mathcal{H} and define the bounded invertible operator S on $\mathcal{H} \oplus \mathcal{H}$ by $S[u, v] = [v, u]$. Then $\Gamma(T^{-1}) = S\Gamma(T)$, since

$$\begin{aligned}\Gamma(T) &= \{[u, v] : u \in \mathcal{D}_T \text{ and } v = Tu\} \\ \Gamma(T^{-1}) &= \{[v, u] : v \in \mathcal{D}_{T^{-1}} \text{ and } u = T^{-1}v\}.\end{aligned}$$

Thus the subspace $\Gamma(T^{-1})$ is closed if and only if the subspace $\Gamma(T)$ is closed. Q.E.D.

The concept of a closable operator is also transparent when viewed from the graph perspective. We can always close the graph of the operator T to get the closed space $\overline{\Gamma(T)}$. The question is now if this closure is itself the graph of some operator \overline{T} , i.e., if $\overline{\Gamma(T)} = \Gamma(\overline{T})$. The reader can verify that the closure is a graph if and only if T is closable and \overline{T} is the closure of T .

Theorem 8 *T^* is a closed operator.*

ALTERNATE PROOF: Let $B: \mathcal{H} \oplus \mathcal{H} \rightarrow \mathcal{H} \oplus \mathcal{H}$ such that $B[u, v] = [v, -u]$. Note that B preserves inner product. Then $\Gamma(T^*) = [B\Gamma(T)]^\perp$, because $[x, x] \in \Gamma(T^*)$ if and only if $z = T^*x$ and $(Tu, x) - (u, z) = 0$ for all $u \in \mathcal{D}_T$. This last expression can be written as

$$([Tu, -u], [x, z]) = (B[u, Tu], [x, z]) = 0.$$

Since $[B\Gamma(T)]^\perp$ is a closed space, T^* must be a closed operator. Q.E.D.

Theorem 9 *The operator T is closable if and only if $\overline{\mathcal{D}_{T^*}} = \mathcal{H}$.*

PROOF: \Leftarrow Suppose \mathcal{D}_{T^*} is dense in \mathcal{H} , and suppose there is a sequence $\{u_n\}$ in \mathcal{D}_T such that $u_n \rightarrow \theta$ and $Tu_n \rightarrow v$. Then for any $w \in \mathcal{D}_{T^*}$ we have $(Tu_n, w) = (u_n, T^*w)$ and, in the limit as $n \rightarrow \infty$, $(v, w) = 0$. Thus $v \perp \mathcal{D}_{T^*}$, so $v = \theta$ and T is closable.

\Rightarrow Suppose there is a nonzero $w \in \mathcal{D}_{T^*}^\perp$. Then $[w, \theta] \perp \Gamma(T^*)$. Since $\Gamma(T^*) = [B\Gamma(T)]^\perp$ we have $\Gamma(T^*)^\perp = \overline{B\Gamma(T)}$, so $[\theta, w] \in \overline{\Gamma(T)}$. Thus T is not closable. Q.E.D.

Theorem 10 *Let A be a symmetric operator on \mathcal{H} . Then $\overline{A} = A^{**}$.*

PROOF: Note that $A^{**} = (A^*)^*$ is a closed operator and A is closable. We have $\Gamma(A^*) = [B\Gamma(A)]^\perp$ and $\Gamma(A^{**}) = [B\Gamma(A^*)]^\perp = B\Gamma(A^*)^\perp$ (since B preserves inner product), so $\overline{\Gamma(A)} = B\Gamma(A^*)^\perp = \Gamma(A^{**})$. Q.E.D.

The following deep result (whose proof uses the axiom of choice) is not necessary for the development in these notes, but is important. A proof can be found in

Theorem 11 *(Closed Graph) A closed operator T with $\mathcal{D}_T = \mathcal{H}$ is bounded.*

Thus non-bounded operators can only have a proper subspace of \mathcal{H} as a domain.

1.3.2 Symmetric Sturm-Liouville operators

Now we investigate the necessary and sufficient conditions that the general S-L operator A be symmetric. Recall that $\mathcal{H} = L_c^2([\ell, m], k)$, with complex inner product

$$(u, v) = \int_\ell^m u(x) \overline{v(x)} k(x) dx, \quad u, v \in L_c^2([\ell, m], k),$$

and

$$Au = \frac{1}{k(x)} [-(p(x)u')' + q(x)u], \quad u \in \mathcal{D}_A \quad (1.10)$$

where

$$\mathcal{D}_A = \{u \in C^2[\ell, m] : B_1u = B_2u = 0\}, \quad (1.11)$$

and

$$\begin{aligned} \alpha_{11}u(\ell) + \alpha_{12}u'(\ell) + \alpha_{13}u(m) + \alpha_{14}u'(m) &\equiv B_1u = 0, \\ \alpha_{21}u(\ell) + \alpha_{22}u'(\ell) + \alpha_{23}u(m) + \alpha_{24}u'(m) &\equiv B_2u = 0. \end{aligned} \quad (1.12)$$

The matrix of real numbers

$$\begin{pmatrix} \alpha_{11}, & \alpha_{12}, & \alpha_{13}, & \alpha_{14} \\ \alpha_{21}, & \alpha_{22}, & \alpha_{23}, & \alpha_{24} \end{pmatrix}$$

is of rank 2.

If $u, v \in \mathcal{D}_A$ we can integrate by parts twice to obtain

$$\begin{aligned} (Au, v) &= - \int_{\ell}^m (pu')' \bar{v} \, dx + \int_{\ell}^m qu \bar{v} \, dx \\ &= \int_{\ell}^m u \overline{-(pv')' + qv} \, dx + p(x) \left[u(x) \overline{v'(x)} - u'(x) \overline{v(x)} \right]_{\ell}^m \\ &= (u, Av) + B(u, v) \end{aligned} \tag{1.13}$$

where the boundary term is defined by

$$B(u, v) = p(x) \left[u(x) \overline{v'(x)} - u'(x) \overline{v(x)} \right]_{\ell}^m. \tag{1.14}$$

Thus A is symmetric if and only if $B(u, v) = 0$ for all $u, v \in \mathcal{D}_A$.

Theorem 12 *The S-L operator A is symmetric in \mathcal{H} if and only if*

$$p(l)(\alpha_{13}\alpha_{24} - \alpha_{14}\alpha_{23}) = p(m)(\alpha_{11}\alpha_{22} - \alpha_{12}\alpha_{21}). \tag{1.15}$$

Before proving the theorem we consider one of its consequences and some examples.

Corollary 2 *If A is an ordinary S-L operator, then it is symmetric.*

PROOF: If A is ordinary S-L then $\alpha_{13} = \alpha_{14} = \alpha_{21} = \alpha_{22} = 0$. It follows from the theorem that A is symmetric. Q.E.D.

Example 1 *Let*

$$A = -u'', \quad \mathcal{H} = L_c^2([0, \pi], 1), \quad B_1 u = u(0) = 0, \quad B_2 u = u(\pi) = 0.$$

Then A is symmetric and the eigenvalue equation is $-u'' = \lambda u$, $u(0) = u(\pi) = 0$. The eigenvalues are $\lambda_n = n^2$, $n = 1, 2, 3, \dots$ and the corresponding normalized eigenfunctions are $u_n(x) = \sqrt{\frac{2}{\pi}} \sin nx$, $n = 1, 2, 3, \dots$. We already know from the theory of Fourier sine series that the $\{u_n\}$ form an ON basis for \mathcal{H}

Example 2 *The same formal operator and Hilbert space as in the previous example, but boundary conditions $u(0) = u'(0) = u(\pi) = u'(\pi) = 0$. (Note that these are not of the form $B_1u = B_2u = 0$.) Here*

$$\mathcal{D}_A = \left\{ f \in C^2[0, \pi] : f(0) = f'(0) = f(\pi) = f'(\pi) = 0 \right\}.$$

In this case A is symmetric but has no eigenvalues or eigenvectors.

PROOF OF THE THEOREM: The proof is more transparent if we express the conditions for A to be symmetric in terms of 2×2 determinants. Thus the requirement that $B(u, v) = 0$ for all u, v in the domain of A can be written as

$$p(x) \begin{vmatrix} u & \overline{v} \\ u' & \overline{v'} \end{vmatrix}_\ell^m = 0. \quad (1.16)$$

Further, a consequence of the requirements $B_1u = B_2u = \overline{B_1v} = \overline{B_2v} = 0$, always true for u, v in the domain of A , is the determinantal identity

$$\begin{vmatrix} \alpha_{11}u(\ell) + \alpha_{12}u'(\ell) & \alpha_{11}\overline{v(\ell)} + \alpha_{12}\overline{v'(\ell)} \\ \alpha_{21}u(\ell) + \alpha_{22}u'(\ell) & \alpha_{21}\overline{v(\ell)} + \alpha_{22}\overline{v'(\ell)} \end{vmatrix} = \begin{vmatrix} \alpha_{13}u(m) + \alpha_{14}u'(m) & \alpha_{13}\overline{v(m)} + \alpha_{14}\overline{v'(m)} \\ \alpha_{23}u(m) + \alpha_{24}u'(m) & \alpha_{23}\overline{v(m)} + \alpha_{24}\overline{v'(m)} \end{vmatrix}.$$

(Note that each matrix element on the right is the negative of the corresponding matrix element on the left.) We recast this identity in the form

$$\begin{vmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \end{vmatrix} \cdot \begin{vmatrix} u(\ell) & \overline{v(\ell)} \\ u'(\ell) & \overline{v'(\ell)} \end{vmatrix} = \begin{vmatrix} \alpha_{13} & \alpha_{14} \\ \alpha_{23} & \alpha_{24} \end{vmatrix} \cdot \begin{vmatrix} u(m) & \overline{v(m)} \\ u'(m) & \overline{v'(m)} \end{vmatrix}. \quad (1.17)$$

Now the requirement (1.16) can be written as

$$p(\ell) \begin{vmatrix} u(\ell) & \overline{v(\ell)} \\ u'(\ell) & \overline{v'(\ell)} \end{vmatrix} = p(m) \begin{vmatrix} u(m) & \overline{v(m)} \\ u'(m) & \overline{v'(m)} \end{vmatrix}. \quad (1.18)$$

for $p(\ell)p(m) \neq 0$. The only way that both these equations can hold is if

$$p(\ell) \begin{vmatrix} \alpha_{13} & \alpha_{14} \\ \alpha_{23} & \alpha_{24} \end{vmatrix} = p(m) \begin{vmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \end{vmatrix}. \quad (1.19)$$

Thus, condition (1.18) implies condition (1.19).

Now assume that condition (1.19) holds. Then

$$\begin{vmatrix} \alpha_{13} & \alpha_{14} \\ \alpha_{23} & \alpha_{24} \end{vmatrix} \neq 0 \implies \begin{vmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \end{vmatrix} \neq 0$$

so we can solve (1.19) for the first determinant and substitute into (1.17) to obtain condition (1.18). On the other hand the case

$$\begin{vmatrix} \alpha_{13} & \alpha_{14} \\ \alpha_{23} & \alpha_{24} \end{vmatrix} = 0 \implies \begin{vmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \end{vmatrix} = 0.$$

Since the matrix of real numbers

$$\begin{pmatrix} \alpha_{11} & \alpha_{12} & \alpha_{13} & \alpha_{14} \\ \alpha_{21} & \alpha_{22} & \alpha_{23} & \alpha_{24} \end{pmatrix}$$

is of rank 2, we can then take linear combinations of boundary conditions B_1, B_2 to obtain a new basis of separated boundary conditions

$$\tilde{B}_1 u = \alpha_1 u(\ell) + \beta_1 u'(\ell), \quad \tilde{B}_2 u = \alpha_2 u(m) + \beta_2 u'(m).$$

This implies that for $u, v \in \mathcal{D}_A$ we must have

$$\begin{vmatrix} u(\ell) & \overline{v(\ell)} \\ u'(\ell) & \overline{v'(\ell)} \end{vmatrix} = \begin{vmatrix} u(m) & \overline{v(m)} \\ u'(m) & \overline{v'(m)} \end{vmatrix} = 0.$$

Thus condition (1.18) holds. Q.E.D.

We now extend the definition of Sturm-Liouville operators to partial differential operators on n variables that act on function spaces on normal domains in real n -dimensional Euclidean space R_n . We denote points in R_n by $x = (x_1, \dots, x_n)$. A **normal domain** $D \subset R_n$ is an open, simply connected, bounded set with boundary ∂D (so that $\overline{D} = D \cup \partial D$), and a real vector field

$$\nu(x) = (\nu_1(x), \dots, \nu_n(x)), \quad \|\nu\| = 1,$$

the bf outer normal vector such that for every function $u(x) = u(x_1, \dots, x_n) \in C^1(\overline{D})$ we have

$$\int_D u_{x_i}(x) dx = \int_{\partial D} u(x) \nu_i(x) dS, \quad i = 1, \dots, n.$$

Here $dx = dx_1 \cdots dx_n$ and dS is the surface element on ∂D , i.e.,

$$dx_1 \cdots \hat{dx}_i \cdots dx_n = \pm \nu_i(x) dS,$$

where the plus or minus sign is chosen depending on whether the outer normal is pointed in the positive x_i -direction or the negative x_i -direction. In particular, if $u = vw$ then we have the integration by parts formula

$$\int_D v(x) w_{x_i}(x) dx + \int_D v_{x_i}(x) w(x) dx = \int_{\partial D} v(x) w(x) \nu_i(x) dS. \quad (1.20)$$

Our Hilbert space is

$$\mathcal{H} = \left\{ u(x), \text{ real valued} : \int_D |u(x)|^2 k(x) dx < \infty \right\},$$

$$(u, v) = \int_D u(x)v(x)k(x) dx, \quad u, v \in \mathcal{H}.$$

Formally, the Sturm-Liouville operator is

$$Au = \frac{1}{k(x)} \left[- \sum_{i,j=1}^n (p_{ij}(x)u_{x_j})_{x_i} + q(x)u \right] \quad (1.21)$$

This formal operator enables us to define three operators, A_1, A_2, A_3 with domains

$$\mathcal{D}_{A_1} = \left\{ u \in C^2(\overline{D}) : u = 0 \text{ for } x \in \partial D \right\}, \quad (1.22)$$

$$\mathcal{D}_{A_2} = \left\{ u \in C^2(\overline{D}) : Ru \equiv \sum_{i,j=1}^n p_{ij}(x)u_{x_j}(x)\nu_{x_j}(x) = 0, \quad x \in \partial D \right\} \quad (1.23)$$

$$\mathcal{D}_{A_3} = \left\{ u \in C^2(\overline{D}) : Ru + \sigma(x)u = 0, \quad x \in \partial D, \quad \sigma(x) \in C^0(\partial D) \right\}, \quad (1.24)$$

respectively. We require

1. $p_{ij}(x), k(x), q(x)$ real and $p_{ij} = p_{ji}$
2. $p_{ij}(x) \in C^1(\overline{D}), \quad k, q \in C^0(\overline{D})$
3. $k > 0$ for $x \in \overline{D}$
4. $\sum_{i,j=1}^n p_{ij}(x)\xi_i\xi_j \geq c_0 \sum_{i=1}^n \xi_i^2$ for all $x \in \overline{D}$ and arbitrary real ξ_i . Here c_0 is a strictly positive constant.

Theorem 13 *S-L operators A_1, A_2, A_3 are symmetric.*

PROOF: Clearly, $\overline{\mathcal{D}_{A_1}} = \overline{\mathcal{D}_{A_2}} = \overline{\mathcal{D}_{A_3}} = \mathcal{H}$. Using the integration by parts formula (1.20) we find

$$(Au, v) - (u, Av) = \int_D \sum_{i,j=1}^n [-(p_{ij}u_{x_j})_{x_i}v + (p_{ij}v_{x_j})_{x_i}u] dx$$

$$= \int_{\partial D} \sum_{i,j=1}^n p_{ij}(-u_{x_j}v + v_{x_i}u)\nu_i dS = \int_{\partial D} (uRv - vRu) dS = 0,$$

for each of the three boundary conditions. Q.E.D.

Recall that A is bounded below if there is a real constant a such that $(Au, u) \geq a||u||^2$ for all u in the domain of A .

Theorem 14 *The operators A_1, A_2 and A_3 (for $\sigma(x) \geq 0$) are bounded below.*

PROOF: Integrating by parts once we find

$$\begin{aligned} (Au, u) &= \int_D \left[- \sum_{i,j=1}^n (p_{ij}u_{x_j})_{x_i} + q(x)u \right] u \, dx \\ &= \int_D \left[\sum_{i,j} p_{ij}u_{x_j}u_{x_i} + qu^2 \right] dx - \int_{\partial D} \sum_{i,j} p_{ij}u_{x_j}\nu_i u \, dS \\ &\geq c_0 \int_D \sum_{i=1}^n (u_{x_i})^2 dx + \int_D qu^2 dx - \int_{\partial D} uRu \, dS. \end{aligned}$$

For A_1 and A_2 the boundary term vanishes and it is clear that $(Au, u) \geq \inf_{x \in D} \frac{q(x)}{k(x)} ||u||^2$. In the case of A_3 we have $Ru + \sigma(x)u = 0$ on the boundary, so

$$(Au, u) \geq c_0 \int_D \sum (u_{x_i})^2 dx + \int_D qu^2 dx + \int_{\partial D} \sigma u^2 dS.$$

Set $\sigma_0 = \inf_{x \in \partial D} \sigma(x)$, $\gamma_0 = \inf\{\sigma_0, c_0\}$. Then

$$\begin{aligned} (Au, u) &\geq \gamma_0 \left[\int_D \sum_{i=1}^n (u_{x_i})^2 dx + \int_{\partial D} u^2 dS \right] + \int_D qu^2 dx \\ &\geq \inf_{x \in D} \frac{q(x)}{k(x)} ||u||^2. \end{aligned}$$

Q.E.D.

Note that the ordinary S-L operator A on an interval in R_1 (with separated boundary values) is a special case of A_2 .

Corollary 3 *The ordinary S-L operator on an interval is symmetric and bounded below.*

1.3.3 The Schrödinger model

Many of the ordinary and partial differential operators studied in these notes appear in the Schrödinger model for quantum mechanical systems. In this section we describe, briefly, how these equations arise. In classical mechanics the state of a system with n degrees of freedom is described by a $2n$ -tuple of Hamiltonian variables: $q_1, \dots, q_n, p_1, \dots, p_n$. The q_j are position variables and the p_j are momentum variables. The states are vectors in the real $2n$ -dimensional state space R_{2n} . The evolution of a state in time is determined by the Hamiltonian $H(q_1, \dots, q_n, p_1, \dots, p_n)$. Indeed the time evolution $q(y), p(t)$ of a system in state q^0, p^0 at time $t = t_0$ is obtained by solving Hamilton's equations

$$\dot{q}_k(t) = \frac{\partial H}{\partial p_k}, \quad \dot{p}_k = -\frac{\partial H}{\partial q_k}, \quad k = 1, \dots, n \quad (1.25)$$

with initial conditions $q_k(t_0) = q_k^0, p_k(t_0) = p_k^0$. Observable quantities for the system are functions $a(q, p, t)$.

In quantum mechanics the state space is a separable complex Hilbert space \mathcal{H} , subject to the following axioms:

1. To every observable quantity a there corresponds a unique self-adjoint operator A in \mathcal{H} .
2. The state of a physical system at time t is represented by a normalized vector u in \mathcal{H} .
3. If a is associated with A , then the expectation $E_u a$ of the observable a in the state u is given by (Au, u) , (a real number, since A is symmetric.)
4. If O_k, P_k are the operators associated with the classical observables q_k, p_k (in Cartesian coordinates) then these operators satisfy the **commutation relations**

$$[Q_k, P_\ell] \equiv Q_k P_\ell - P_\ell Q_k = i\hbar \delta_{k,\ell}, \quad [Q_k, Q_\ell] = [P_k, P_\ell] = 0 \quad 1 \leq k, \ell \leq n \quad (1.26)$$

on some dense subspace of \mathcal{H} , where $\hbar = h/2\pi$ and $h > 0$ is **Planck's constant**, and $i = \sqrt{-1}$.

5. The time evolution $u(t)$ of a quantum system in state u^0 at time $t = t_0$ is obtained by solving the **time dependent Schrödinger equation**

$$i\hbar \frac{\partial}{\partial t} u(t) = H u(t), \quad u(t_0) = u^0.$$

(This formal expression can be made rigorous.) Here H is the **Hamiltonian operator**, or energy operator, the quantum operator corresponding to the classical Hamiltonian energy observable.

There are other statistical axioms that we shall not discuss here.

In the case where H is independent of time, we can partially solve the time dependent Schrödinger equation. Indeed, suppose $u(t)$ is an eigenvector of H with eigenvalue λ . Then $i\hbar \dot{u}(t) = \lambda u(t)$. This equation has the solution $u(t) = \exp(-i\lambda t/\hbar)u^0$ where u^0 is a unit vector in \mathcal{H} that is independent of t and is a solution of the **time independent Schrödinger equation**

$$Hu^0 = \lambda u^0. \quad (1.27)$$

The most commonly used prescription for passing from the classical description to the quantum description of a physical system is the **Schrödinger model**. Corresponding to a classical system with n degrees of freedom we have the Hilbert space $\mathcal{H} = L_c^2(R_n)$ of complex Lebesgue square integrable functions in n -dimensional Euclidean space, with weight function $k(x) = 1$. The state of the system is given by function $u(q_1, \dots, q_n) \in L_c^2(R_n)$ where the q_j are Cartesian coordinates in R_n . The operators Q_k, P_k are defined formally by $Q_k = q_k$, $P_k = -i\hbar \partial_{q_k}$, i.e.,

$$Q_k u(q_1, \dots, q_n) = q_k u(q_1, \dots, q_n), \quad P_k u(q_1, \dots, q_n) = -i\hbar \partial_{q_k} u(q_1, \dots, q_n), \quad (1.28)$$

for $k = 1, \dots, n$. These operators formally satisfy the commutation relations (1.26).

Definition 16 *Two symmetric operators A and B have the **Heisenberg commutation property** if*

1. $\mathcal{R}_A \subseteq \mathcal{D}_B$, $\mathcal{R}_B \subseteq \mathcal{D}_A$
2. $ABu - BAu = -i\hbar u$, for all $u \in \mathcal{D}_A \cap \mathcal{D}_B$ such that $Au \in \mathcal{D}_B$, $Bu \in \mathcal{D}_A$.

Recall that if a is an observable associated with the self-adjoint operator A , then the expectation $E_u a = \alpha$ of a in the state u , ($\|u\| = 1$) is given by

$$E_u(a) = (Au, u).$$

Definition 17 *The **dispersion** of a in the state u is $D_u a = E_u(a - \alpha)^2$.*

If the observable $(a - \alpha)^2$ is associated with the operator $(A - \alpha I)^2$, then

$$D_u a = (u, (A - \alpha I)^2 u) = \|(A - \alpha I)u\|^2, \quad \text{if } \mathcal{R}_A \subseteq \mathcal{D}_A.$$

Note also that

1. $D_u a = 0 \iff Au = \alpha u.$
2. $D_u a = \|(A - \alpha I)u\|^2 = \|Au\|^2 - 2\alpha(Au, u) + \alpha^2 = \|Au\|^2 - \alpha^2.$

Theorem 15 (*Heisenberg uncertainty relation*) *Let A, B be symmetric operators satisfying the Heisenberg commutation property, and associated with observables a, b , respectively. Let $u \in \mathcal{D}_A \cap \mathcal{D}_B$, $\|u\| = 1$, and set $\alpha = (Au, u) = E_u a$, $\beta = (Bu, u) = E_u b$. Then $D_u a \cdot D_u b \geq \frac{\hbar^2}{4}$.*

PROOF: Set $A' = A - \alpha I$, $B' = B - \beta I$. Note that A', B' are symmetric and satisfy the Heisenberg commutation property $A'B' - B'A'u = -i\hbar u$. Also

$$\begin{aligned} i\hbar = (u, -i\hbar u) &= (u, A'B'u - B'A'u) = (A'u, B'u) - (B'u, A'u) \\ &= (A'u, B'u) - \overline{(A'u, B'u)} \\ &= 2i\Im(A'u, B'u) \end{aligned}$$

so (where $\Im c$ is the imaginary part of c)

$$\hbar/2 = \Im(A'u, B'u) \leq |(A'u, B'u)| \leq \|A'u\| \cdot \|B'u\|.$$

We conclude that

$$\frac{\hbar^2}{4} \leq \|A'u\|^2 \cdot \|B'u\|^2 = D_u a \cdot D_u b.$$

Q.E.D.

This theorem says that if A, B satisfy the Heisenberg commutation property then we cannot measure the values of the observables a and b with arbitrary precision in any state u .

We conclude this section by examining some implications of the Schrödinger model for energy operators. Suppose we have a classical system describing the motion of a single particle of mass m in a potential field $V(x_1, x_2, x_3)$. In classical physics the total energy of this system is given by

$$\frac{m}{2}(\dot{x}_1^2 + \dot{x}_2^2 + \dot{x}_3^2) + V(x_1, x_2, x_3)$$

so the Hamiltonian is

$$H(x_1, x_2, x_3, p_1, p_2, p_3) = \frac{1}{2m}(p_1^2 + p_2^2 + p_3^2) + V(x_1, x_2, x_3), \quad p_k = m\dot{x}_k.$$

The quantum Hamiltonian is thus

$$H = \frac{1}{2m}(P_1^2 + P_2^2 + P_3^2) + V(Q_1, Q_2, Q_3).$$

In the Schrödinger model $\mathcal{H} = L_c^2(R_3)$, the state functions are $u(x_1, x_2, x_3)$ and the Hamiltonian operator is

$$H = -\frac{\hbar^2}{2m}\Delta_3 + V(x_1, x_2, x_3), \quad \Delta_3 = \partial_{x_1}^2 + \partial_{x_2}^2 + \partial_{x_3}^2. \quad (1.29)$$

To make precise sense of these formal manipulations we need to solve the following problems

1. Find a dense subspace \mathcal{D}_H of \mathcal{H} such that H is defined and self-adjoint on \mathcal{D}_H .
2. Find the spectral resolution of H , e.g., find the eigenvalues and eigenvectors of H on \mathcal{D}_H .

Note that the eigenvalue equation for (1.29) is the time independent Schrödinger equation $Hu = \lambda u$ or

$$-\frac{\hbar^2}{2m}\Delta_3 u + V(x_1, x_2, x_3)u = \lambda u. \quad (1.30)$$

REMARK: In the special case that

$$V(x_1, x_2, x_3) = V_1(x_1) + V_2(x_2) + V_3(x_3)$$

we can use the separation of variables method and try to solve (1.27) formally through the ansatz $u(x_1, x_2, x_3) = u_1(x_1)u_2(x_2)u_3(x_3)$. We then obtain three ordinary differential equations of the form

$$-u_k'' + f_k(x_k)u_k = \lambda_k u_k, \quad k = 1, 2, 3, \quad -\infty < x_k < \infty$$

Instead of boundary conditions we have the requirement that the solutions be square integrable:

$$\int_{-\infty}^{\infty} |u_k(x_k)|^2 dx_k < \infty.$$

This is an example of the Weyl-Stone eigenvalue problem, or **singular Sturm-Liouville problem**.

1.4 Symmetric quantum mechanical operators

For quantum mechanical operators obtained from the Schrödinger model it is typical that they act on Hilbert spaces $\mathcal{H} = L_c^2(R_n, k)$ with inner product

$$(u, v) = \int_{R_n} u(x) \overline{v(x)} k(x) dx, \quad x = (x_1, \dots, x_n).$$

For these spaces the domain of integration is unbounded and this leads to complications that were not an issue in our earlier treatment of regular Sturm-Liouville operators. For example:

1. We have the intuitive notion that square integrable functions $u(x)$ on an infinite domain go to zero for x large: $|u(x)| \rightarrow 0$ as $|x| \rightarrow \infty$. This isn't necessarily true. Consider for example $n = 1, k = 1$ and the function

$$u(x) = \begin{cases} \ell + 1 & \text{if } \ell \leq |x| \leq \ell + \frac{1}{(\ell+1)^2}, \\ 0 & \text{otherwise.} \end{cases} \quad \ell = 0, 1, \dots$$

This function is square integrable, but unbounded as $|x|$ grows.

2. If A is a S-L operator and $u \in C^2(R_n)$ then Au is defined, but it doesn't necessarily follow that $Au \in \mathcal{H}$. That is Au may not be square integrable.

We will encounter these delicate issues as we consider the operators of quantum mechanics in detail.

We first consider the momentum operator P in R_1 . here,

$$\mathcal{H} = L_c^2(R_1), \quad Pu = -i\hbar \frac{du}{dx},$$

$$\mathcal{D}_P = \left\{ u \in \mathcal{H} : u \in C^1(R_1) \text{ and } Au \in \mathcal{H} \right\}.$$

Theorem 16 *P in H is symmetric but not self-adjoint.*

PROOF: First we show that P is symmetric. Since all infinitely differentiable functions with compact support are in the domain of P , it is clear that $\overline{\mathcal{D}_P} = \mathcal{H}$. Now let $u, v \in \mathcal{D}_P$. Then

$$(Pu, v) = -i\hbar \int_{-\infty}^{\infty} u'(x) \overline{v(x)} dx = -i\hbar \lim_{a \rightarrow -\infty} \lim_{b \rightarrow +\infty} \int_a^b u'(x) \overline{v(x)} dx$$

$$\begin{aligned}
&= i\hbar \lim_a \lim_b \int_a^b u(x) \overline{v'(x)} dx - i\hbar \lim_a \lim_b u(x) \overline{v(x)} \Big|_a^b \\
&= (u, Pv) + i\hbar \lim_{a \rightarrow -\infty} u(a) \overline{v(a)} - i\hbar \lim_{b \rightarrow +\infty} u(b) \overline{v(b)},
\end{aligned}$$

where each of the limits exists separately in the last equality. Setting $u = v \in \mathcal{D}_P$ in these expressions we see that the following limits exist: $\lim_{b \rightarrow +\infty} |u(b)|^2 = \beta^2$, $\lim_{a \rightarrow -\infty} |u(a)|^2 = \alpha^2$. Thus

$$\lim_{b \rightarrow +\infty} |u(b)| = \beta, \quad \lim_{a \rightarrow -\infty} |u(a)| = \alpha.$$

If $\beta > 0$ then clearly $\int_0^\infty |u(x)|^2 dx$ diverges. This is impossible, so $\beta = 0$. Similarly $\alpha = 0$. Therefore, if $u \in \mathcal{D}_P$ then $\lim_{b \rightarrow +\infty} u(b) = \lim_{a \rightarrow -\infty} u(a) = 0$. Hence $(Pu, v) = (u, Pv)$.

Now we show that P is not self-adjoint. Let

$$w(x) = \begin{cases} 0, & x < 1 \\ 1 - x^2, & -1 \leq x \leq 1 \\ 0, & x > 1. \end{cases}$$

Clearly, w is square integrable but, because of the discontinuities in the first derivative at $x = \pm 1$, w does not belong to the domain of P . Now for $u \in \mathcal{D}_P$ we have

$$(Pu, w) = -i\hbar \int_{-1}^1 u'(x)(1 - x^2) dx = -2i\hbar \int_{-1}^1 u(x)x dx.$$

Therefore,

$$|(Pu, w)| \leq 2\hbar \int_{-1}^1 |u(x)| dx \leq 2\sqrt{2}\hbar \sqrt{\int_{-1}^1 |u(x)|^2 dx} \leq 2\sqrt{2}\hbar \|u\|.$$

Thus (Pu, w) is a bounded linear function of u , so $w \in \mathcal{D}_{P^*}$ and $P \subset P^*$, where the inclusion is proper, so P is not self-adjoint. Q.E.D.

REMARK: We will show later that \overline{P} is self-adjoint.

Now we treat a general class of S-L operators in R_n that arise in quantum mechanics. These are formally similar to operators treated earlier, but here the boundary conditions on finite domains are replaced by square integrability requirements on the infinite domain R_n . Our Hilbert space is

$$\mathcal{H} = L_c^2(R_n, k) = \left\{ u(x) : \int_{R_n} |u(x)|^2 k(x) dx < \infty \right\},$$

$$(u, v) = \int_{R_n} u(x) \overline{v(x)} k(x) dx, \quad u, v \in \mathcal{H}.$$

Formally, the Sturm-Liouville operator is

$$Au = \frac{1}{k(x)} \left(- \sum_{\ell, j=1}^n D_j [(p_{j\ell}(x) D_\ell u] + q(x)u \right), \quad D_j = i\partial_{x_j} + b_j(x). \quad (1.31)$$

We require

1. $p_{j\ell}, b_j, k, q$ real and $p_{\ell j} = p_{j\ell}$
2. $p_{j\ell}, b_j \in C^1(R_n)$, $k, q \in C^0(R_n)$
3. $k > 0$ for $x \in R_n$
4. $\sum_{j,\ell=1}^n p_{j\ell}(x) \xi_j \overline{\xi_\ell} \geq \rho(x) \sum_{j=1}^n \|\xi_j\|^2$ for all $x \in R_n$ and arbitrary complex ξ_j . Here ρ is real valued and $\rho(x) > 0$ on R_n .

This formal operator enables us to define two operators, A_0, A_1 with domains

$$\mathcal{D}_{A_0} = \left\{ u \in \mathcal{H} : u \in \overset{o}{C}^2(R_n) \right\}, \quad (1.32)$$

$$\mathcal{D}_{A_1} = \left\{ u \in \mathcal{H} : u \in C^2(R_n) \text{ and } Au \in \mathcal{H} \right\}, \quad (1.33)$$

respectively. Here $\overset{o}{C}^2(R_n)$ is the space of twice continuously differentiable functions with compact support in R_n .

Theorem 17 *S-L operators A_0 , and A_1 (with some additional technical assumptions, see Hellwig, page 85) are symmetric in H .*

PROOF: (sketch) It is clear that $\overline{\mathcal{D}_{A_0}} = \overline{\mathcal{D}_{A_1}} = \mathcal{H}$. Now, for $u, v \in \mathcal{D}_{A_j}$,

$$(Au, v) = \int_{R_n} Au(x) \overline{v(x)} k(x) dx = \lim_{r \rightarrow \infty} \int_{|x| \leq r} Au \overline{v} k dx.$$

Now we integrate by parts on the ball $|x| \leq r$, where

$$|x|^2 = x_1^2 + \cdots + x_n^2, \quad \nu_j(x) = \frac{x_j}{|x|} \text{ on } |x| = r.$$

$$\begin{aligned}
\int_{|x| \leq r} Au \bar{v} k dx &= \int_{|x| \leq r} [\sum D_j (p_{j\ell} D_\ell u) \bar{v} + qu \bar{v}] dx \\
&= \int_{|x| \leq r} [\sum p_{j\ell} D_\ell u \overline{D_j v} + qu \bar{v}] dx + i \int_{|x|=r} (\sum \frac{x_j}{|x|} p_{j\ell} D_\ell u) \bar{v} dS \\
&= \int_{|x| \leq r} u \overline{Av} k dx + i \int_{|x|=r} \sum_{j,\ell} [\frac{x_j}{|x|} p_{j\ell} (\bar{v} D_\ell u + u \overline{D_\ell v})] dS.
\end{aligned}$$

Let

$$\Psi(r) = \int_{|x| \leq r} (u \overline{Av} - Au \bar{v}) dx = -i \int_{|x|=r} [\cdot] dS.$$

Then

$$(Au, v) = (u, Av) - \lim_{r \rightarrow \infty} \Psi(r).$$

If $u, v \in \mathcal{D}_{A_0}$ then $\Psi(r) = 0$ for r sufficiently large. hence A_0 is symmetric. If, however, $u, v \in \mathcal{D}_{A_1}$ then additional technical assumptions are needed to show that $\lim_{r \rightarrow \infty} \Psi(r) = 0$, see Hellwig, page 85. With these assumptions A_1 is symmetric. Q.E. D.

Theorem 18 Suppose $\frac{q(x)}{k(x)} \geq -K$ for all x , where K is a positive constant. The A_0 is bounded below by $-K$. If in addition there is a constant $c_1 > 0$ such that

$$\frac{1}{k(x)} \sum p_{j\ell}(x) \frac{x_j x_\ell}{|x|^2} \leq c_1 |x|^2,$$

then A_1 is bounded below by $-K$ and $\int_{R_n} \sum p_{j\ell} D_\ell u \overline{D_j u} dx$ exists for all $u \in \mathcal{D}_{A_1}$.

PROOF:

$$\int_{|x| \leq r} (Au) \bar{u} k dx = \int_{|x| \leq r} [\sum p_{j\ell} D_\ell u \overline{D_j u} + q|u|^2] dx + i \int_{|x|=r} [\sum \frac{x_j}{|x|} p_{j\ell} D_\ell u] \bar{u} dS.$$

If $u \in \mathcal{D}_{A_0}$ we have

$$\begin{aligned}
(Au, u) &= \lim_{r \rightarrow \infty} \int_{|x| \leq r} (Au) \bar{u} k dx = \int_{R_n} [\sum p_{j\ell} D_\ell u \overline{D_j u} + q|u|^2] dx \\
&\geq \int_{R_n} \frac{q}{k} |u|^2 k dx \geq -K ||u||^2.
\end{aligned}$$

If $u \in \mathcal{D}_{A_1}$ then by the previous theorem A_1 is symmetric, and technical lemmas give

$$(Au, u) = \int_{R_n} [\sum p_{j\ell} D_\ell u \overline{D_j u} + q|u|^2] dx \geq -K ||u||^2.$$

Q.E.D.

Example 3 If $k = 1$ and $Au = -\Delta_3 u + q(x)u$ and $q(x) \geq -K|x|^2$ for sufficiently large $|x|$, then A_1 is symmetric.

A further essential extension of the theory concerns Schrödinger operators with singular potential. Here,

$$\mathcal{H} = L_c^2(R_n), \quad Au = -\Delta_n u + q(x)u, \quad x = (x_1, \dots, x_n), \quad q \text{ real},$$

$$\mathcal{D}_A \{u \in \mathcal{H} : u \in \overset{o}{C}_c^2(R_n) \text{ and } Au \in \mathcal{H}\}.$$

The complication is that q may be singular, e.g., the Coulomb potential

$$q(x_1, x_2, x_3) = -\frac{e^2}{\sqrt{x_1^2 + x_2^2 + x_3^2}} = -\frac{e^2}{r}.$$

Theorem 19 If $u, v \in \mathcal{D}_A$ then $(Au, v) = (u, Av)$.

PROOF: Integrating by parts twice, we have

$$\begin{aligned} (Au, v) &= \int_{R_n} [-\Delta_n u \bar{v} + qu\bar{v}] dx \\ &= \int_{R_n} [\sum_{j=1}^n u_{x_j} \overline{v_{x_j}} + qu\bar{v}] dx = \int_{R_n} [-u \Delta_n \bar{v} + qu\bar{v}] dx \\ &= (u, Av). \end{aligned}$$

Q.E.D.

If $\overline{\mathcal{D}_A} = \mathcal{H}$ then the above simple argument shows that A is symmetric. However, for singular q it may not be true that the domain of A is dense in \mathcal{H} . To determine this we need to look at the behavior of q in the neighborhood of a singularity and, also, the behavior of q as $|x| \rightarrow \infty$.

As an extremely important example consider the rotationally symmetric potential $q(x_1, x_2, x_3) = \frac{a}{r}$ where A is a nonzero constant. (If a is negative, this is the Coulomb potential.) I claim that in this case

$$\mathcal{D}_A = \{u \in \mathcal{H} : u \in \overset{o}{C}_c^2(R_n)\},$$

i.e., that if u belongs to this space then, necessarily, $Au \in \mathcal{H}$. Thus, it is clear that the domain of A is dense in \mathcal{H} .

To prove this we note that

$$\begin{aligned} \int_{R_3} |Au|^2 dx &= \int_{R_3} |\Delta_3 u|^2 dx - \int_{R_3} (\Delta_3 u) q \bar{u} dx - \int_{R_3} q u \Delta_3 \bar{u} dx + \int_{R_3} q^2 |u|^2 dx \\ &\leq c_0 + c_1 \int_{R_3} |qu| dx + \int_{R_3} q^2 |u|^2 dx, \end{aligned}$$

where c_0, c_1 are finite positive constants. Now we need to show that the two integrals on the right-hand side are finite, for any $u \in \overset{o}{C}_c^2(R_n)$. Note that any such u is bounded and vanishes outside some ball with center at the origin and radius r_0 . Thus there is a positive constant $M < \infty$ such that

$$\int_{R_3} |qu| dx \leq M \int_{S_2} \left[\int_0^{r_0} |q| r^2 dr \right] d\omega < \infty$$

where S_2 is the unit sphere, centered at the origin. Similarly

$$\int_{R_3} |qu|^2 dx \leq N \int_{S_2} \left[\int_0^{r_0} |q|^2 r^2 dr \right] d\omega < \infty,$$

so $Au \in \mathcal{H}$.

This operator is also bounded below. The proof is simplest if $a \geq 0$. Then

$$(Au, u) = \int_{S_2} \int_0^\infty \left[\sum_{j=1}^3 |u_{x_j}|^2 + \frac{a}{r} |u|^2 \right] r^2 dr d\omega \geq 0.$$

Now suppose $a = -\alpha < 0$ (the case for the Coulomb problem). Note that for any positive constant b we can find a positive constant c such that

$$\frac{\alpha}{r} < \frac{b}{r} + c$$

for all $r > 0$. Therefore

$$\int_{R_3} \frac{\alpha}{r} |u|^2 dx \leq b \int_{R_3} \frac{|u|^2}{r^2} dx + c \int_{R_3} |u|^2 dx.$$

Lemma 9 $\int_{R_3} \frac{|u|^2}{r^2} dx \leq 4 \int_{R_3} \sum_{j=1}^3 |u_{x_j}|^2 dx.$

PROOF: Without loss of generality, we can assume that u is real. Set $v = u\sqrt{r}$. Then, using the chain rule, we have $\sum_{j=1}^3 u_{x_j}^2 = \frac{1}{r} \sum_{j=1}^3 v_{x_j}^2 - \frac{1}{r^2} v \frac{\partial v}{\partial r} + \frac{v^2}{4r^3}$. Therefore,

$$\int_{R_3} \sum_{j=1}^3 |u_{x_j}|^2 dx \geq -\frac{1}{2} \int_{R_3} \frac{\partial(v^2)}{\partial r} \frac{1}{r^2} dx + \frac{1}{4} \int_{R_3} \frac{v^2}{r^3} dx$$

$$= -\frac{1}{2} \int_{S_2} \left[\int_0^\infty \frac{\partial}{\partial r} (ru^2) dr \right] d\omega + \frac{1}{4} \int_{R_3} \frac{u^2}{r^2} dx.$$

Note that the integral in the brackets is zero. Q.E.D.

Now we see that A is bounded below, because

$$\begin{aligned} (Au, u) &\geq \int_{R_3} \left[\frac{|u|^2}{4r^2} + \frac{a|u|^2}{r} \right] dx \\ &\geq \left(\frac{1}{4} - b \right) \int_{R_3} \frac{|u|^2}{r^2} dx - c \int_{R_3} |u|^2 dx \geq -c \int_{R_3} |u|^2 dx, \end{aligned}$$

if we choose $b \leq \frac{1}{4}$.

1.4.1 Some important operators and their adjoints

Recall that a symmetric operator A is closable, but not necessarily closed. The adjoint operator A^* is always closed and $A \subseteq A^*$.

Definition 18 *A symmetric operator is **essentially self-adjoint** if $\overline{A} = A^*$.*

Thus, since $A^* = \overline{A}^*$, to obtain a self-adjoint operator from one that is essentially self-adjoint, we need only take the closure.

As an important example, we consider the formal operator $A = -(\partial_{x_1}^2 + \partial_{x_2}^2 + \partial_{x_3}^2) = -\Delta_3$, acting on the Hilbert space $\mathcal{H} = L^2(R_3)$. Now we define two different operators A_0, A_1 with formal action defined by A and domains

$$\mathcal{D}_{A_0} = \left\{ u \in \overset{o}{C}^2(R_3) \right\}, \quad \mathcal{D}_{A_1} = \left\{ u \in C^2(R_3) : u \in \mathcal{H} \text{ and } Au \in \mathcal{H} \right\},$$

respectively. Note that $\mathcal{D}_{A_0} \subset \mathcal{D}_{A_1}$. Furthermore it is easy to check that $(A_0 u, v) = (u, A_1 v)$ for all $u \in \mathcal{D}_{A_0}$ and $v \in \mathcal{D}_{A_1}$. It follows that A_0 is symmetric and

$$A_0 \subset A_1 \subseteq A_0^*$$

and, since taking adjoints reverses the inclusions,

$$\overline{A_0} = A_0^{**} \subseteq A_1^* \subseteq A_0^*.$$

Note: If A_0 is essentially self-adjoint, then $\overline{A_0} = A_0^*$ and we can combine the above inclusions to obtain $A_1 \subseteq A_1^* \implies A_1$ is symmetric. A fact that isn't obvious since the validity of integration by parts isn't clear.

We will show that A_0 is essentially self-adjoint, in steps. The (unitary) Fourier transform

$$\hat{u}(y) = \mathcal{F}u(y) \equiv \frac{1}{(2\pi)^{\frac{3}{2}}} \lim_{r \rightarrow \infty} \int \int \int_{|x| \leq r} e^{-ix \cdot y} u(x) dx,$$

where $x = (x_1, x_2, x_3)$, $y = (y_1, y_2, y_3)$ is a unitary mapping of \mathcal{H} onto $\hat{\mathcal{H}} = L^2(R_3)$ (in the y coordinates), i.e., the map is 1-1, onto and preserves inner product. Now if $u \in \mathcal{D}_{A_0}$ then

$$\hat{A}u(y) = -\frac{1}{(2\pi)^{\frac{3}{2}}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-ix \cdot y} \Delta_3 u(x) dx = |y|^2 \hat{u}(y).$$

Now let K be the operator with maximal domain that multiplies by $|y|^2$ in $\hat{\mathcal{H}}$:

$$\mathcal{D}_K = \{ \hat{v} \in \hat{\mathcal{H}} : |y|^2 \hat{v}(y) \in \hat{\mathcal{H}} \}.$$

Clearly, $K = K^*$. Let A be the operator on \mathcal{H} defined by $A = \mathcal{F}^{-1} K \mathcal{F}$. (Note that $\mathcal{F}^{-1} = \mathcal{F}^*$ since \mathcal{F} is unitary. So $(Au, v) = (\mathcal{F}^{-1} K \mathcal{F}u, v) = (K \mathcal{F}u, \mathcal{F}v) = (K \hat{u}, \hat{v})$, where (\cdot, \cdot) is the inner product on $\hat{\mathcal{H}}$.) We see that A is an extension of A_0 . Further, $A = A^*$, since $K = K^*$. Thus A_0 has a self-adjoint extension. We will show later that, in fact, $A = \overline{A_0}$. The graph inner product provides us with a convenient way of posing the problem. Consider the graphs of A_0 and A_0^* :

$$\Gamma(A_0) = \{ [u, A_0 u] : u \in \mathcal{D}_{A_0} \}, \quad \Gamma(A_0^*) = \{ [u, A_0^* u] : u \in \mathcal{D}_{A_0^*} \}.$$

Now $\overline{\Gamma(A_0)} = \Gamma(\overline{A_0}) \subseteq \Gamma(A_0^*)$. If $\Gamma(\overline{A_0}) \subset \Gamma(A_0^*)$ then there exists a nonzero $v \in \mathcal{D}_{A_0^*}$ such that $[v, A_0^* v] \perp \Gamma(A_0)$. This means that

$$(u, v) + (A_0 u, A_0^* v) = 0$$

for all $u \in \mathcal{D}_{A_0}$. But this shows that $A_0^* v \in \mathcal{D}_{A_0}$ and $(A_0 u, A_0^* v) = (u, A_0^* A_0^* v)$, so $(A_0^*)^2 v = -v$.

Lemma 10 $\overline{A_0} \subset A_0^*$ and $\overline{A_0} \neq A_0^*$ if and only if there is a nonzero $v \in \mathcal{D}_{A_0^*}$ such that $(A_0^*)^2 v = -v$.

Note: Since $(u, (A_0^*)^2 v) = (A_0^2 u, v)$ for all $u \in \mathcal{D}_{A_0^2}$ this is equivalent to the statement that $(A_0^2 u + u, v) = 0$ for all $u \in \mathcal{D}_{A_0^2}$. Thus, v must satisfy the relation

$$(A_0^2 u + u, v) = 0, \quad \text{for all } u \in \mathcal{D}_{A_0^2}.$$

If we transfer this expression to the Fourier transform Hilbert space $\hat{\mathcal{H}}$ we have the requirement

$$\int_{R_3} (|y|^4 + 1) \hat{u}(y) \overline{\hat{v}(y)} dy = 0.$$

Thus if the functions $(|y|^4 + 1) \hat{u}(y)$ are dense in $\hat{\mathcal{H}}$ as u runs over $\mathcal{D}_{A_0^2}$ it will follow that $\hat{v} = \theta$, hence that $v = \theta$. Rather than developing the technical details from Fourier theory, at this point, to show that these functions are in fact dense, we will return to this problem later when we use operator theory to demonstrate that the range of $A_0^2 + I$ is dense in \mathcal{H} .

For our next example, we first recall some facts about absolutely continuous functions. A complete treatment is given in our Lebesgue theory notes.

Definition 19 *A function f is **absolutely continuous** on $[a, b]$ if there exist a function $g \in L^1[a, b]$ such that $f(t) = c + \int_a^t g(x) dx$, $c = f(a)$, for all $t \in [a, b]$.*

Theorem 20 *If f is absolutely continuous then $f'(t)$ exists for almost every $t \in [a, b]$ and $f(t) = f(a) + \int_a^t f'(x) dx$.*

Theorem 21 *f is absolutely continuous on $[a, b]$ if and only if for every $\epsilon > 0$ there exists a $\delta > 0$ such that $\sum_{k=1}^n |f(x_k + \delta_k) - f(x_k)| \leq \epsilon$ for every finite family of non-overlapping subintervals $(x_k, x_k + \delta_k)$ in $[a, b]$ of total length $\sum \delta_k \leq \delta$.*

Theorem 22 *if f_1, f_2 are absolutely continuous on $[a, b]$, then $f_1 f_2$ is absolutely continuous on $[a, b]$ and $\frac{d}{dx}(f_1 f_2) = f_1' f_2 + f_1 f_2'$.*

For our next example we consider the momentum operator $A = i \frac{d}{dx}$ on $[a, b]$ with domain

$$\mathcal{D}_A = \left\{ f \in L_c^2[a, b] = \mathcal{H} : f \text{ abs. cont. and } f' \in L_c^2[a, b] \right\}.$$

Let's compute A^* . We look for all pairs $g, h \in \mathcal{H}$ such that $(Af, g) = (f, h)$ for all $f \in \mathcal{D}_A$. Setting $z(x) = \int_a^x h(t) dt$, so z is absolutely continuous, we have the integration by parts formula

$$i \int_a^b \frac{df}{dx} \bar{g} dx = \int_a^b f \bar{h} dx = - \int_a^b \frac{df}{dx} \overline{z(x)} dx + f(b) \overline{z(b)}.$$

Thus

$$\int_a^b \frac{df}{dx} (i\bar{g} + \bar{z}) dx = f(b) \overline{z(b)}.$$

Now let f run over $C_c^\infty[a, b]$, dense in \mathcal{H} , (so $f(b) = 0$) and then $\frac{df}{dx}$ also runs over $C_c^\infty[a, b]$. Thus $g = -iz$ almost everywhere. Since z is absolutely continuous, then by redefining g on a set of measure zero if necessary, we can assume g is absolutely continuous, so $g' = -iz' = -ih$ almost everywhere. Thus, $h = i\frac{dg}{dx}$. From this it follows that $A^* = i\frac{d}{dx}$,

$$\mathcal{D}_{A^*} = \{f \in \mathcal{H} : f \text{ abs. cont.}, f' \in \mathcal{H}, f(a) = f(b) = 0\}.$$

Similarly, from the integration by parts formula

$$i \int_a^b \frac{df}{dx} \bar{g} dx = -i \int_a^b \frac{df}{dx} \overline{g(x)} dx + i(f(b)\overline{g(b)} - f(a)\overline{g(a)})$$

for f, g absolutely continuous, we see that the operator $A_1 = i\frac{d}{dx}$ with domain

$$\mathcal{D}_{A_1} = \left\{ f \in L_c^2[a, b] = \mathcal{H} : f \text{ abs. cont. and } f' \in L_c^2[a, b], \text{ and } f(a) = f(b) \right\},$$

is self-adjoint.

Chapter 2

Completely Continuous Operators

As we have seen differential operators are normally unbounded, and their domains do not include the entire Hilbert space. However, the inverses of differential operators, when they exist, are typically integral operators that are bounded and, even better, completely continuous. For this reason it is frequently advantageous to transfer problems about a differential operator to problems about its inverse. With this motivation, we begin a study of completely continuous operators on a Hilbert space H .

Definition 20 *The operator A with $\overline{\mathcal{D}_A} = \mathcal{H}$ is **completely continuous** if for every bounded sequence $u_1, u_2, \dots \in \mathcal{D}_A$ (i.e., there exists a constant $b > 0$ such that $\|u_i\| \leq b$ for $i = 1, 2, \dots$) the collection $\{Au_1, Au_2, \dots\}$ has a convergent subsequence.*

Theorem 23 *A completely continuous $\implies A$ bounded.*

PROOF: Assume A not bounded. Then there exists a sequence $u_1, u_2, \dots \in \mathcal{D}_A$ such that $\|u_n\| = 1$ and $\|Au_n\| > n$ for $n = 1, 2, \dots$. Clearly u_1, u_2, \dots is bounded and Au_1, Au_2, \dots contains no convergent subsequence. Impossible! Q.E.D.

REMARKS:

1. A bounded operator on a finite dimensional inner product space is completely continuous. This is just the Bolzano- Weierstrass theorem, proved in the Lebesgue notes.

2. In an infinite dimensional Hilbert space a bounded operator may not be completely continuous. Example: the identity operator I .

Theorem 24 *If A is completely continuous with $\overline{\mathcal{D}_A} = \mathcal{H}$ then \overline{A} with domain \mathcal{H} is also completely continuous (i.e., we can always assume that the domain of a completely continuous operator is \mathcal{H}).*

PROOF: Let u_1, u_2, \dots be a bounded sequence in \mathcal{H} , ($\|u_n\| < b$, $n = 1, 2, \dots$). Then for every n there exists a vector $v_n \in \mathcal{D}_A$ such that $\|u_n - v_n\| < \frac{1}{n}$. Now $\|v_n\| \leq \|u_n\| + \|v_n - u_n\| < b + 1$ by the triangle inequality, so v_1, v_2, \dots is a bounded sequence. Thus there is a convergent subsequence $\{Av_{n_j} : j = 1, 2, \dots\}$. But

$$\|\overline{A}u_{n_j} - \overline{A}u_{n_k}\| = \|\overline{A}u_{n_j} - Av_{n_j}\| + \|Av_{n_j} - Av_{n_k}\| + \|Av_{n_k} - \overline{A}u_{n_k}\| \quad (2.1)$$

by the triangle inequality. Since $\|\overline{A}\| = \|A\|$ the first term on the right hand side of (2.1) is bounded by $\|A\|/n_j$, and the third term by $\|A\|/n_k$. Given any $\epsilon > 0$ we can choose j, k so large that the middle term is less than ϵ . Thus $\|\overline{A}u_{n_j} - \overline{A}u_{n_k}\| \rightarrow 0$ as $j, k \rightarrow \infty$. It follows that the sequence $\{\overline{A}u_{n_j}\}$ is Cauchy, hence convergent. Q.E.D.

Recall the following properties of the operator norm, proved in the Lebesgue theory notes. If A is a bounded operator on H the operator norm is defined by

$$\|A\| = \sup_{u \in \mathcal{D}_A, u \neq \theta} \frac{\|Au\|}{\|u\|} = \sup_{u \in \mathcal{D}_A, \|u\|=1} \|Au\|. \quad (2.2)$$

Lemma 11 *If A, B are bounded operators on \mathcal{H} and α is a complex number then*

1. $\|\alpha A\| = |\alpha| \cdot \|A\|$
2. $\|A + B\| \leq \|A\| + \|B\|$
3. $\|AB\| \leq \|A\| \cdot \|B\|$
4. $\|A^n\| \leq \|A\|^n, \quad n = 1, 2, \dots$

An application to quantum mechanics.

Theorem 25 *Let A, B be bounded operators on H such that $[A, B] = -i\hbar I$. Then the relation*

$$ABu - BAu = -i\hbar u \quad \text{for all } u \in \mathcal{H}$$

cannot hold.

PROOF: Assume that the theorem is false and that there exist bounded operators A, B such that $AB - BA = -\hbar I$ and $\|A\| \cdot \|B\| > 0$. By induction we can show that

$$-\hbar n B^{n-1} = AB^n - B^n A = [A, B^n], \quad n = 1, 2, \dots \quad (2.3)$$

Thus

$$\hbar n \|B^{n-1}\| \leq 2\|A\| \cdots \|B^n\| \leq 2\|A\| \cdot \|B\| \cdot \|B^{n-1}\|.$$

Suppose $\|B^{n-1}\| \neq 0$ for all n . Then $\hbar n \leq 2\|A\| \cdot \|B\|$ for all n Impossible! Thus $\|B^n\| = 0$, so $B^n = 0$ for sufficiently large n . Then (2.3) implies that $B^{n-1} = 0$, and it follows that $B^1 = B = 0$, so $\|B\| = 0$, which is impossible. Q.E.D.

Theorem 26 *Suppose A is symmetric and bounded. Then $|(Au, u)| \leq \alpha \|u\|^2$ for all $u \in \mathcal{D}_A$ for $\alpha = \|A\|$ and $\|A\|$ is the smallest number α that will work. Thus*

$$\|A\| = \sup_{u \in \mathcal{D}_A, u \neq \theta} \left| \frac{(Au, u)}{\|u\|^2} \right| = \sup_{u \in \mathcal{D}_A, \|u\|=1} |(Au, u)|.$$

PROOF: We have

$$|(Au, u)| \leq \|Au\| \cdot \|u\| \leq \|A\| \cdot \|u\|^2.$$

Now let

$$L = \sup_{u \in \mathcal{D}_A, u \neq \theta} \left| \frac{(Au, u)}{\|u\|^2} \right|.$$

Clearly, $L \leq \|A\|$. Now we must show $L \geq \|A\|$. Consider the identity

$$(A(u+v), u+v) - (A(u-v), u-v) = 2(Au, v) + 2(Av, u)$$

for all $u, v \in \mathcal{H}$. Note that the inner products on the left-hand side are real, by the symmetry of A . Thus

$$(A(u+v), u+v) \leq L\|u+v\|^2, \quad (A(u-v), u-v) \geq -L\|u-v\|^2$$

which implies that

$$2(Au, v) + 2(Av, u) \leq L(\|u + v\|^2 + \|u - v\|^2),$$

expanding to

$$(Au, v) + (Av, u) \leq L(\|u\|^2 + \|v\|^2).$$

Now choose a u such that $Au \neq \theta$ and substitute $v = (\|u\|/\|Au\|)Au$ into this last inequality to obtain $\|Au\| \leq L\|u\|$ for $Au \neq \theta$. This result is obviously true also if $Au = \theta$. Therefore $\|A\| \leq L$. Q.E.D.

Thus if A is bounded and symmetric, we have $\|A\| = \sup_{\|u\|=1} |(Au, u)|$, where we assume without loss of generality that $\mathcal{D}_A = \mathcal{H}$.

REMARK: If \mathcal{H} is n dimensional, where n is finite, and $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigenvalues of A then we know that $\|A\| = \max\{|\lambda_1|, \dots, |\lambda_n|\} = |\lambda_i|$ and there exists a nonzero vector u_0 such that $\|A\| = |(Au_0, u_0)|$ and $Au_0 = \lambda_i u_0$. We will see that symmetric completely continuous operators preserve many of the eigenvalue features of self-adjoint matrices.

Theorem 27 *let A be bounded and symmetric on \mathcal{H} . There exists a sequence $\{u_k\}$, $\|u_k\| = 1$, such that $\lim_{k \rightarrow \infty} (Au_k - \lambda_1 u_k) = \theta$ in the norm, where $\lambda_1 = \|A\|$, or $-\|A\|$.*

PROOF: Since $\|A\| = \sup_{\|u\|=1} |(Au, u)|$, there exists a sequence $\{v_\ell\}$ such that $\|v_\ell\| = 1$ and $\lim_{\ell \rightarrow \infty} |(Av_\ell, v_\ell)| = \|A\|$. Then $\{v_\ell\}$ contains a subsequence $\{u_k\}$ such that either $(Au_k, u_k) \rightarrow \|A\|$ as $k \rightarrow \infty$ or $(Au_k, u_k) \rightarrow -\|A\|$. Therefore $(Au_k, u_k) \rightarrow \lambda_1$ as $k \rightarrow \infty$. Now

$$\|Au_k - \lambda_1 u_k\|^2 = \|Au_k\|^2 - 2\lambda_1(Au_k, u_k) + \lambda_1^2 \|u_k\|^2 \leq \lambda_1^2 - 2\lambda_1(Au_k, u_k) + \lambda_1^2 \rightarrow 0$$

as $k \rightarrow \infty$. Q.E.D.

Theorem 28 *Let A be symmetric and completely continuous (and to avoid a trivial case assume $\|A\| > 0$). Then either $\lambda_1 = \|A\|$ or $\lambda_1 = -\|A\|$ is an eigenvalue of A . Furthermore, if λ is another eigenvalue of A then $|\lambda_1| \geq |\lambda|$.*

PROOF: Let $\lambda_1, \{u_k, k = 1, 2, \dots\}, \|u_k\| = 1$ be as in the last theorem. Since A is completely continuous there is a subsequence $\{w_j\}$ of $\{u_k\}$ such that

Aw_j converges to some vector, say $\lambda_1 w$, as $j \rightarrow \infty$. Now $\|Aw_j - \lambda_1 w_j\| \rightarrow 0$ as $j \rightarrow \infty$ by the preceding theorem. Therefore

$$|\lambda_1| \cdot \|w - w_j\| = \|\lambda_1 w - \lambda_1 w_j\| \leq \|\lambda_1 w - Aw_j\| + \|Aw_j - \lambda_1 w_j\|$$

by the triangle inequality, and each of the terms on the right-hand side goes to zero as $j \rightarrow \infty$. Thus $\lim_{j \rightarrow \infty} w_j = w$ and $\|w\| = \lim_{j \rightarrow \infty} \|w_j\| = 1$. Finally

$$\|Aw - \lambda_1 w\| \leq \|Aw - Aw_j\| + \|Aw_j - \lambda_1 w_j\| + \|\lambda_1 w_j - \lambda_1 w\|$$

by the triangle inequality, and each of the terms on the right-hand side goes to zero as $j \rightarrow \infty$. Therefore $Aw = \lambda_1 w$. Q.E.D.

REMARK: This last result is not true for an arbitrary bounded symmetric operator A . First A may have no point eigenvalues at all. Even if A has a basis of eigenvectors the theorem fails to hold.

Example 4 Let \mathcal{H} be an infinite dimensional Hilbert space with an ON basis $\{u_n\}$ of eigenvectors of A such that

$$Au_n = \frac{n}{n+1}u_n, \quad n = 1, 2, \dots$$

Then any unit vector u in \mathcal{H} can be written uniquely in the form $u = \sum_n \alpha_n u_n$ with $\sum_n |\alpha_n|^2 = 1$. We see that $Au = \sum_n \alpha_n \frac{n}{n+1} u_n$. Now $\|A\| = \sup_{\|u\|=1} |(Au, u)|$ and

$$|(Au, u)| = \sum_n |\alpha_n|^2 \frac{n}{n+1} < \sum_n |\alpha_n|^2 = 1.$$

Therefore $\|A\| = 1$ but there is no unit vector $\tilde{u} \in \mathcal{H}$ such that $|(A\tilde{u}, \tilde{u})| = 1$.

Theorem 29 (Spectral Theorem for symmetric completely continuous operators.) Let A be a nonzero symmetric completely continuous operator on the separable Hilbert space \mathcal{H} . Then

1. Every nonzero eigenvalue of A has finite multiplicity.
2. A has countably (or finitely) many eigenvalues $\lambda_1, \lambda_2, \dots$. They can be ordered so that

$$\|A\| = |\lambda_1| \geq |\lambda_2| \geq |\lambda_3| \geq \dots$$

with each nonzero eigenvalue counted a number of times equal to its multiplicity.

3. $\lim_{j \rightarrow \infty} \lambda_j = 0$ if there are an infinite number of eigenvalues.
4. We can choose an eigenvalue ϕ_j corresponding to each eigenvalue λ_j such that $(\phi_j, \phi_k) = \delta_{jk}$.
5. $|\lambda_j| = |(A\phi_j, \phi_j)| = \max_{u \in \mathcal{H}_j, \|u\|=1} |(Au, u)|$ where

$$\mathcal{H}_1 = \mathcal{H} \quad \mathcal{H}_j = \{v \in \mathcal{H} : v \perp \phi_1, \phi_2, \dots, \phi_{j-1}\}.$$

Here, $\mathcal{H} = \mathcal{H}_1 \supset \mathcal{H}_2 \supset \mathcal{H}_3 \supset \dots$.

6. If $u \in \mathcal{R}_A$, i.e., $u = Av$ for some $v \in \mathcal{H}$, then

$$u = \sum_k (u, \phi_n) \phi_n = \sum_n (av, \phi_n) \phi_n = \sum_n \lambda_n (v, \phi_n) \phi_n.$$

The $\{\phi_n\}$ form an ON basis for $\overline{\mathcal{R}_A}$.

PROOF:

1. Let $\lambda \neq 0$ be an eigenvalue of A and $S_\lambda = \{v \in \mathcal{H} : Av = \lambda v\}$. Suppose $\dim S_\lambda = \infty$ and let $\{v_j\}$ be an ON basis for S_λ . Now $\{v_j\}$ is bounded in norm and A is completely continuous, so the set $\{Av_j\} = \{\lambda v_j\}$ contains a convergent subsequence. Impossible! Therefore $\dim S_\lambda$ is finite.
2. By a previous theorem there exists an eigenvalue λ_1 and a unit eigenvector ϕ_1 such that $|\lambda_1| = \|A\|$ and $A\phi_1 = \lambda_1 \phi_1$. let $\mathcal{H}_2 = \{v \in \mathcal{H} : v \perp \phi_1\}$. Then $A\mathcal{H}_2 \subset \mathcal{H}_2$. Indeed, let $v \in \mathcal{H}_2$. Then

$$(\phi_1, Av) = (A\phi_1, v) = \lambda_1(\phi_1, v) = 0,$$

so $Av \in \mathcal{H}_2$. If $A\mathcal{H}_2 = \{\theta\}$ then we are done. Otherwise keep going and use previous theorem to show that there exists an eigenvalue λ_2 and a unit eigenvector ϕ_2 so that

$$|\lambda_2| = \max_{\|u\|=1, u \in \mathcal{H}_2} |(Au, u)|.$$

Clearly $(\phi_1, \phi_2) = 0$. We proceed in this way step by step. At the n th step, either $\mathcal{H}_n = \{\theta\}$ in which case we stop, or we find a unit vector

$$\phi_n \in \mathcal{H}_n = \{v \in \mathcal{H} : v \perp \phi_1, \phi_2, \dots, \phi_{n-1}\}, \quad A\phi_n = \lambda_n$$

where

$$|\lambda_n| = \max_{\|u\|=1, u \in \mathcal{H}_n} |(Au, u)|,$$

etc. Clearly $(\phi_n, \phi_j) = 0$ for $j = 1, \dots, n-1$. Since $\mathcal{H}_1 \supset \mathcal{H}_2 \supset \mathcal{H}_3 \supset \dots$ we have $|\lambda_1| \geq |\lambda_2| \geq |\lambda_3| \geq \dots$.

3. Since $\{\phi_n, n = 1, 2, \dots\}$ is bounded and A is completely continuous, there exists a convergent sequence $\{A\phi_{n_j} = \lambda_{n_j}\phi_{n_j}\}$. Thus

$$\|A\phi_{n_k} - A\phi_{n_j}\|^2 = \|\lambda_{n_k}\phi_{n_k} - \lambda_{n_j}\phi_{n_j}\|^2 = \lambda_{n_k}^2 + \lambda_{n_j}^2 \rightarrow 0 \quad \text{as } j, k \rightarrow \infty,$$

so $\lambda_{n_k} \rightarrow 0$ as $k \rightarrow \infty$ which implies that $\lambda_n \rightarrow 0$ as $n \rightarrow \infty$.

4. Let $u \in \mathcal{R}_A$, $u = Av$ and note that $(u, \phi_k) = (Av, \phi_k) = \lambda_k(v, \phi_k)$. For any integer n , set

$$w_n = v - \sum_{k=1}^n (v, \phi_k) \phi_k.$$

Then $w_n \perp \phi_1, \dots, \phi_n$ which implies $w_n \in \mathcal{H}_{n+1}$. Therefore $|(Aw_n, w_n)| \leq |\lambda_{n+1}| \cdot \|w_n\|^2$ and $\|Aw_n\| \leq |\lambda_{n+1}| \cdot \|w_n\|$. Now

$$\|w_n\|^2 = \|v\|^2 - \sum_{k=1}^n |(v, \phi_k)|^2 \leq \|v\|^2.$$

Therefore $\|w_n\| \leq \|v\|$ for all n . Thus $\|Aw_n\| \rightarrow 0$ as $n \rightarrow \infty$, since $\lambda_{n+1} \rightarrow 0$ as $n \rightarrow \infty$. But

$$Aw_n = Av - \sum_{k=1}^n (v, \phi_k) \lambda_k \phi_k = u - \sum_{k=1}^n (u, \phi_k) \phi_k.$$

Therefore $u = \sum_{k=1}^{\infty} (u, \phi_k) \phi_k$

We haven't quite completed the proof, since we need to show that our procedure has found all of the nonzero eigenvalues. To do this we first review some simple material involving the ranges and null spaces of operators. Let B be an operator on \mathcal{H} with dense domain and let $\mathcal{N}_B = \{u \in \mathcal{D}_B : Bu = \theta\}$, $\mathcal{R}_B = \{v \in \mathcal{H} : v = Bu \text{ for some } u \in \mathcal{D}_B\}$, be the **null space** and the **range** of B , respectively.

Lemma 12 \mathcal{N}_B and \mathcal{N}_{B^*} are closed, and

$$\mathcal{R}_B^\perp = \mathcal{N}_{B^*}, \quad \mathcal{N}_{B^*}^\perp = \overline{\mathcal{R}_B}.$$

PROOF: The proof that the null spaces are closed is elementary. Suppose that $w \perp \mathcal{R}_B$. Then $(w, Bu) = 0$ for all $u \in \mathcal{D}_B$. This implies that $w \in \mathcal{D}_{B^*}$ and $(B^*w, u) = 0$, so $w \in \mathcal{N}_{B^*}$. On the other hand, if $w \in \mathcal{N}_{B^*}$ then $B^*w = \theta$ so $(B^*w, u) = 0$ for all $u \in \mathcal{D}_B$ which implies $(w, Au) = 0$ or $w \perp \mathcal{R}_B$. Q.E.D.

Now again we assume that A is symmetric and completely continuous. This implies also that A is self-adjoint. Thus we have

$$\mathcal{R}_A^\perp = \mathcal{N}_{A^*} = \mathcal{N}_A, \quad \mathcal{N}_A^\perp = \overline{\mathcal{R}_A}.$$

This implies that \mathcal{H} decomposes into the direct sum $\mathcal{H} = \mathcal{N}_A \oplus \overline{\mathcal{R}_A}$ of two closed subspaces. We choose an ON basis $\gamma_1, \gamma_2, \dots$ for \mathcal{N}_A and the ON basis of eigenvectors ϕ_1, ϕ_2, \dots for \mathcal{R}_A .

Corollary 4 *let A be symmetric and completely continuous. Let $\{\gamma_k\}$ be an ON basis for \mathcal{N}_A and $\{\phi_k\}$ be the ON basis for $\overline{\mathcal{R}_A}$ constructed above. Then $\{\gamma_k, \phi_k\}$ is an ON basis for \mathcal{H} , i.e., $\mathcal{H} = \mathcal{N}_A \oplus \overline{\mathcal{R}_A}$.*

CONTINUATION OF PROOF OF THE SPECTRAL THEOREM: have we missed any nonzero eigenvalues of A in the list $\{\lambda_k\}$? Suppose $\lambda \neq 0$ is an eigenvalue with eigenvector ϕ and such that λ is not in the list constructed above. Since $\frac{1}{\lambda}A\phi = \phi$ we see that $\phi \in \mathcal{R}_A$. Therefore $\phi = \sum_{k=1}^{\infty} (\phi, \phi_k) \phi_k$. However, by construction $(\phi, \phi_k) = 0$ for all k , hence $\phi = \theta$. This is impossible, so the list is complete. Q.E.D.

QUESTION: The theorem shows that every $u \in \overline{\mathcal{R}_A}$ can be expanded in an ON basis of the eigenvectors of A , corresponding to nonzero eigenvalues, where the series converges in the Hilbert space sense. However, in the case that \mathcal{H} is a space of functions one can ask about pointwise convergence of the series. Also there is the question of the nature of the eigenfunctions ϕ_k . Are they continuous, differentiable, ...? We will develop some machinery that will help us answer these questions for specific Hilbert spaces and operators.

We say that **Condition I** holds for a symmetric completely continuous operator on \mathcal{H} if

1. $\|A\| \neq 0, \overline{\mathcal{D}_A} = \mathcal{H}, \mathcal{R}_A \subseteq \mathcal{D}_A$.
2. For every bounded sequence $\{u_n\}$ in \mathcal{D}_A there is a subsequence $\{v_n\}$ such that $Av_n \rightarrow v \in \mathcal{D}_A$ as $n \rightarrow \infty$.

REMARKS:

1. If condition I holds then by the spectral theorem, all of the eigenfunctions ϕ_k belong to \mathcal{D}_A .
2. Suppose the following two requirements are satisfied.
 - a) For every nonzero $u \in \mathcal{D}_A$ there exists a real number $[u] > 0$ such that $\|u\| \leq \alpha[u]$ where α is a fixed positive constant, independent of u .
 - b) For every $u = Av \in \mathcal{R}_A$, $v \in \mathcal{D}_A$ there exists a $w \in \mathcal{D}_A$ such that

$$\lim_{n \rightarrow \infty} \left[w - \sum_{k=1}^n a_k \phi_k \right] = 0, \quad a_k = (\phi, \phi_k).$$

Then $w = u$ and $\lim_{n \rightarrow \infty} [u - \sum_{k=1}^n a_k \phi_k] = 0$.

PROOF:

$$\left[w - \sum_{k=1}^n a_k \phi_k \right] \geq \alpha \left\| w - \sum_{k=1}^n a_k \phi_k \right\|.$$

Since the term on the left goes to 0 as $n \rightarrow \infty$, so does the term on the right. Hence $w = u$ Q.E.D.

Example 5 Let $\mathcal{H} = L_c^2(D)$, where D is a bounded domain in R_n . Thus the inner product is $(u, v) = \int_D u \bar{v} dx$. Let A be a symmetric completely continuous operator with $\mathcal{D}_A = \{u : u \in \overset{\circ}{C}(\bar{D})\}$. Set $[u] = \max_{x \in \bar{D}} |u(x)|$ and define the **volume** of D by $V(D) = \int_D dx$. Then if $u \in \mathcal{D}_A$ we have

$$\|u\| = \sqrt{\int_D |u(x)|^2 dx} \leq \sqrt{V(D)} \max_{x \in \bar{D}} |u(x)| = \alpha[u], \quad \alpha = \sqrt{V(D)}.$$

2.1 Separable operators

We say that an operator A on the Hilbert space \mathcal{H} is **separable** if it can be obtained in the following way. Let n be a finite integer and let $\{u_1, u_2, \dots, u_n\}$ be a linearly independent subset of \mathcal{H} , and $\{v_1, v_2, \dots, v_n\}$ be any subset. Then for any $w \in \mathcal{H}$ we define

$$Aw = \sum_{j=1}^n (w, v_j) u_j.$$

Now

$$\|Aw\| \leq \left(\sum_{j=1}^n \|v_j\| \cdot \|u_j\|\right) \|w\|,$$

so A is bounded. Furthermore, A maps \mathcal{H} into a finite-dimensional subspace of \mathcal{H} , so A is completely continuous.

Example 6 Let $\mathcal{H} = L_c^2([a, b], k)$ and define A by

$$Aw(x) = \int_a^b K(x, y)w(y)k(y)dy, \quad K(x, y) = \sum_{j=1}^n u_j(x)\overline{v_j(y)},$$

for $u_j, v_j \in \mathcal{H}$ and $\{u_j\}$ linearly independent. The kernel $K(x, y)$ defined here is said to be **separable**. Note that A is symmetric if $K(x, y) = \overline{K(y, x)}$, i.e., if $K(x, y) = \sum_{j=1}^n u_j(x)\overline{u_j(y)}$.

Theorem 30 Let A be a bounded operator on \mathcal{H} such that there exists a sequence $\{A_n\}$ of completely continuous operators on \mathcal{H} with $\mathcal{D}_{A_n} = \mathcal{H}$ and $\lim_{n \rightarrow \infty} \|A - A_n\| = 0$. Then A is completely continuous.

PROOF: Let $\{u_n\}$ be a bounded sequence in \mathcal{D}_A , ($\|u_n\| \leq \alpha$). We use the Cantor diagonalization argument:

A_1 completely continuous \implies

there exists a subsequence $\{u_n^{(1)}\}$ of $\{u_n\}$ such that $\{A_1 u_n^{(1)}\}$ is convergent.

A_2 completely continuous \implies

there exists a subsequence $\{u_n^{(2)}\}$ of $\{u_n^{(1)}\}$ such that $\{A_2 u_n^{(2)}\}$ is convergent.

A_3 completely continuous \implies

there exists a subsequence $\{u_n^{(3)}\}$ of $\{u_n^{(2)}\}$ such that $\{A_3 u_n^{(3)}\}$ is convergent.

\vdots

A_k completely continuous \implies

there exists a subsequence $\{u_n^{(k)}\}$ of $\{u_n^{(k-1)}\}$ such that $\{A_k u_n^{(k)}\}$ is convergent.

\vdots

Now consider the diagonal sequence $u_1^{(1)}, u_2^{(2)}, u_3^{(3)}, u_4^{(4)}, \dots$. Clearly $\{A_k u_j^{(j)} : j = 1, 2, \dots\}$ is convergent for each k , since $u_j^{(j)} \subset \{u_n^{(k)}\}$ for $j \geq k$. Then for any $\epsilon > 0$ we have

$$\begin{aligned} \|Au_j^{(j)} - Au_\ell^{(\ell)}\| &\leq \|Au_j^{(j)} - A_k u_j^{(j)}\| + \|A_k u_j^{(j)} - A_k u_\ell^{(\ell)}\| + \|A_k u_\ell^{(\ell)} - Au_\ell^{(\ell)}\| \\ &\leq \|A - A_k\| \cdot [\|u_j^{(j)}\| + \|u_\ell^{(\ell)}\|] + \|A_k u_j^{(j)} - A_k u_\ell^{(\ell)}\| < \frac{\epsilon}{4\alpha}(2\alpha) + \frac{\epsilon}{2} = \epsilon, \end{aligned}$$

if we choose k so large that $\|A - A_k\| < \frac{\epsilon}{4\alpha}$ and j, ℓ so large that $\|A_k u_j^{(j)} - A_k u_\ell^{(\ell)}\| < \frac{\epsilon}{2}$. Thus the subsequence $\{Au_j^{(j)}\}$ converges, which implies that A is completely continuous. Q.E.D.

Let Q be one of the intervals $[a, b]$, $(a, b]$, $[a, b)$, (a, b) , where $(-\infty, b]$, $[a, \infty)$, $(-\infty, \infty)$ are permitted.

Theorem 31 Let $k \in C(Q)$ $k(x) > 0$ for $x \in Q$, $\mathcal{H} = L_c^2(Q, k)$. Suppose $K(x, y)$ is complex valued and continuous in (x, y) for all $(x, y) \in Q \times Q$, and

$$\int_Q \int_Q |K(x, y)|^2 k(x) k(y) dx dy < \infty.$$

Then the operator defined on \mathcal{H} by

$$Au(x) = \int_Q K(x, y) u(y) k(y) dy = (u, \overline{K(x, \cdot)}), \quad u \in \mathcal{H} \quad (2.4)$$

is completely continuous.

PROOF: From expression (2.4) we have

$$|Au(x)|^2 \leq \int_Q |K(x, y)|^2 k(y) dy \cdot \int_Q |u(y)|^2 k(y) dy$$

so

$$\|Au\|^2 = \int_Q |Au(x)|^2 k(x) dx \leq \|u\|^2 \int_Q \int_Q |K(x, y)|^2 k(x) k(y) dx dy$$

and

$$\|A\|^2 \leq \int_Q \int_Q |K(x, y)|^2 k(x) k(y) dx dy.$$

Thus A is bounded. Now let $\{u_n\}$ be an ON basis for \mathcal{H} . Then $\{u_n(x) \overline{u_n(y)}\}$ is an ON basis for $\mathcal{K} = L_c^2(Q \times Q, k(x)k(y))$ and $K(\cdot, \cdot) \in \mathcal{K}$. We have the expansion

$$K(x, y) = \sum_{j, \ell} a_{j\ell} u_j(x) \overline{u_\ell(y)}, \quad a_{j\ell} = \int_Q \int_Q |K(x, y)|^2 \overline{u_j(x)} u_\ell(y) k(x) k(y) dx dy,$$

where convergence is in \mathcal{K} , not pointwise. Parseval's equality gives

$$\sum_{j\ell} |a_{j\ell}|^2 = \int_Q \int_Q |K(x, y)|^2 k(x)k(y) dx dy.$$

Now consider the sequence of separable kernels

$$K_n = \sum_{j+\ell=1}^n a_{j\ell} u_j(x) \overline{u_\ell(y)}, \quad n = 2, 3, \dots$$

and operators A_n on \mathcal{H} given by $A_n w(x) = \int_Q K_n(x, y) w(y) k(y) dy$. Clearly each A_n is completely continuous and

$$\|A - A_n\|^2 \leq \int_Q \int_Q |K(x, y) - K_n(x, y)|^2 k(x)k(y) dx dy = \sum_{j\ell=n+1}^{\infty} |a_{j\ell}|^2 \rightarrow 0$$

as $n \rightarrow \infty$. It follows from Theorem 30 that A is completely continuous. Q.E.D.

Corollary 5 *If $Q = Q_1 \times Q_2 \times \dots \times Q_n \subseteq R_n$ (a boxlike domain in Euclidean n space) where each Q_j is an interval on the x_j axis as defined above, then the analogous result to Theorem 31 holds in R_n .*

Definition 21 *We say that the integral operator (2.4) is **Hilbert-Schmidt** if $K \in L_c^2(Q \times Q, k(x)k(y))$, i.e., if $\int_Q \int_Q |K(x, y)|^2 k(x)k(y) dx dy < \infty$.*

Corollary 6 *If Q is as in Corollary 5 and A is Hilbert-Schmidt, then A is completely continuous.*

ASIDE: We will make frequent use of the following basic result from Lebesgue theory.

Theorem 32 (Fubini) *Let $\mathcal{B}_1 = L_c^1(R_n, k_1)$, $\mathcal{B}_2 = L_c^1(R_m, k_2)$, $\mathcal{B} = L_c^1(R_{n+m}, k_1 k_2)$, where $k_1 = k_1(x)$, $k_2 = k_2(y)$, $x = (x_1, \dots, x_n)$, $y = (y_1, \dots, y_m)$. If any one of the Lebesgue integrals*

$$\begin{aligned} \int_{R_{n+m}} |f(x, y)| k_1(x) k_2(y) dx dy, \quad \int_{R_m} \left(\int_{R_n} |f(x, y)| k_1(x) dx \right) k_2(y) dy, \\ \int_{R_n} \left(\int_{R_m} |f(x, y)| k_2(y) dy \right) k_1(x) dx, \end{aligned}$$

*is finite, then all are finite and **equal**. Furthermore, if $f \in \mathcal{B}$ then*

$$\int_{R_{n+m}} f k_1 k_2 dx dy = \int_{R_m} \left(\int_{R_n} f k_1 dx \right) k_2 dy = \int_{R_n} \left(\int_{R_m} f k_2 dy \right) k_1 dx.$$

Thus, if f is a measurable function on R_{n+m} and $|f|$ is integrable, then so is f integrable and each of these integrals can be evaluated as iterated integrals in lower dimensional spaces. The order of iteration is immaterial. (In general it is not permitted to change the order of iteration if f is only conditionally integrable.)

We will not give here the extensive technical details needed to prove this result. However, the idea behind the proof is relatively simple. It is sufficient to consider the case $n = m = 1, k_1 \equiv k_2 \equiv 1$. In our earlier online notes we defined the space of Lebesgue integrable functions $L^1(R_1)$ by first defining the integrals of step functions and then completing the space of step functions in the L^1 norm. Every Lebesgue integrable function was obtained as the a.e pointwise convergent limit of a Cauchy sequence of step functions. Any step function s on the line is associated with a partition $\{x_j : \dots < x_{j-1} < x_j < x_{j+1} < \dots, \quad j = 0, \pm 1, \pm 2, \dots\}$ of the real line. Then the step function is defined by $s(x) = c_j$ for $x_j \leq x < x_{j+1}$, where only a finite number of the constants c_j are nonzero. The integral of s is defined by $\int s dx = \sum_j c_j (x_{j+1} - x_j)$. The sum of two step functions (with different partitions) is again a step function with a refined partition of the real line.

To define the Lebesgue space $L^1(R_2)$ we proceed in an analogous manner. A step function s is associated with a double partition

$$\{(x_j, y_k) : \dots < x_{j-1} < x_j < x_{j+1} < \dots, \quad \dots < y_{k-1} < y_k < y_{k+1} < \dots\}$$

of the real plane, where $j, k = 0, \pm 1, \pm 2, \dots$. The step function is defined by $s(x, y) = c_{j,k}$ for $x_j \leq x < x_{j+1}, y_k \leq y < y_{k+1}$, where only a finite number of the constants $c_{j,k}$ are nonzero. The integral of s is defined by $\int s dx = \sum_{j,k} c_{j,k} (x_{j+1} - x_j) (y_{k+1} - y_k)$. The sum of two step functions (with different partitions) is again a step function with a refined partition of the real plane. Now it is a simple matter to verify the identities

$$\int_{R_s} s dx dy = \int_{R_1} \left(\int_{R_1} s dx \right) dy = \int_{R_1} \left(\int_{R_1} s dy \right) dx.$$

Indeed, for each \tilde{x} or \tilde{y} , $s(\tilde{x}, y)$ or $s(x, \tilde{y})$ is a step function on the line. The rest of the proof of Fubini's theorem involves showing that this identity continues to hold in the limit as we take Cauchy sequences of step functions.

BACK TO COMPLETELY CONTINUOUS OPERATORS

Corollary 7 *Let D be a bounded normal domain in R_n and $\mathcal{H} = L_c^2(D, k)$.*

Let K be a function on $D \times D$ such that

$$\int_{D_y} \int_{D_x} |K(x, y)|^2 k(x) k(y) dx dy = \int_{R_{2n}} |K(x, y)|^2 k(x) k(y) \chi_D(x) \chi_D(y) dx dy < \infty$$

where χ_D is the characteristic function of D , i.e., the operator A such that

$$Aw(x) = \int_D K(x, y) w(y) k(y) dy$$

for $w \in \mathcal{H}$ is Hilbert-Schmidt. Then A is completely continuous.

Example 7 Let the domain D be as in the corollary and suppose

1. $K(x, y) = \frac{a(x, y)}{|x - y|^\alpha}$ for $x, y \in R_n$.
2. a is complex-valued and continuous for $x, y \in \overline{D}$, $0 < \alpha < \frac{n}{2}$. NOTE: A kernel K with properties 1 and 2 is said to be **weakly singular**.
3. $a(x, y) = \overline{a(y, x)}$, for all $x, y \in \overline{D}$.
4. $\mathcal{H} = L_c^2(D, k)$.

According to Hellwig (Theorem 3, Section 4.3)

$$\int_D \frac{dy}{|x - y|^\beta} \leq \frac{\omega_n}{n - \beta} \left(\frac{nV}{\omega_n} \right)^{1 - \frac{\beta}{n}}$$

if $0 < \beta < n$, where ω_n is the area of the unit n -sphere and V is the volume of D . Indeed, for fixed x we can write $y - x$ in polar coordinates centered at x . Then dy is proportional to $r^{n-1} dr d\omega_n$, where $d\omega_n$ is the differential of area measure on the unit n -sphere. Then an estimate for the integral is $\int_0^B \frac{r^{n-1}}{r^\beta} dr = \frac{B^{n-\beta}}{n-\beta}$ where D is contained in a ball of radius B about x . It follows that $\int_{D \times D} |K(x, y)|^2 k(x) k(y) dx dy < \infty$, so the weakly singular kernel $K(x, y)$ defines a symmetric Hilbert-Schmidt operator on \mathcal{H} .

2.2 Pointwise convergence of expansion formulas

Suppose A is a non-zero symmetric Hilbert-Schmidt operator in $L_c^2(D, k)$ with weakly singular or continuous kernel, as above, on the bounded domain

D . Then A has non-zero eigenvalues $\{\lambda_n\}$ with $|\lambda_1| \geq |\lambda_2| \geq \dots$ and corresponding normalized eigenvectors $\{\phi_n\}$ such that they form an ON basis for \mathcal{R}_A . Thus if $u \in \mathcal{R}_A$ then $u = \sum_{n=1}^{\infty} (u, \phi_n) \phi_n$. When is this convergence pointwise?

Theorem 33 *Suppose the kernel K is continuous or weakly singular on the bounded normal domain D , and $\overline{\mathcal{D}_A} = L_c^2(D, k)$. Then $\mathcal{R}_A \subseteq C(\overline{D})$.*

PROOF: let $v = Au$, $u \in \mathcal{D}_A$. Then

$$\begin{aligned} |v(x_1) - v(x_2)|^2 &= \left| \int_D [K(x_1, y) - K(x_2, y)] k(y) u(y) dy \right|^2 \\ &\leq \int_D |K(x_1, y) - K(x_2, y)|^2 k(y) dy \int_D |u(y)|^2 k(y) dy \\ &\leq k_0 \|u\|^2 \int_D |K(x_1, y) - K(x_2, y)|^2 dy, \end{aligned}$$

where $k_0 = \max_{y \in \overline{D}} k(y)$. Now recall that we have verified the inequality

$$\int_{S(x,b)} \frac{dy}{|x-y|^\alpha} \leq c_0^2 b^{n-\alpha}, \quad S(x,b) = \{y \in R_n : |x-b| \leq b\}$$

for $n > \alpha$, where $c_0 > 0$. Let $|x_1 - x_2| < b$ and write

$$\begin{aligned} \int_D |K(x_1, y) - K(x_2, y)|^2 dy &= \int_{D \cap S(x_1, b)} |K(x_1, y) - K(x_2, y)|^2 dy \\ &\quad + \int_{D - D \cap S(x_1, b)} |K(x_1, y) - K(x_2, y)|^2 dy. \end{aligned}$$

The first integral on the right-hand side is bounded above by

$$2 \int_{D \cap S(x_1, b)} (|K(x_1, y)|^2 + |K(x_2, y)|^2) dy \leq c_1 b^{n-\alpha}$$

where $c_1 > 0$ and we have used our inequality. The kernel in the second integral on the right is uniformly continuous in x_1, x_2 , so both integrals go to 0 as $b = |x_1 - x_2| \rightarrow 0$. Thus v is a continuous function. Q.E.D.

Corollary 8 *Let A be an integral operator with weakly singular kernel, $\overline{\mathcal{D}_A} = \mathcal{H}$, and ϕ an eigenfunction of A with nonzero eigenvalue λ . Then $\phi \in C(\overline{D})$.*

PROOF: $A\phi = \lambda\phi \implies A(\lambda^{-1}\phi) = \phi \implies \phi \in \mathcal{R}_A \subseteq C(\overline{D})$. Q.E.D.

Let D be a bounded normal domain and K a weakly singular kernel with $K(x, y) = \overline{K(y, x)}$ for all $x, y \in \overline{D}$, and $\mathcal{H} = L_c^2(D, k)$. Then K defines a symmetric completely continuous operator A (A is Hilbert-Schmidt) with $\mathcal{D}_A = C^0(\overline{D})$. We know that A has nonzero eigenvalues $\lambda_1, \lambda_2, \dots$ with $|\lambda_1| \geq |\lambda_2| \geq \dots \rightarrow 0$ and corresponding normalized eigenfunctions ϕ_1, ϕ_2, \dots , each of which is continuous on \overline{D} .

Theorem 34 *let A be as above. If $u \in \mathcal{R}_A$, $u = Av$, $v \in \mathcal{D}_A$ then $u(x) = \sum_{n=1}^{\infty} (u, \phi_n) \phi_n(x)$ for $x \in \overline{D}$ where the convergence is pointwise uniform absolute on \overline{D} .*

PROOF: Assume there are an infinite number of nonzero eigenvalues. (Otherwise the theorem is trivial.) Recall that $(\phi_i, \phi_j) = \delta_{ij}$ and $A\phi_j = \lambda_j\phi_j$. For $u \in \mathcal{R}_A$ with $u = Av$ we have

$$(u, \phi_j) = (Av, \phi_j) = (v, A\phi_j) = \lambda_j(v, \phi_j).$$

1. Let $S_k(x) = \sum_{n=1}^k (u, \phi_n) \phi_n(x) \in C^0(\overline{D})$ for each integer k . We will show that $\{S_k(x)\}$ is a uniformly pointwise convergent sequence of continuous functions on \overline{D} , so that it converges to a continuous function $w(x)$ in \overline{D} . Indeed, for $k > \ell$,

$$\begin{aligned} |S_k(x) - S_\ell(x)|^2 &= \left| \sum_{n=\ell+1}^k (u, \phi_n) \phi_n(x) \right|^2 \\ &= \left| \sum_{n=\ell+1}^k \lambda_n(v, \phi_n) \phi_n(x) \right|^2 \leq \sum_{n=\ell+1}^k |(v, \phi_n)|^2 \cdot \sum_{n=\ell+1}^k |\lambda_n \phi_n(x)|^2. \end{aligned}$$

Later we will show that $\sum_{n=\ell+1}^k |\lambda_n \phi_n(x)|^2 < \beta^2 < \infty$ for all $x \in \overline{D}$. Assuming this, we see that

$$|S_k(x) - S_\ell(x)| \leq \beta \sqrt{\sum_{n=\ell+1}^k |(v, \phi_n)|^2} \rightarrow 0$$

uniformly in x as $k, \ell \rightarrow \infty$. Thus $\lim_{k \rightarrow \infty} S_k(x) = w(x)$ and, since D is bounded, $\|S_k - w\| \rightarrow 0$ as $k \rightarrow \infty$.

2. $S_k(x) \rightarrow u(x)$, uniformly as $k \rightarrow \infty$. Indeed

$$\|u - w\| \leq \|u - S_k\| + \|S_k - w\| \rightarrow 0$$

as $k \rightarrow \infty$, so $u = w$ in \mathcal{H} and, since u, w are both continuous, we have $u(x) \equiv w(x)$ for all $x \in \overline{D}$.

3. Finally, we have to show that $\sum_{n=1}^{\infty} |\lambda_n \phi_n(x)|^2$ is uniformly bounded on \overline{D} . Now $u(x) = Av(x) = \int_D K(x, y)v(y)k(y)dy = (K(x, \cdot), \overline{v})$, so

$$\begin{aligned} \sum_{n=1}^{\infty} |\lambda_n \phi_n(x)|^2 &= \sum_{n=1}^{\infty} |A\phi_n(x)|^2 \\ &= \sum_{n=1}^{\infty} |(K(x, \cdot), \overline{\phi_n})|^2 \leq (K(x, \cdot), K(x, \cdot)) \end{aligned}$$

by Bessel's inequality. However the right hand side of the last expression is just $\int_D |K(x, y)|^2 k(y)dy < \beta^2 < \infty$ since K is weakly singular. Therefore

$$\sum_{n=1}^{\infty} |\lambda_n \phi_n(x)|^2 \leq \beta^2 < \infty$$

for all $x \in \overline{D}$. Q.E.D.

Let A be symmetric and completely continuous on the Hilbert space \mathcal{H} , and reorder the nonzero eigenvalues $\{\lambda_n\}$ of A so that

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0 \geq \cdots \geq \lambda_{-n} \geq \cdots \geq \lambda_{-1},$$

with associated normalized eigenvectors

$$\phi_1, \phi_2, \dots, \phi_n, \dots, \phi_{-n}, \dots, \phi_{-1}.$$

Theorem 35

$$\begin{aligned} \lambda_1 &= \max_{\|u\|=1, u \in \mathcal{H}} (Au, u), & \lambda_{-1} &= \min_{\|u\|=1, u \in \mathcal{H}} (Au, u), \\ \lambda_n &= \max_{\|u\|=1, u \perp \phi_1, \dots, \phi_{n-1}} (Au, u), & \lambda_{-n} &= \min_{\|u\|=1, u \perp \phi_{-n+1}, \dots, \phi_{-1}} (Au, u), \\ & & n &= 2, 3, \dots \end{aligned}$$

PROOF: We give only the proof of the characterization of λ_1 . The remaining characterizations have similar proofs. If $u \in \mathcal{H}$ with $\|u\| = 1$ then, setting $a_j = (u, \phi_j)$, we have $\sum_j |a_j|^2 = \sum_j |(u, \phi_j)|^2 \leq 1$. Now

$$Au = \sum_j (Au, \phi_j) \phi_j = \sum_j \lambda_j (u, \phi_j) \phi_j$$

so

$$\begin{aligned} (Au, u) &= \sum_j \lambda_j |(u, \phi_j)|^2 = \overbrace{\lambda_1 |a_1|^2 + \lambda_2 |a_2|^2 + \cdots}^{\text{positive}} + \overbrace{\cdots + \lambda_{-2} |a_{-2}|^2 + \lambda_{-1} |a_{-1}|^2}^{\text{negative}} \\ &\leq \lambda_1 \left(\sum_j |a_j|^2 \right) \leq \lambda_1. \end{aligned}$$

But $(A\phi_1, \phi_1) = \lambda_1$. Q.E.D.

2.3 Relationships between completely continuous and S-L operators. Green's functions

Consider a general regular S-L operator in R_1 , (1.10). Here,

$$Au = \frac{1}{k(x)} [-(p(x)u')' + q(x)u], \quad \mathcal{H} = L_c^2([\ell, m], k),$$

$$\mathcal{D}_A = \{u \in \mathcal{H} : u \in C^2([\ell, m]); B_1 u = B_2 u = 0\}$$

$$B_j u = \alpha_{j1} u(\ell) + \alpha_{j2} u'(\ell) + \alpha_{j3} u(m) + \alpha_{j4} u'(m), \quad j = 1, 2,$$

and the $\alpha_{j\ell}$ are real. Assume B_1, B_2 are linearly independent and such that A is a symmetric operator.

If the complex number μ is not an eigenvalue of A then $(A - \mu I)^{-1}$ exists. Further $\mathcal{D}_{(A - \mu I)^{-1}} = \mathcal{R}_{A - \mu I} = C^0([\ell, m])$, $\mathcal{R}_{(A - \mu I)^{-1}} = \mathcal{D}_{A - \mu I} = \mathcal{D}_A$ and

$$(A - \mu I)^{-1} f(x) = \int_{\ell}^m g(x, y, \mu) f(y) k(y) dy, \quad f \in C^0([\ell, m])$$

where $g(x, y, \mu) = g(y, x, \mu)$ is symmetric, bounded and continuous on $[\ell, m]$.

Theorem 36 *Let A be a general non-singular symmetric S-L operator as defined above. Then*

1. *A has a countably infinite number of eigenvalues $\lambda_1 \leq \lambda_2 \leq \dots$, all real with only $+\infty$ as a limit point. The multiplicity of an eigenvalue is at most 2.*
2. *Let $\{\phi_j\}$ be the corresponding normalized eigenvectors of the $\{\lambda_j\}$, $A\phi_j = \lambda_j\phi_j$. Then the $\{\phi_j\}$ form an ON basis for \mathcal{D}_A , hence for \mathcal{H} . Furthermore, if $u \in \mathcal{D}_A$ then*

$$u(x) = \sum_{j=1}^{\infty} (u, \phi_j) \phi_j(x)$$

where the convergence is pointwise uniformly absolute.

3. *The eigenvalues are characterized by the minimization properties*

$$\lambda_1 = \min_{\|u\|=1, u \in \mathcal{D}_A} (Au, u) \quad \lambda_j = \min_{\|u\|=1, u \in \mathcal{D}_A, u \perp \phi_1, \dots, \phi_{j-1}} (Au, u).$$

PROOF: Choose μ real and not an eigenvalue of A . Let $B = A - \mu I$. Then B^{-1} exists and

$$B^{-1}f(x) = \int_{\ell}^m g(x, y, \mu) k(y) f(y) dy$$

and the kernel is real and symmetric in (x, y) , so B^{-1} is a symmetric completely continuous operator. Further, $\mathcal{D}_{B^{-1}} = \mathcal{R}_A$, $\mathcal{R}_{B^{-1}} = \mathcal{D}_A$. it follows that B^{-1} has real nonzero eigenvalues $\{\Lambda_j\}$ and corresponding normalized eigenvectors $\{\phi_j\}$ such that $B^{-1}\phi_j = \Lambda_j\phi_j$ and $\{\phi_j\}$ is an ON basis for $\mathcal{R}_{B^{-1}} = \mathcal{D}_A$. B^{-1} has no zero eigenvalues.

If $u \in \mathcal{D}_A$ then $u(x) = \sum_j (u, \phi_j) \phi_j(x)$ where the convergence is pointwise uniform and absolute. Now

$$\begin{aligned} (A - \mu I)^{-1} \phi_j &= B^{-1} \phi_j = \Lambda_j \phi_j \iff \Lambda_j (A - \mu I) \phi_j = \phi_j \\ &\iff A \phi_j = (\mu + \frac{1}{\Lambda_j}) \phi_j = \lambda_j \phi_j. \end{aligned}$$

Therefore, $\lambda_j = \mu + \frac{1}{\Lambda_j}$ is an eigenvalue of A if and only if Λ_j is a nonzero eigenvalue of B^{-1} . Also the $\{\phi_j\}$ are the eigenvectors corresponding to $\{\lambda_j\}$. Since A is bounded below, we can order the eigenvalues of A so that

$$\lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \dots \rightarrow +\infty.$$

There are an infinite number of eigenvalues because \mathcal{D}_A is infinite dimensional. This proves statements 1 and 2. Statement 3 follows immediately from Theorem 35. Q.E.D.

Example 8 *Let*

$$A = -\frac{d^2}{dx^2}, \quad \mathcal{H} = L_c^2([0, 2\pi], 1),$$

$$\mathcal{D}_A = \left\{ u \in \mathcal{H} : u \in C^2[0, 2\pi], u(0) = u(2\pi), u'(0) = u'(2\pi) \right\}.$$

Note that A is symmetric. Indeed, for $u, v \in \mathcal{D}_A$

$$(Au, v) = - \int_0^{2\pi} \frac{d^2 u}{dx^2} \bar{v} dx = - \frac{du}{dx} \bar{v} \Big|_0^{2\pi} + \int_0^{2\pi} \frac{du}{dx} \frac{d\bar{v}}{dx} dx = - \int_0^{2\pi} u \frac{d^2 \bar{v}}{dx^2} dx = (u, Av).$$

To find the eigenvectors and eigenvalues we solve $Au = \lambda u$ for $u \in \mathcal{D}_A$ or $-u'' = \lambda u$. Applying the boundary conditions we find that the eigenvalues are $\lambda_n = n^2$, $n = 0, \pm 1, \pm 2, \dots$ and the corresponding eigenvectors are $\phi_n = e^{inx}/\sqrt{2\pi}$. Thus each eigenvalue is of multiplicity 2 if $n \neq 0$ and the eigenvalue 0 is of multiplicity 1. The $\{u_n\}$ form an ON basis for $\text{cal } H$. If $u \in \mathcal{D}_A$ then $u(x) = \sum_{n=-\infty}^{\infty} (u, u_n) u_n(x)$ where the convergence is pointwise uniform and absolute. Note that this expansion

$$u(x) = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} \left[\int_0^{2\pi} u(y) e^{-iny} dy \right] e^{inx}$$

is just the complex form of Fourier series.

REMARK: In the above examples, and examples to follow, of symmetric S-L operators A with completely continuous inverses A^{-1} , the S-L operators are, in fact, essentially self-adjoint. (If A has 0 as an eigenvalue, just choose a real μ that isn't an eigenvalue so that $A - \mu I$ is invertible. Our argument will then show that $A - \mu I$ is essentially self-adjoint, which implies that A is essentially self-adjoint.)

To see this note that the bounded operator $\overline{A}^{-1} = \overline{A^{-1}}$ is self-adjoint and $\mathcal{D}_{\overline{A^{-1}}} = \mathcal{H}$. Thus $\mathcal{R}_{\overline{A}} = \mathcal{D}_{\overline{A^{-1}}} = \mathcal{H}$ and $\mathcal{D}_{\overline{A}} = \mathcal{R}_{\overline{A^{-1}}}$. Since A is symmetric we have $\overline{A} \subseteq A^* = \overline{A}^*$. Now let $v \in \mathcal{D}_{\overline{A}^*}$. Then

$$(\overline{A}u, v) = (u, \overline{A}^*v)$$

for all $u \in \mathcal{D}_{\overline{A}} = \mathcal{R}_{\overline{A^{-1}}}$. Every such u is of the form $u = \overline{A}^{-1}w$, where $w \in \mathcal{H}$, and every $w \in \mathcal{H}$ is of the form $w = \overline{A}u$. Thus the above equation reads

$$(w, v) = (\overline{A}^{-1}w, \overline{A}^*v) = (w, \overline{A}^{-1}\overline{A}^*v),$$

for all $w \in \mathcal{H}$. (The last identity follows from the fact that the bounded operator \overline{A}^{-1} is self-adjoint.) We conclude that $v = \overline{A}^{-1}\overline{A}^*v$, so $v \in \mathcal{D}_{\overline{A}}$ and $\overline{A}v = \overline{A}^*v$. This shows that $A^* \subseteq \overline{A}$, so $A^* = \overline{A}$. Q.E.D.

2.3.1 Extension to an S-L operator in R_n

We will sketch a treatment of pointwise convergence for expansions in terms of eigenfunctions of S-L operators in R_n . Let D be a bounded normal domain and $\mathcal{H} = L^2(D)$. We consider only the S-L operator (1.21)

$$Au = -\Delta_n u, \quad \Delta_n = \sum_{j=1}^n \frac{\partial^2}{\partial x_j^2},$$

and

$$\mathcal{D}_A = \left\{ u : u \in C^1(\overline{D}) \cap C^2(D), Au \in \mathcal{H}, \text{ and } u = 0 \text{ for } x \in \partial D \right\}.$$

Recall that A is symmetric, bounded below, and strictly positive.

Assume $n \geq 2$. We give a sketch of the construction of A^{-1} . The functions $u = S_n$ where

$$S_n(x, y) = \begin{cases} \frac{1}{(n-2)\omega_n|x-y|^{n-2}}, & \text{for } n > 2 \\ -\frac{1}{2\pi} \ln|x-y|, & \text{for } n = 2, \end{cases} \quad (2.5)$$

$x, y \in R_n$ and ω_n is the area of the unit n -sphere, are called **principal solutions** of the equation $\Delta_n u = 0$. For a discussion of these functions, see Titchmarsh, "Eigenfunction Expansions, Part II," Oxford, 1958. There the following result from potential theory is proved:

Theorem 37 *Let $f \in C^1(\overline{D})$ and define u by*

$$u(x) = - \int_D S_n(x, y) f(y) dy.$$

Then $u \in C^1(\overline{D}) \cap C^2(D)$ and $\Delta_n u(x) = f(x)$ in D .

Suppose that D is such that the **Dirichlet problem** can be solved: Given a continuous function $g(x)$ on ∂D find a unique function $v \in C^2(D) \cap C^0(\overline{D})$ such that $\Delta_n v = 0$ and $v(x) = g(x)$ for all $x \in \partial D$. Then for every $y \in \overline{D}$ we can find a solution $\gamma(x, y)$ of $\Delta_n \gamma = 0$ and $\gamma(x, y) = -S_n(x, y)$, for all $x \in \partial D$. We define the **Green's function** for this problem by

$$g(x, y) = \gamma(x, y) + S_n(x, y).$$

Then $\Delta_n g(x, y) = 0$ for $x \neq y$, and if f is defined as in Theorem 37, the function

$$u(x) = - \int_D g(x, y) f(y) dy$$

satisfies $u \in \mathcal{D}_A$ and $\Delta_n u = f(x)$ in D . Thus we have inverted the equation $Au = f$ to find the unique solution $u = A^{-1}f$. It follows that $C^1(\overline{D}) \subseteq \mathcal{D}_{A^{-1}}$ and

$$A^{-1}f(x) = - \int_D g(x, y) f(y) dy$$

if $f \in C^1(\overline{D})$.

One can show that $g(x, y)$ is an Hilbert-Schmidt kernel if $n = 2, 3$ so then A^{-1} is completely continuous. Furthermore, since A is symmetric we have that A^{-1} is symmetric. Therefore the expansion theorem for completely continuous symmetric operators applies to A^{-1} . Keep in mind that

$$A\phi = \lambda\phi \iff \frac{1}{\lambda}\phi = A^{-1}\phi.$$

We conclude that A has an infinite number of eigenvalues $\lambda_1 \leq \lambda_2 \leq \dots$ and corresponding normalized eigenvectors ϕ_1, ϕ_2, \dots with $\phi_n \in C^1(\overline{D})$ and each eigenvalue of finite multiplicity. Further, if $u \in \mathcal{D}_A \cap C^3(\overline{D})$ then $Au \in C^1(\overline{D})$ and

$$u(x) = \sum_{n=1}^{\infty} (u, \phi_n) \phi_n(x)$$

where the convergence is uniform and absolute on \overline{D} .

The following result enlarges the domain of functions with a pointwise convergence expansion.

Theorem 38 1) If $u \in \mathcal{D}_A$ then $u(x) = \int_D g(x, y) f(y) dy$ where $f(x) = -\Delta_n u(x)$. 2) If $f \in C^1(\overline{D})$ then the function $u(x) = \int_D g(x, y) f(y) dy$ is an element of $C^2(D) \cap C^1(\overline{D})$ and $\Delta_n u = -f$ in D .

SKETCH OF PROOF OF 1): This is a standard potential theory argument, making use of the integration by parts formula (1.20). We choose a point $x \in D$ and let $J_\epsilon \subset D$ be a ball of radius ϵ about x . Then we apply a variant of formula (1.20) to the domain $D - J_\epsilon$:

$$\int_{\partial D + \partial J_\epsilon} u \frac{\partial g}{\partial n} d_y S - \int_{\partial D + \partial J_\epsilon} g \frac{\partial u}{\partial n} d_y S = \int_{D - J_\epsilon} u \Delta_n g \, dy - \int_{D - J_\epsilon} g \Delta_n u \, dy.$$

Now $\Delta_n g = 0$ and $\Delta_n u = -f$ in $D - J_\epsilon$, whereas $u = g = 0$ on ∂D . Thus the equation reduces to

$$\int_{\partial J_\epsilon} u \frac{\partial g}{\partial n} d_y S - \int_{\partial J_\epsilon} g \frac{\partial u}{\partial n} d_y S = \int_{D - J_\epsilon} g f \, dy.$$

The behavior of the two integrals on the left is entirely determined by the singularity at x of the principal solution $S_n(x, y)$. It is straightforward to show that as $\epsilon \rightarrow 0$ the first integral on the left goes to $u(x)$, whereas the second integral goes to 0. As $\epsilon \rightarrow 0$ the integral on the right obviously converges to $\int_D g f \, dy$. Thus $u = \int_D g f \, dy$. Q.E.D.

We conclude from this last result that if $u \in \mathcal{D}_A$ then $f = \Delta_n u \in \mathcal{R}_A$, so $u(x) = \sum_{n=1}^{\infty} (u, \phi_n) \phi_n(x)$ where the convergence is uniform and absolute on \overline{D} .

2.3.2 Extension to mixed initial and boundary value problems

Here we consider a mixed initial and boundary value problem $Au + \dot{u} = f$ where A is an S-L operator, $f(x, t)$ is a given function and both f and $u(x, t)$, and all functions in the function space, are real valued. We choose A to be an ordinary S-L operator on an interval on the real line

$$Au = \frac{1}{k(x)} \left[-\frac{\partial}{\partial x} \left(p(x) \frac{\partial u}{\partial x} \right) + q(x)u \right], \quad x \in [\ell, m],$$

with separated boundary conditions

$$B_1 u(x, t) = \alpha_{11} u(\ell, t) + \alpha_{12} \frac{\partial u}{\partial x}(\ell, t) = 0,$$

$$B_2 u(x, t) = \alpha_{21} u(m, t) + \alpha_{22} \frac{\partial u}{\partial x}(m, t) = 0,$$

for $0 < t < \infty$. Here B_1, B_2 are assumed linearly independent. For each $0 < t < \infty$, A acts on the Hilbert space

$$\mathcal{H}_t = \left\{ u(x, t) : \int_{\ell}^m u^2(x, t) k(x) dx < \infty \right\}, \quad (u, v)_t = \int_{\ell}^m u(x, t) v(x, t) k(x) dx.$$

The domain of A at time t is

$$\mathcal{D}_A^t = \left\{ u(x, t) \in \mathcal{H}_t : u \in C^2[\ell, m], \quad B_1 u = B_2 u = 0 \right\}.$$

Theorem 39 *Suppose we are given functions $u_0(x) \in C^0[\ell, m]$, $f \in C^0(\ell \leq x \leq m, 0 < t < \infty)$. Then*

1. *There exists at most one solution u of the equation $Au + \frac{\partial u}{\partial t} = f$ such that $u \in \mathcal{D}_A^t$, $\frac{\partial u}{\partial t} \in C^0(\ell \leq x \leq m, 0 < t < \infty)$, and $u(x, 0) = u_0(x)$ for all $x \in [\ell, m]$.*
2. *If the solution u exists, it is given by the expression*

$$u(x, t) = \sum_{j=1}^{\infty} \left[(u_0, \phi_j) + \int_0^t (f, \phi_j) e^{\lambda_j \tau} d\tau \right] \cdot e^{-\lambda_j t} \phi_j(x)$$

where $\lambda_1 \leq \lambda_2 \leq \dots$ are the eigenvalues of A and the $\{\phi_j\}$ are the corresponding normalized eigenvectors.

3. *If a) $u_0(x), \frac{\partial u_0}{\partial x}, \frac{\partial^2 u}{\partial x^2} \in C^0[\ell, m]$, b) $f \equiv 0$, and c) $B_1 u_0 = B_2 u_0 = 0$, then a solution u exists.*

REMARK: Formally, assertion 2. states that the solution of $Au + \dot{u} = f$ is

$$u = e^{-tA} u_0 + e^{-tA} \int_0^t e^{\tau A} f d\tau.$$

Lemma 13 *let $x \in [a, b]$ and suppose*

1. $\sum_{j=1}^{\infty} v_j(x) = v(x)$ for all $x \in [a, b]$.
2. $v_j(x) \in C^1[a, b]$, for all j .
3. $\sum_{j=1}^{\infty} v'_j(x) = g(x)$ where the convergence is pointwise uniform on $[a, b]$.

Then $v \in C^1[a, b]$ and $v'(x) = \sum_{j=1}^{\infty} v'_j(x)$ for all $x \in (a, b)$.

PROOF OF THE LEMMA: Let $s_n(x) = \sum_{j=1}^n v_j(x)$. Then $s_n \in C^1[a, b]$ and $s_n(x) \rightarrow v(x)$, $s'_n(x) \rightarrow g(x)$ as $n \rightarrow \infty$, where the convergence is uniform. By the Fundamental Theorem of Calculus, $s_n(x) - s_n(a) = \int_a^x s'_n(y) dy$ goes in the limit as $n \rightarrow \infty$ to $v(x) - v(a) = \int_a^x g(y) dy$ since the convergence is uniform. Also, since each v'_j is continuous and the convergence is uniform, then g is continuous. Thus, by the Fundamental Theorem of Calculus again, we have $v'(x) = g(x)$ for all $x \in (a, b)$. Q.E.D.

PROOF OF THE THEOREM: Assume a solution u exists. Then $u \in \mathcal{D}_A^t$ for all $t \in (0, \infty)$, so

$$u(x, t) = \sum_{j=1}^{\infty} (u, \phi_j)_t \phi_j(x)$$

where the convergence is uniform and absolute in x . Set $\alpha_j(t) = (u, \phi_j)_t$.

Remarks:

- $\alpha_j(0) = (u_0, \phi_j)$.
- We have

$$\begin{aligned} Au + \dot{u} = f &\implies (Au, \phi_j)_t + (\dot{u}, \phi_j)_t = (f, \phi_j)_t \\ &\implies \lambda_j (u, \phi_j)_t + \frac{\partial}{\partial t} (u, \phi_j)_t = (f, \phi_j)_t \\ &\implies \dot{\alpha}_j(t) + \lambda_j \alpha_j(t) = (f, \phi_j)_t. \end{aligned}$$

- Thus

$$\alpha_j(t) = e^{-\lambda_j t} \left[\int_0^t (f, \phi_j)_\tau e^{\lambda_j \tau} d\tau + (u_0, \phi_j) \right].$$

This proves assertions 1. and 2. of the theorem. To prove assertion 3. it is enough to show that the series $\sum_{j=1}^{\infty} (u_0, \phi_j) e^{-\lambda_j t} \phi_j(x)$ converges to a function u that is a solution of the boundary value problem.

Remarks:

- $\sum_{j=1}^{\infty} (u_0, \phi_j) \phi_j(x)$ converges uniformly and absolutely to $u_0(x)$.
- $\lambda_j \rightarrow +\infty$ as $j \rightarrow \infty$.
- $e^{-\lambda_j t} \rightarrow 0$ as $j \rightarrow \infty$. Thus $\sum_{j=1}^{\infty} (u_0, \phi_j) e^{-\lambda_j t} \phi_j(x) = u(x, t)$ converges uniformly and absolutely in x and t .

- Let $u_j(x, t) = (u_0, \phi_j)e^{-\lambda_j t}\phi_j(x)$. Clearly $Au_j + \dot{u}_j = 0$.
- It is enough to show that the series $\sum_j \dot{u}_j$, $\sum_j \frac{\partial u_j}{\partial x}$, and $\sum_j \frac{\partial^2 u_j}{\partial x^2}$ converge uniformly in the interval $\ell \leq x \leq m$, $0 < t_0 \leq t < \infty$, for every $t_j > 0$.
- $\sum_j \dot{u}_j = -\sum_j (u_0, \phi_j)\lambda_j e^{-\lambda_j t}\phi_j(x)$ and $\lambda_j e^{-\lambda_j t} \rightarrow 0$, as $j \rightarrow \infty$, uniformly for all $t > t_0 > 0$. Therefore $\sum_j \dot{u}_j$ converges uniformly $\Rightarrow \dot{u}(x, t)$ exists and $\dot{u}(x, t) = \sum_j \dot{u}_j(x, t)$.
- $\sum_j \frac{\partial u_j}{\partial x} = \sum_j (u_0, \phi_j)e^{-\lambda_j t}\phi_j'(x)$. Assume that 0 is not an eigenvalue of A . Then

$$A\phi_j = \lambda_j\phi_j \iff \phi_j = \lambda_j A^{-1}\phi_j = \lambda_j \int_{\ell}^m g(x, y, 0)k(y)\phi_j(y)dy,$$

where

$$g(x, y, 0) = \begin{cases} -\frac{v_2(x)v_1(y)}{p(\ell)w(\ell)}, & \ell \leq y \leq x \leq m, \\ -\frac{v_1(x)v_2(y)}{p(\ell)w(\ell)}, & \ell \leq x \leq y \leq m, \end{cases}$$

with $Av_1 = av_2 = \theta, B_1v_1 = B_2v_2 = 0$. Thus

$$\begin{aligned} \phi_j(x) &= -\lambda_j v_2(x) \int_{\ell}^x \frac{v_1(y)k(y)\phi_j(y)}{pw} dy - \lambda_j v_1(x) \int_x^m \frac{v_2(y)k(y)\phi_j(y)}{pw} dy \\ \Rightarrow \phi_j'(x) &= -\lambda_j v_2'(x) \int_{\ell}^x \frac{v_1(y)k(y)\phi_j(y)}{pw} dy - \lambda_j v_1'(x) \int_x^m \frac{v_2(y)k(y)\phi_j(y)}{pw} dy. \end{aligned}$$

Therefore, $\sum_j (u_0, \phi_j)e^{-\lambda_j t}\phi_j'(x)$ converges uniformly.

- $A\phi_j = \lambda_j\phi_j \Rightarrow \phi_j'' = \frac{1}{p}[-p'\phi_j' + q\phi_j - \lambda_2 k\phi_j] \Rightarrow \sum_j (u_0, \phi_j)e^{-\lambda_j t}\phi_j''$ converges uniformly. Q.E.D.

The corresponding problem for $Au + \ddot{u} = f$ has a very similar treatment.

Chapter 3

Spectral Theory for Self-Adjoint Operators

We start by reformulating the expansion theorem for symmetric completely continuous operators in a manner that will generalize to all self-adjoint operators. Let A be symmetric and completely continuous on the Hilbert space \mathcal{H} , and let $\{\lambda_j\}$ (including the zero eigenvalue if it exists) be the eigenvalues of A . Denoting by ϕ_j the corresponding normalized eigenvectors, we now have that $\{\phi_j\}$ is an ON basis for \mathcal{H} , not just $\overline{\mathcal{R}_A}$. If $u \in \mathcal{H}$ then

$$u = \sum_{j=1}^{\infty} (u, \phi_j) \phi_j.$$

Note that the eigenvectors ϕ_j are not uniquely determined, since the eigenspaces corresponding to nonzero eigenvalues could have finite multiplicity, and the zero eigenspace may even have countably infinite multiplicity. It is only the eigenspaces themselves that are unique. The following statements are easy to verify.

Theorem 40 *Let λ be a real number and define the operator E_λ by*

$$E_\lambda u = \sum_{\{j: \lambda_j \leq \lambda\}} (u, \phi_j) \phi_j$$

for any $u \in \mathcal{H}$.

1. E_λ is a linear operator in \mathcal{H} , with $\mathcal{D}_{E_\lambda} = \mathcal{H}$.

2. E_λ is symmetric.
3. E_λ is bounded and $\|E_\lambda\| = 1$ if $E_\lambda \neq 0$.
4. $E_\lambda^2 = E_\lambda$.
5. If $\lambda \geq \|A\|$ then $E_\lambda = I$.
6. If $\lambda < -\|A\|$ then $E_\lambda = 0$.
7. $E_\lambda E_\mu = E_\mu E_\lambda = E_\omega$ where $\omega = \min(\mu, \lambda)$.

Let \mathcal{S}_{λ_j} be the eigenspace corresponding to eigenvalue λ_j . (Note that we may have $\mathcal{S}_{\lambda_j} = \mathcal{S}_{\lambda_k}$, provided $\lambda_j = \lambda_k$.)

Remarks:

1. Let $\mathcal{M}_\lambda = \{v \in \mathcal{H} : v \perp \mathcal{S}_{\lambda_j} \text{ for all } \lambda_j > \lambda\}$. Then \mathcal{M}_λ is closed and its definition is independent of the choice of basis $\{\phi_j\}$. Furthermore $\mathcal{H} = \mathcal{M}_\lambda \oplus \mathcal{M}_\lambda^\perp$.

2. We have

$$v \in \mathcal{M}_\lambda \iff v = \sum_{\{j: \lambda_j \leq \lambda\}} (v, \phi_j) \phi_j,$$

$$v \in \mathcal{M}_\lambda^\perp \iff v = \sum_{\{j: \lambda_j > \lambda\}} (v, \phi_j) \phi_j,$$

3. Given $u \in \mathcal{H}$ we can write $u = u_1 + u_2$, with $u_1 \in \mathcal{M}_\lambda$, $u_2 \in \mathcal{M}_\lambda^\perp$ and the decomposition is unique. Clearly, $u = \sum_j (u, \phi_j) \phi_j$

$$\implies u_i = \sum_{\{j: \lambda_j \leq \lambda\}} (u, \phi_j) \phi_j, \quad u_2 = \sum_{\{j: \lambda_j > \lambda\}} (u, \phi_j) \phi_j.$$

4. $E_\lambda u = u_1 =$ projection of u on \mathcal{M}_λ , independent of the choice of basis $\{\phi_j\}$.

5. We have

$$E_\lambda u = u \iff u \in \mathcal{M}_\lambda \iff u = \sum_{\{j: \lambda_j \leq \lambda\}} (u, \phi_j) \phi_j.$$

6. We have

$$E_\lambda u = \theta \iff u \in \mathcal{M}_\lambda^\perp \iff u = \sum_{\{j:\lambda_j > \lambda\}} (u, \phi_j) \phi_j.$$

Let $\rho(\lambda) = (E_\lambda u, v)$ for $u, v \in \mathcal{H}$. This defines ρ on the interval $(-\infty, \infty)$.

Theorem 41 ρ is a step function and right continuous, i.e., $\lim_{\lambda \rightarrow \lambda_0+} \rho(\lambda) = \rho(\lambda_0)$. Also, $\rho(\lambda) = 0$ if $\lambda < -\|A\|$, $\rho(\lambda) = (u, v)$ if $\lambda \geq \|A\|$.

PROOF: Explicitly,

$$\begin{aligned} \rho(\lambda) &= (E_\lambda u, v) = \left(\sum_{\{j:\lambda_j \leq \lambda\}} (u, \phi_j) \phi_j, \sum_{\{j:\lambda_j \leq \lambda\}} (v, \phi_j) \phi_j \right) \\ &= \sum_{\{j:\lambda_j \leq \lambda\}} (u, \phi_j) \overline{(v, \phi_j)}. \end{aligned}$$

Q.E.D.

Note that the eigenvalues of A are located at the jump discontinuities of ρ .

At this point we recall the Riemann-Stieltjes integral, a very useful tool for representing the spectral resolutions of operators. Let $[a, b]$ $a < b$ be a bounded interval on the real line. For any partition

$$\Delta: \quad a = x_0 < x_1 < \cdots < x_n = b$$

we define the maximum partition width $\|\Delta\| = \max_{i=1, \dots, n} \{x_i - x_{i-1}\}$. Given functions $f(x), g(x)$ on $[a, b]$ choose y_k such that $x_{k-1} \leq y_k \leq x_k$, $k = 1, \dots, n$.

Definition 22 The Riemann-Stieltjes integral $\int_a^b f dg$ is defined by

$$\int_a^b f(x) dg(x) = \lim_{\|\Delta\| \rightarrow 0} \sum_{k=1}^n f(y_k) \{g(x_k) - g(x_{k-1})\},$$

if the limit exists.

Here we are taking the limit over all partitions as the partition width goes to 0. This is just the ordinary Riemann integral if $g(x) = x$. However the Riemann-Stieltjes integral makes sense for functions g with jump discontinuities. The **improper Riemann-Stieltjes integral** is defined by

$$\int_{-\infty}^{\infty} f(x) dg(x) = \lim_{b \rightarrow +\infty} \lim_{a \rightarrow -\infty} \int_a^b f(x) dg(x),$$

if the limits exist.

Theorem 42 *let A be a symmetric completely continuous operator as defined above. Then*

$$(Au, v) = \int_{-\infty}^{\infty} \lambda \, d\rho_{u,v}(\lambda) = \int_{-\infty}^{\infty} \lambda \, d(E_{\lambda}u, v) = \sum_j \lambda_j (u, \phi_j)(\phi_j, v),$$

where the integral is Riemann-Stieltjes.

Note: We can also write $A = \int_{-\infty}^{\infty} \lambda \, dE_{\lambda}$ because

$$\lim_{\|\Delta\| \rightarrow 0} \sum_{k=1}^n \xi_k (E_{x_k} - E_{x_{k-1}}) = A,$$

where the limit is taken with respect to the operator norm. Further we can write

$$Au = \int_{-\infty}^{\infty} \lambda \, dE_{\lambda}u = \sum_k \lambda_k (u, \phi_k)$$

because

$$\lim_{\|\Delta\| \rightarrow 0} \sum_{k=1}^n \xi_k (E_{x_k}u - E_{x_{k-1}}u) = Au,$$

where the limit is taken with respect to the Hilbert space norm.

3.1 Projection operators

Let \mathcal{M} be a closed subspace of the Hilbert space \mathcal{H} . Then

$$\mathcal{H} = \mathcal{M} \oplus \mathcal{M}^{\perp},$$

i.e., every $u \in \mathcal{H}$ can be written uniquely as $u = u_1 + u_2$, where $u_1 \in \mathcal{M}$, $u_2 \in \mathcal{M}^{\perp}$. Define the operator $P : \mathcal{H} \rightarrow \mathcal{H}$ by $Pu = u_1$ for all $u \in \mathcal{H}$. P is called the **orthogonal projection operator** onto \mathcal{M} .

Theorem 43 *let P be the orthogonal projection operator of \mathcal{H} onto \mathcal{M} . Then*

1. P is linear and symmetric
2. The projection operator onto \mathcal{M}^{\perp} is $Q = I - P$.
3. $P^2 = P$.

4. If $P \neq 0$ then $\|P\| = 1$.
5. $P \neq 0$ is a positive operator.
6. $\mathcal{R}_P = \mathcal{M}$, $\mathcal{N}_P = \mathcal{M}^\perp$, and $\mathcal{D}_P = \mathcal{H}$.

PROOF:

1. Let $u, v \in \mathcal{H}$, $\alpha, \beta \in \mathbb{C}$, $u = u_1 + u_2$, $v = v_1 + v_2$, with $u_1, v_1 \in \mathcal{M}$, $u_2, v_2 \in \mathcal{M}^\perp$. Then $\alpha u + \beta v = (\alpha u_1 + \beta v_1) + (\alpha u_2 + \beta v_2)$ where the first term is in \mathcal{M} and the second in \mathcal{M}^\perp . Thus $Pu = u_1$, $Pv = v_1$ and

$$P(\alpha u + \beta v) = \alpha u_1 + \beta v_1 = \alpha Pu + \beta Pv.$$

Also

$$(Pu, v) = (u_1, v_1 + v_2) = (u_1, v_1) = (u_1 + u_2, v_1) = (u, Pv).$$

2. $Qu = u_2$. But also $(I - P)u = u_1 + u_2 - u_1 = u_2$.
3. $PPu = Pu_1 = u_1 = Pu$.
4. If $P \neq 0$ then

$$\|Pu\|^2 = \|u_1\|^2 \leq \|u_1\|^2 + \|u_2\|^2 = \|u\|^2, \implies \|P\| \leq 1.$$

But if $u \in \mathcal{R}_P = \mathcal{M}$ then $\|Pu\| = \|u\|^2$, so $\|P\| = 1$.

5. $(Pu, u) = (PPu, u) = (Pu, Pu) = \|Pu\|^2 \geq 0$.
6. This is evident. Q.E.D.

Theorem 44 *If R is symmetric, $\mathcal{D}_R = \mathcal{H}$, and $R^2 = R$, then R is an orthogonal projection on \mathcal{R}_R . In particular, \mathcal{R}_R is closed.*

PROOF: Note that for any $u \in \mathcal{H}$,

$$\|Ru\|^2 = (Ru, Ru) = (Ru, u) \leq \|Ru\| \cdot \|u\|,$$

so $\|Ru\| \leq \|u\|$ and R is bounded with $\|R\| \leq 1$. Now let $\mathcal{M} = \mathcal{R}_R$. Then $u = Ru + (u - Ru) = u_1 + u_2$ and $R(Ru) = Ru$, so $u_1 = Ru_1 \in \mathcal{M}$. Now $u_2 = u - Ru$ and for any $v \in \mathcal{H}$ we have

$$(u_2, Rv) = (u - Ru, Rv) = (u, Rv) - (Ru, Rv) = (u, Rv) - (u, Rv) = 0.$$

Therefore $u - Ru \in \mathcal{M}^\perp$. Finally, we must show that \mathcal{M} is closed. Clearly, $\mathcal{M} \subseteq (\mathcal{M}^\perp)^\perp = \overline{\mathcal{M}}$. let $v \in (\mathcal{M}^\perp)^\perp$. Then also $Rv \in \mathcal{M} \subseteq v - Rv(\mathcal{M}^\perp)^\perp$, so $v - Rv \in \mathcal{M}^\perp \cap (\mathcal{M}^\perp)^\perp$. Thus $v - Rv = \theta$, so $v \in \mathcal{M}$. Thus $\mathcal{M} = (\mathcal{M}^\perp)^\perp = \overline{\mathcal{M}}$. Q.E.D.

The proof of the following is straight forward.

Theorem 45 *Let P_1, P_2 be orthogonal projections on the closed subspaces $\mathcal{M}_1, \mathcal{M}_2$, respectively. Then*

1. *If $P_1P_2 = P_2P_1$ then P_1P_2 is the orthogonal projection onto $\mathcal{M}_1 \cap \mathcal{M}_2$.*
2. *If $P_1P_2 = 0$ then $(P_1P_2)^* = 0 = P_2P_1$ and $\mathcal{M}_1 \perp \mathcal{M}_2$. We say that P_1 and P_2 are **orthogonal** to one another. In this case $P_1 + P_2$ is the orthogonal projection onto $\mathcal{M}_1 \oplus \mathcal{M}_2$.*
3. *If $P_1P_2 = P_2P_1$ then $P_1 + P_2 - P_1P_2$ is the orthogonal projection onto $\mathcal{M}_1 + \mathcal{M}_2$.*
4. *$P_1P_2 = P_2 \implies P_2P_1 = P_2$ and this is true if and only if $\mathcal{M}_2 \subseteq \mathcal{M}_1$.*

3.2 The spectrum of an operator

Recall the following facts about closed operators B :

1. If B^{-1} exists then B^{-1} is closed.
2. if B^{-1} is bounded then \mathcal{R}_B is a closed set.
3. If \mathcal{D}_B is a closed set then B is bounded.

Now let A be a closed operator (not necessarily symmetric) on the Hilbert space \mathcal{H} with $\overline{\mathcal{D}_A} = \mathcal{H}$. Let λ be a complex number. Then the operator $A - \lambda I$ is also closed. There are exactly four possibilities for λ :

1. $(A - \lambda I)^{-1}$ exists and is bounded, with $\mathcal{R}_{A - \lambda I} = \mathcal{H}$. In this case we say that λ is a **regular value** of A . The set of all regular values of A is called the **resolvent set** of A . The set of all non-regular values is called the **spectrum** of A .
2. The equation $(A - \lambda I)u = \theta$ has a nonzero solution $u \in \mathcal{D}_A$. We say that λ is an **eigenvalue** of A . The set of eigenvalues forms the **point spectrum** of A .

3. $(A - \lambda I)^{-1}$ exists with $\overline{\mathcal{R}_{A-\lambda I}} = \mathcal{H}$, but the inverse isn't bounded. Hence $\mathcal{R}_{A-\lambda I} \neq \mathcal{H}$. We say the λ belongs to the **continuous spectrum** of A .
4. $(A - \lambda I)^{-1}$ exists but $\overline{\mathcal{R}_{A-\lambda I}} \neq \mathcal{H}$. We say the λ belongs to the **residual spectrum** of A . The **deficiency** of λ is $\dim [\mathcal{R}_{A-\lambda I}^\perp]$.

The sets $\sigma_P(A), \sigma_C(A), \sigma_R(A)$ comprise the complex numbers λ in the point spectrum of A , the continuous spectrum of A , and the residual spectrum of A , respectively.

Theorem 46 *Let $\lambda \in \sigma_R(A)$. Then the deficiency of λ is m if and only if $\bar{\lambda} \in \sigma_P(A^*)$ with multiplicity m .*

PROOF: Let v_1, \dots, v_m be a basis for $\mathcal{R}_{A-\lambda I}^\perp$, where m may be infinite. Then $([A - \lambda I]u, v_j) = 0$ for all $u \in \mathcal{D}_A$, so $v_j \in \mathcal{D}_{[A-\lambda I]^*}$ and $[A - \lambda I]^*v_j = A^*v_j - \bar{\lambda}v_j = \theta$. The converse is similar. Q.E.D.

Recall that if A is symmetric and $\lambda \in \sigma_P(A)$ then λ is real.

Lemma 14 *Let A be symmetric and $\lambda = \alpha + i\beta$, with α, β real. Then $\|(A - \lambda I)u\|^2 \geq \beta^2\|u\|^2$.*

PROOF: We have

$$\begin{aligned} \|(A - \lambda I)u\|^2 &= (Au - \lambda u, Au - \lambda u) = \|Au\|^2 + |\lambda|^2\|u\|^2 - \lambda(u, Au) - \bar{\lambda}(u, Au) \\ &= \|Au\|^2 + (\alpha^2 + \beta^2)\|u\|^2 - 2\alpha(u, Au) \geq \|Au\|^2 + (\alpha^2 + \beta^2)\|u\|^2 - 2|\alpha| \cdot \|u\| \cdot \|Au\| \\ &= [\|Au\| - |\alpha| \cdot \|u\|]^2 + \beta^2\|u\|^2 \geq \beta^2\|u\|^2, \end{aligned}$$

where we have made use of the fact that $(Au, u) = (u, Au)$ is real for a symmetric operator. Q.E.D.

Theorem 47 *If A is symmetric and $\lambda \in \sigma_C(A)$ then λ is real.*

PROOF: Suppose $\lambda \in \sigma_C(A)$, $\lambda = \alpha + i\beta$, and $\beta \neq 0$. Then $\|(A - \lambda I)u\|^2 \geq \beta^2\|u\|^2$ for all $u \in \mathcal{D}_A$. Let $v \in \mathcal{R}_{A-\lambda I}$, so $v = (A - \lambda I)u$ for some $u \in \mathcal{D}_A$. Then $\|v\|^2 \geq \beta^2\|(A - \lambda I)^{-1}v\|^2$, so $(A - \lambda I)^{-1}$ is bounded. Impossible! Q.E.D.

We conclude from these results that if A is symmetric then the sets $\sigma_P(A)$ and $\sigma_C(A)$ contain only real elements. In general, we can't say anything about the reality of $\sigma_R(A)$ for A symmetric.

Recall that a self-adjoint operator is closed.

Theorem 48 *If A is self-adjoint then the spectrum of A lies on the real axis and $\sigma_R(A)$ is the empty set.*

PROOF: $\sigma_P(A)$ and $\sigma_C(A)$ are real, since A is symmetric. If $\lambda \in \sigma_R(A)$ then $0 < \dim \mathcal{R}_{A-\lambda I}^\perp = \dim \mathcal{N}_{A^*-\bar{\lambda}I}$, so $Av = A^*v = \bar{\lambda}v$ for some nonzero $v \in \mathcal{D}_{A^*}$. Thus $\bar{\lambda} \in \sigma_P(A)$, so $\bar{\lambda} = \lambda$ is real and $\lambda \in \sigma_P(A)$. Impossible! Q.E.D.

We have achieved a considerable simplification in the spectral classification for a self-adjoint operator A . There are just three possibilities:

1. λ is regular $\iff \mathcal{R}_{A-\lambda I} = \mathcal{H}$.
2. $\lambda \in \sigma_P(A) \iff \overline{\mathcal{R}_{A-\lambda I}} \neq \mathcal{H} \iff \mathcal{N}_{A-\lambda I} \neq \{\theta\}$.
3. $\lambda \in \sigma_C(A) \iff \mathcal{R}_{A-\lambda I} \neq \mathcal{H}$ but $\overline{\mathcal{R}_{A-\lambda I}} = \mathcal{H}$.

Example 9 *Let $A = i\frac{\partial}{\partial x}$, acting on the Hilbert space $\mathcal{H} = L_2^c(-\infty, \infty)$ of complex-valued square integrable functions on the real line. Here, $\mathcal{D}_A = \{u \text{ absolutely continuous} : u, u' \in \mathcal{H}\}$. We will show later that $A = A^*$, and assume this here. We classify the spectra of A . Let $\lambda \in \mathbb{R}$. Then*

$$Au = \lambda u \implies iu' = \lambda u \implies u(x) = ce^{-i\lambda x}.$$

Clearly $u \in \mathcal{H} \iff c = 0$. Therefore $\lambda \notin \sigma_P(A)$. Now choose $v \in \mathcal{H}$ and consider the equation $(A - \lambda E)u = v$, or $iu' - \lambda u = v$. Writing this equation in the form

$$\frac{d}{dx}(e^{i\lambda x}u) = -ie^{i\lambda x}v$$

, we see that the general solution is

$$e^{i\lambda x}u(x) = -i \int_{-\infty}^x e^{i\lambda t}v(t)dt + c.$$

We must have $c = 0$, for otherwise u could not be square integrable. Hence

$$u(x) = (A - \lambda E)^{-1}v = -i \int_{-\infty}^x e^{i\lambda(t-x)}v(t)dt.$$

We will show that $\mathcal{R}_{A-\lambda E} \neq \mathcal{H}$. Suppose $v(t) = \chi[0, 1](t)$. Then

$$u(x) = \begin{cases} 0 & \text{if } x \leq 0 \\ -i \int_0^x e^{i\lambda(t-x)}dt = \frac{e^{-i\lambda x}-1}{\lambda} & \text{if } 0 < x < 1 \\ -i \int_0^1 e^{i\lambda(t-x)}dt = -\frac{e^{-i\lambda x}}{\lambda}(e^{i\lambda}-1) & \text{if } x \geq 1 \end{cases}$$

It follows that $u \notin \mathcal{H}$, so $v \notin \mathcal{R}_{A-\lambda E}$. Thus $\lambda \in \sigma_C(A)$ for all real λ .

Example 10 Let $B = i\frac{\partial}{\partial x}$, acting on the Hilbert space $\mathcal{H} = L_2^c[0, \infty)$. Here, $\mathcal{D}_B = \{u \text{ absolutely continuous} : u, u' \in \mathcal{H}, u(0) = 0\}$. In this case B is symmetric and closed. The adjoint operator is given by $B^* = i\frac{\partial}{\partial x}$ with $\mathcal{D}_{B^*} = \{u \text{ absolutely continuous} : u, u' \in \mathcal{H}\}$. (Note that if $u \in \mathcal{D}_B$ and $v \in \mathcal{D}_{B^*}$ then

$$(Bu, v) = \int_0^\infty iu' \bar{v} \, dx = \int_0^\infty u \overline{iv'} \, dx + iu\bar{v} \Big|_0^\infty = (u, B^*v),$$

since the boundary term at ∞ vanishes and $u(0) = 0$.

Now let λ be a complex number. If $Bu = \lambda u$ then $u(x) = ce^{-i\lambda x}$ and this is square integrable only if $c = 0$. Thus $\sigma_P(B) = \emptyset$. Recall that $\bar{\lambda} \in \sigma_P(B) \iff \lambda \in \sigma_P(B) \cup \sigma_R(B)$, and in this case $\sigma_P(B) = \emptyset$. Now $B^*u = \bar{\lambda}u$ implies $iu' = \bar{\lambda}u$ so $u(x) = ce^{-i\bar{\lambda}x} \in \mathcal{H}$ if $\text{Im}(\bar{\lambda}) < 0 \implies \text{Im}(\lambda) > 0$. We conclude that if $\lambda = \alpha + i\beta$ with $\beta > 0$ then $\lambda \in \sigma_R(B)$. Here, the deficiency of λ is 1 and $e^{-i\bar{\lambda}x}$ spans $\mathcal{R}_{B-\lambda E}^\perp$.

3.3 Square roots of positive symmetric bounded operators

The space of bounded operators on a Hilbert space \mathcal{H} is closed under the operator norm.

Theorem 49 Let $\{B_n\}$ be a sequence of bounded operators that is Cauchy in the operator norm, i.e., $\|B_n - B_m\| \rightarrow 0$ as $n, m \rightarrow \infty$. Then there exists a unique bounded operator B such that $\|B - B_n\| \rightarrow 0$ as $n \rightarrow \infty$.

PROOF: For every $u \in \mathcal{H}$ define $Bu = \lim_{n \rightarrow \infty} B_n u$, where the convergence is in the Hilbert space norm. Then

1. B is well-defined: $\|B_n u - B_m u\| \leq \|B_n - B_m\| \cdot \|u\| \rightarrow 0$ as $n, m \rightarrow \infty$. Therefore, $\lim_{n \rightarrow \infty} B_n u$ exists.
2. B is linear: Let $u, v \in \mathcal{H}$, $\alpha, \beta \in \mathbb{C}$. Then

$$\begin{aligned} & \|B(\alpha u + \beta v) - (\alpha Bu + \beta Bv)\| \leq \\ & \|B(\alpha u + \beta v) - B_n(\alpha u + \beta v)\| + \|(\alpha B_n u + \beta B_n v) - (\alpha Bu + \beta Bv)\| \\ & \leq \|B(\alpha u + \beta v) - B_n(\alpha u + \beta v)\| + |\alpha| \cdot \|\alpha B_n u - Bu\| + |\beta| \cdot \|B_n v - Bv\| \rightarrow 0 \\ & \text{as } n, m \rightarrow \infty. \text{ Therefore } B(\alpha u + \beta v) = \alpha Bu + \beta Bv. \end{aligned}$$

3. B is bounded: Let $u \in \mathcal{H}$, $\|u\| = 1$. Then

$$\|Bu\| \leq \|Bu - B - nu\| + \|B_n u\|.$$

The first term on the right can be made ≤ 1 by choosing n sufficiently large. The second term on the right is bounded, say $\|B_n\| \leq a$ because $\{B_n\}$ is Cauchy in the operator norm. Hence $\|Bu\| \leq a = 1$, so B is bounded.

4. $\|B\| = \lim_{n \rightarrow \infty} \|B_n\|$ and $\|B - B_n\| \rightarrow 0$ as $n \rightarrow \infty$: Let $u \in \mathcal{H}$, $\|u\| = 1$. Then

$$\|Bu - B_n u\| \leq \|Bu - B_m u\| + \|B_m u - B_n u\| \leq \|Bu - B_m u\| + \|B_m - B_n\|.$$

Given $\epsilon > 0$, we can make the first term on the right hand side $< \frac{\epsilon}{2}$ by choosing m sufficiently large, and the second term $< \frac{\epsilon}{2}$ by choosing m and n sufficiently large. Thus $\|B - B_n\| \leq \epsilon$ for n sufficiently large. Q.E.D.

Now let A be a bounded, symmetric and positive operator on \mathcal{H} . (recall that A is **positive** if $(Au, u) \geq 0$ for all $u \in \mathcal{H}$. The main purpose of this section is to define and construct the positive square root of A . That is, we will define $B = \sqrt{A}$ such that 1) B is bounded, symmetric and positive, and 2) $B^2 = A$.

Note: This is easy in the special case $A = C$ where C is a symmetric completely continuous positive operator. Then C has nonzero eigenvalues $\{\lambda_j\}$ and corresponding normalized eigenvectors $\{\phi_j\}$ such that

$$Cu = \sum_j \lambda_j (u, \phi_j) \phi_j.$$

Since C is positive, we have $\lambda_j \geq 0$ for all j . Thus, denoting by $\sqrt{\lambda_j}$ the positive square root of λ_j , we can define

$$\sqrt{C}u = \sum_j \sqrt{\lambda_j} (u, \phi_j) \phi_j$$

and this operator has the correct properties.

Lemma 15 *Let T be a bounded operator on \mathcal{H} . Then the operators TT^* and T^*T are symmetric and positive.*

Remark: Recall that if T is bounded then so is T^* . It follows that TT^* and T^*T are bounded.

PROOF OF THE LEMMA: $(TT^*)^* = T^{**}T^* = TT^*$. Also

$$(TT^*u, u) = (T^*u, T^*u) = \|T^*u\|^2 \geq 0.$$

The proof for T^*T is similar. Q.E.D.

Theorem 50 *If A is a bounded symmetric positive operator, there exists a unique bounded symmetric positive operator B such that $B^2 = A$.*

PROOF: Without loss of generality we can re-scale A , if necessary, so that

$$0 \leq (Au, u) \leq \|u\|^2,$$

i.e., $\|A\| \leq 1$. Therefore $(u, u) \geq (u - Au, u) \geq 0$, so the operator $A' = I - A$ is positive and symmetric, and $\|A'\| \leq 1$. Now $A = I - A'$ and, formally,

$$[I - A']^{\frac{1}{2}} = I - \frac{1}{2}A' + \frac{\frac{1}{2}(\frac{1}{2} - 1)}{1 \cdot 2}(A')^2 - \frac{\frac{1}{2}(\frac{1}{2} - 1)(\frac{1}{2} - 2)}{1 \cdot 2 \cdot 3}(A')^3 + \dots.$$

I claim that the series

$$s = 1 + \frac{1}{2}\|A'\| + \frac{1}{2 \cdot 4}\|A'\|^2 + \frac{1 \cdot 3}{2 \cdot 4 \cdot 6}\|A'\|^3 + \dots + \frac{1 \cdot 3 \dots (2n-3)}{2 \cdot 4 \dots (2n)}\|A'\|^n + \dots,$$

for $n \geq 2$, converges for all $\|A'\| \leq 1$. If $\|A'\| < 1$ this is true by the ratio test. Suppose $\|A'\| = 1$. Then

$$\left| \frac{a_{n+1}}{a_n} \right| = \frac{2n-1}{2n+2} = 1 - \frac{3}{2n+2} < 1 - \frac{4}{3n}$$

if $n > 17$. Now consider the series $\sum_{n=1}^{\infty} \frac{1}{n^\alpha}$ that we know to be convergent for $\alpha > 1$. From Taylor's theorem with remainder we know that the expansion

$$f(x) = (1-x)^\alpha = 1 - \alpha x + \frac{\alpha(\alpha-1)}{2!}x^2(1-y)^{\alpha-2}$$

holds for any $x < 1$, $\alpha > 1$ where y satisfies $0 < y < x < 1$. Thus the remainder term is positive and $(1-x)^\alpha > 1 - \alpha x$. Clearly, the ratio between successive terms in $\sum_{n=1}^{\infty} \frac{1}{n^\alpha}$ is

$$\frac{\frac{1}{n^\alpha}}{\frac{1}{(n-1)^\alpha}} = \left(1 - \frac{1}{n}\right)^\alpha > 1 - \frac{\alpha}{n},$$

so, by the comparison test, there is a positive constant c_0 such that

$$s \leq c_0 \sum_{n=1}^{\infty} \frac{1}{n^{\frac{4}{3}}} < \infty.$$

It follows from this that the formal series $[I - A']^{\frac{1}{2}}$ actually converges absolutely to a bounded symmetric operator B , and $B^2 - ([I - A']^{\frac{1}{2}})^2 = I - A' = A$. Further,

$$\begin{aligned} (Bu, u) &= (u, u) - \frac{1}{2}(A'u, u) + \frac{\frac{1}{2}(\frac{1}{2} - 1)}{2!}((A')^2, u, u) + \dots \\ &\geq \|u\|^2 - \left(\frac{1}{2}\|A'\| + \frac{\frac{1}{2}(\frac{1}{2})}{2!}\|A'\|^2 + \dots \right) \|u\|^2 = \|u\|^2 \sqrt{1 - \|A'\|} \geq 0, \end{aligned}$$

so B is positive. Since $B^2 = A$ we have $\|B\|^2 \geq \|A\|$ so $\|B\| \geq \|A\|^{\frac{1}{2}}$. However, $(Bu, Bu) = (B^2u, u) = (Au, u) \leq \|A\| \cdot \|u\|^2$, so $\|B\| \leq \sqrt{\|A\|}$. Thus $\|B\| = \sqrt{\|A\|}$.

Remark: It follows that B commutes with all bounded symmetric operators that commute with A . We signify this through the notation $BccA$.

Finally, we must show that B is unique. let B, B' be positive, symmetric, bounded, such that $B^2 = (B')^2 = A$. Now $B'A = (B')^3 = AB'$, so $B'B = BB'$. For any $u \in \mathcal{H}$ let $v = (B - B')u$. let $\sqrt{B'}, \sqrt{B}$ be bounded, symmetric, positive square roots of B', B , respectively. Then

$$\|\sqrt{B'}v\|^2 + \|\sqrt{B}v\|^2 = (B'v, v) + (Bv, v) =$$

$$(B'Bu - Au, Bu - B'u) + (Au - BB'u, Bu - B'u) = 0,$$

because $BB' = B'B$. Thus $\sqrt{B}v = \sqrt{B'}v = \theta$, which implies $Bv = B'v = \theta$. Now

$$\|v\|^2 = (Bu - B'u, Bu - B'u) = ([B - B']^2u, u) = ([B - B']v, u) = 0,$$

so $v = \theta$ and $B = B'$. Q.E.D.

Theorem 51 *Let B be bounded and closed. If λ belongs to the spectrum of B then $|\lambda| \leq \|B\|$.*

REMARK: The theorem implies that if $|\lambda| > \|B\|$, then λ belongs to the resolvent set of B . Furthermore, if A is bounded and symmetric then the spectrum of A is contained in the interval $[-\|A\|, \|A\|]$.

PROOF OF THEOREM: Suppose $\lambda \in C$, $|\lambda| > \|B\|$. Then $(B - \lambda I) = -\lambda(I - \frac{1}{\lambda}B)$ where $\|\frac{1}{\lambda}B\| < 1$. Formally,

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

and this series converges in the operator norm, since

$$\sum_{n=0}^{\infty} \frac{1}{|\lambda|^{n+1}} \|B\|^n = \frac{1}{|\lambda|} (1 - \frac{\|B\|}{|\lambda|})^{-1} < \infty.$$

Therefore

$$\left(\sum_{n=0}^{\infty} \frac{1}{\lambda^{n+1}} B^n \right) (B - \lambda I) = I,$$

and $(B - \lambda I)^{-1} = \sum_{n=0}^{\infty} \frac{1}{\lambda^{n+1}} B^n$ exists and is bounded. This means that λ belongs to the resolvent set of B . Q.E.D.

Note that if A is a bounded symmetric operator, then A^2 is bounded, symmetric and positive.

Definition 23 *let A, B be bounded symmetric operators on the Hilbert space \mathcal{H} . We say $A \geq B$ if $(Au, u) \geq (Bu, u)$ for all $u \in \mathcal{H}$. In particular $A \geq 0 \iff A$ is positive.*

Note that this definition is quite different from the definition of \geq for extensions of symmetric operators.

By definition, if A is bounded symmetric then $A^2 \geq 0$, so it has a unique positive square root.

Definition 24 *Given a bounded symmetric operator A , we have bounded symmetric operators $|A|, A_+, A_-$ given by*

$$|A| = \sqrt{A^2}, \quad A_+ = \frac{1}{2}(|A| + A), \quad A_- = \frac{1}{2}(|A| - A).$$

Note that $A = A_+ - A_-$.

Example 11 let C be symmetric and completely continuous, with nonzero eigenvalues $\{\lambda_j\}$ and corresponding normalized eigenvectors $\{\phi_j\}$. Then for any $u \in \mathcal{H}$ we have

$$\begin{aligned} Cu &= \sum_j \lambda_j (u, \phi_j) \phi_j, \\ C^2 u &= \sum_j \lambda_j^2 (u, \phi_j) \phi_j, \\ |C|u &= \sqrt{C^2}u = \sum_j |\lambda_j| (u, \phi_j) \phi_j, \\ C_+ u &= \frac{1}{2}(|C| + C)u = \sum_j \lambda_j \geq 0 \lambda_j (u, \phi_j) \phi_j, \\ C_- u &= \frac{1}{2}(|C| - C)u = - \sum_j \lambda_j < 0 \lambda_j (u, \phi_j) \phi_j. \end{aligned}$$

Let

$$\mathcal{M} = \{u \in \mathcal{H} : A_+ u = \theta\} = \mathcal{N}_{A_+},$$

and let P be the orthogonal projection operator on \mathcal{M}

Example 12 Consider the operator C again. Here, $\mathcal{M} = \{v = \sum_{\lambda_j \leq 0} (v, \phi_j) \phi_j\}$ and for $u \in \mathcal{H}$ we have $Pu = \sum_{\lambda_j \leq 0} (u, \phi_j) \phi_j$.

In general, P has the following properties:

1. $P^2 = P$, $P = P_+$
2. $\mathcal{R}_P = \mathcal{M}$
3. $A_+ Pu = \theta$ for all $u \in \mathcal{H}$, so $A_+ P = 0 = PA_+$
4. $|A|ccA^2$ so $|A|ccA$. This implies $A_+ ccA$, $A_- ccA$.
5. $PccA$. Indeed, if D is bounded symmetric and $DA = AD$ then $DA_+ = A_+ D$. If $v \in \mathcal{M}$ then $\theta = DA_+ v = A_+ Dv$, so $Dv \in \mathcal{M}$. Therefore $DPu = PDPu$ for all $u \in \mathcal{H}$ so

$$DP = PDP \implies PDP + PD \implies DP = PD,$$

and $PccA$.

6. $A_-P = PA_- = A_-$. Indeed $|A|ccA$, so

$$A_+A_- = \frac{1}{4}(|A| + A)(|A| - A) = \frac{1}{4}(|A|^2 - A^2) = 0.$$

This implies $A_- \mathcal{H} \subseteq \mathcal{M}$, so $PA_- = A_-$.

7. $(I - P)A = A(I - P) = A_+$. This follows from the previous identity and $A = A_+ - A_-$, which gives $PA = AP = -A_-$.

8. $A_+ + A_- = |A| \geq 0$

9. A_+, A_- are positive operators. Indeed, $A_- = PA_- + PA_+ = P|A|$ and this is a positive operator since

$$(P|A|u, u) = (P^2|A|u, u) = (|A|Pu, Pu) \geq 0.$$

Similarly

$$A_+ = |A| - A_- = |A| - P|A| = (I - P)|A| \geq 0.$$

EXTENSION: Let μ be a real number and set $A_\mu = A - \mu I$. Then again A_μ is bounded and symmetric, and we can define $A_{\mu+}, A_{\mu-}, |A_\mu|, P_\mu, \mathcal{M}_\mu$ in the usual way. We obviously have $P_\mu ccA_\mu, A_{\mu\pm} ccA_\mu$, etc. so $P_\mu ccA, A_{\mu\pm} ccA$.

Definition 25 We say that the set of orthogonal projection operators $\{P_\mu : -\infty < \mu < \infty\}$ is the **spectral family** of A .

Example 13 let C be the symmetric completely continuous operator $Cu = \sum_j \lambda_j (u, \phi_j) \phi_j$. Then

$$C_\mu u = \sum_j [\lambda_j - \mu] (u, \phi_j) \phi_j,$$

$$P_\mu u = \sum_{\lambda_j \leq \mu} (u, \phi_j) \phi_j.$$

Lemma 16 If B, C are positive symmetric bounded operators on \mathcal{H} , and $BC = CB$ then BC is positive symmetric and bounded.

PROOF: Only the statement that BC is positive needs demonstration.

$$(BCu, u) = (\sqrt{B}\sqrt{B}Cu, u) = (C\sqrt{B}u, \sqrt{B}u) \geq 0.$$

Q.E.D.

PROPERTIES OF $\{P_\mu\}$:

1. $P_\mu P_\nu = P_\nu P_\mu$
2. $P_\mu^2 = P_\mu, P_\mu^* = P_\mu$
3. $P_\mu \leq P_\nu$ if $\mu \leq \nu$. PROOF:

$$A_{\mu+} - A_{\nu+} + A_{\nu-} \geq A_{\mu+} - A_{\nu+} + A_{\nu-} - A_{\mu-} = A_\mu - A_\nu = (\nu - \mu)I \geq 0.$$

Now $A_{\nu+} \geq 0 \implies A_{\nu+}(A_{\mu+} - A_{\nu+} + A_{\nu-}) \geq 0$. Recall $A_{\nu+}A_{\nu-} = 0 \implies A_{\nu+}A_{\mu+} \geq A_{\nu+}A_{\nu+}$ so

$$(A_{\nu+}A_{\mu+}u, u) \geq (A_{\nu+}A_{\nu+}u, u) = \|A_{\nu+}u\|^2.$$

Thus $A_{\mu+}u = \theta \implies A_{\nu+}u = \theta \implies \mathcal{M}_\mu \subseteq \mathcal{M}_\nu$. Therefore, $P_\mu P_\nu = P_\nu P_\mu = P_\mu$ and

$$P_\nu - P_\mu = P_\nu - P_\nu P_\mu = P_\nu(I - P_\mu) \geq 0,$$

since the final term is a product of two commuting positive operators.

Q.E.D.

4. Let $M = \sup_{\|u\|=1}(Au, u)$, $m = \inf_{\|u\|=1}(Au, u)$. If $\mu < m$ then $P_\mu = 0$. If $\mu > M$ then $P_\mu = I$.

PROOF: If $\mu < m$ then $A_\mu = A - \mu I \geq 0$ since

$$(Au, u) - \mu(u, u) \geq m(u, u) - \mu(u, u) \geq 0.$$

Thus

$$|A_\mu| = A_\mu \implies A_{\mu+} = A_\mu, \quad A_{\mu-} = 0.$$

Note: $(A_\mu u, u) \geq (m - \mu)(u, u)$, so $A_\mu u = A_{\mu+}u = \theta \implies u = \theta$. Therefore $P_\mu = 0$.

If $\mu > M$ then $-A_\mu = \mu I - A \geq 0$,

$$\implies |A_\mu| = -A_\mu \implies A_{\mu+} = 0 \implies P_\mu = I.$$

Q.E.D.

Before continuing with our list of properties of the family of orthogonal projection operators $\{P_\mu\}$ we introduce and prove a crucial convergence property of monotone increasing sequences of operators.

Definition 26 We say that $\langle \cdot, \cdot \rangle: \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{C}$ is a **positive Hermitian form** on \mathcal{H} if

1. $\langle u, v \rangle$ is linear in the first argument.
2. $\langle u, v \rangle = \overline{\langle v, u \rangle}$
3. $\langle u, u \rangle \geq 0$ for all $u \in \mathcal{H}$

Note that the positive Hermitian form has all of the properties of an inner product, except that $\langle u, u \rangle = 0$ doesn't necessarily imply $u = \theta$. It follows that the Schwarz equality holds for $\langle \cdot, \cdot \rangle$ in the form

$$|\langle u, v \rangle|^2 \leq \langle u, u \rangle \langle v, v \rangle,$$

for all $u, v \in \mathcal{H}$.

Theorem 52 Let $\{A_n\}$ be a sequence of bounded symmetric operators such that $A_1 \leq A_2 \leq \dots$ and $\|A_n\| < \alpha < \infty$ for all n . Then there exists a bounded symmetric operator A such that $Au = \lim_{n \rightarrow \infty} A_n u$ for all $u \in \mathcal{H}$. (We say that A_n **strongly converges** to A , i.e., converges in the Hilbert space norm, not the operator norm.)

PROOF: By adding an appropriate multiple of I to each operator, and then rescaling, we can assume that $0 \leq A_1 \leq A_2 \leq \dots \leq I$. Now let $A_{mn} = A_m - A_n$, so that $A_{mn} \geq 0$ if $m \geq n$. Then $\langle u, v \rangle = (A_{mn}u, v)$ is a positive hermitian form. Therefore

$$\begin{aligned} \|A_{mn}u\|^4 &= (A_{mn}u, A_{mn}u)^2 = |\langle u, A_{mn}u \rangle|^2 \leq \\ &\langle u, u \rangle \langle A_{mn}u, A_{mn}u \rangle = (A_{mn}u, u)(A_{mn}^2u, A_{mn}u). \end{aligned}$$

Now $0 \leq A_{mn} \leq I$ so $\|A_{mn}\| \leq 1$. Therefore $\|A_{mn}u\|^4 \leq (A_{mn}u, u)\|u\|^2$ and

$$\|A_m - A_n\|^4 \leq [(A_mu, u) - (A_nu, u)] \cdot \|u\|^2.$$

But, since $\{(A_nu, u)\}$ is a bounded monotone increasing sequence, it follows from this that $\{A_nu\}$ is a Cauchy sequence in the Hilbert space norm. Therefore $\lim_{n \rightarrow \infty} A_nu = Au$ exists for all $u \in \mathcal{H}$. It is easy to check that A is linear, bounded and symmetric. Q.E.D.

Corollary 9 *If the $\{A_n\}$ of the theorem are orthogonal projection operators, then so is A .*

PROOF: let $u \in \mathcal{H}$.

$$\begin{aligned} \|A^2u - A_n\| &\leq \|A^2u - A_nAu\| + \|A_nAu - A_nA_n\| \\ &\leq \|(A - A_n)Au\| + \alpha\|(A - A_n)u\| \rightarrow 0 \end{aligned}$$

as $n \rightarrow \infty$. Therefore $A_n \rightarrow A^2$ and $A_n \rightarrow A$ as $n \rightarrow \infty$. Thus $A^2 = A$, so A is an orthogonal projection operator. Q.E.D.

Now we return to our listing of properties of the family $\{P_\mu\}$.

5. Set $P_{\lambda\mu} = P_\lambda - P_\mu$, for $\lambda > \mu$. Then

$$\mu P_{\lambda\mu} \leq AP_{\lambda\mu} \leq \lambda P_{\lambda\mu}.$$

Note: $P_{\lambda\mu}$ is a projection operator, since

$$P_{\lambda\mu}^2 = (P_\lambda - P_\mu)^2 = P_\lambda^2 - 2P_\lambda P_\mu + P_\mu^2 = P_\lambda - 2P_\mu + P_\mu = P_\lambda - P_\mu.$$

PROOF: $P_\lambda P_{\lambda\mu} = P_\lambda P_\lambda - P_\lambda P_\mu = P_\lambda - P_\mu = P_{\lambda\mu} = (I - P_\mu)P_{\lambda\mu}$, so

$$(A - \lambda I)P_{\lambda\mu} = A_\lambda P_{\lambda\mu} = A_\lambda P_\lambda P_{\lambda\mu} = -A_\lambda - P_{\lambda\mu} \leq 0,$$

$$(A - \mu I)P_{\lambda\mu} = A_\mu P_{\lambda\mu} = A_\mu(I - P_\mu)P_{\lambda\mu} = -A_\mu + P_{\lambda\mu} \geq 0.$$

Therefore, $AP_{\lambda\mu} \leq \lambda P_{\lambda\mu}$ and $AP_{\lambda\mu} \geq \mu P_{\lambda\mu}$. Q.E.D.

6. $\lim_{\lambda \rightarrow \mu+0} P_\lambda \equiv P_{\mu+0} = P_\mu$, i.e. $S_\mu = \lim_{\lambda \rightarrow \mu+0} P_{\lambda\mu} = 0$, in the sense of strong convergence.

PROOF: The limit S_μ exists, since the $\{P_{\lambda\mu}\}$ is monotone for fixed μ . Furthermore, S_μ is an orthogonal projection operator. Now $\mu P_{\lambda\mu} \leq AP_{\lambda\mu} \leq \lambda P_{\lambda\mu} \implies \mu S_\mu \leq AS_\mu \leq \mu S_\mu \implies AS_\mu = \mu S_\mu \implies A_\mu S_\mu = 0$. Furthermore,

$$(I - P_\mu)P_{\lambda\mu} = P_{\lambda\mu} \implies (I - P_\mu)S_\mu = S_\mu \implies P_\mu S_\mu = 0.$$

Now $A_\mu S_\mu = 0 \implies (I - P_\mu)A_\mu S_\mu = 0 \implies A_{\mu+} S_\mu = 0 \implies S_\mu \mathcal{H} \subset \mathcal{M}_\mu \implies 0 = P_\mu S_\mu = S_\mu$. Q.E.D.

3.4 The spectral calculus

We have shown that the spectral family of orthogonal projection operators $\{P_\mu\}$ associated with the bounded symmetric operator A has the following properties:

1. $P_\mu \leq P_\nu$ for $\mu \leq \nu$
2. $P_\mu P_\nu = P_\nu P_\mu = P_\mu$ for $\mu \leq \nu$
3. $P_{\mu+0} = P_\mu$
4. $\lim_{\mu \rightarrow +\infty} P_\mu = I, \lim_{\mu \rightarrow -\infty} P_\mu = 0$.

Any family of orthogonal projection operators $\{P_\mu\}$ satisfying properties 1.-4. is called a **spectral family**, independent of any association with an operator A .

Now we are at the point where we can discuss Riemann-Stieltjes integrals over a spectral family, and use such integrals to define the spectral resolutions of self-adjoint operators. Let $\{P_\mu\}$ be a spectral family.

Definition 27 *Let δ be an interval on the real line. We define the operator $P(\delta)$ as follows:*

$$\begin{aligned} \delta = (a, b) &\iff P(\delta) = P_{b-0} - P_a \\ \delta = (a, b] &\iff P(\delta) = P_b - P_a \\ \delta = [a, b] &\iff P(\delta) = P_b - P_{a-0} \\ \delta = [a, b) &\iff P(\delta) = P_{b-0} - P_{a-0}. \end{aligned}$$

Here is the basic idea. Let $f(\lambda)$ be a bounded function on the real line and let $\Delta = \{\delta_k : k = 0, \pm 1, \pm 2, \dots\}$ be a decomposition of $(-\infty, \infty) = R_1$ into pairwise disjoint intervals: $R_1 = \cup_k \delta_k$, $\delta_i \cap \delta_j = \{\emptyset\}$ for $i \neq j$. In particular, the left and right-hand endpoints of δ_k are μ_{k-1}, μ_k , respectively (the endpoints may or may not be included in δ_k). Let $|\delta_k| = \mu_k - \mu_{k-1}$ be the length of interval δ_k and set $|\Delta| = \sup_k |\delta_k|$. Now choose a point $\lambda_k \in \delta_k$ for each k . We define the spectral integral of f by

$$\int_{-\infty}^{\infty} f(\lambda) dP_\lambda = \lim_{|\Delta| \rightarrow 0} \sum_{k=-\infty}^{\infty} f(\lambda_k) P(\delta_k),$$

provided the limit exists. Convergence is in the operator norm.

We will construct the integral in stages, starting with the integral of a bounded step function. Let $f(\lambda)$ be such a function. Thus there is a decomposition $\Delta = \{\delta_k\}$ of the real line such that $f(\lambda) = c_k$ for $\lambda \in \delta_k$, and $|c_k| \leq M$ for all k . (It is OK for f to be nonzero on a countably infinite number of intervals.)

Lemma 17 $\sum_{k=1}^{\infty} c_k P(\delta_k)$ converges to a bounded operator on \mathcal{H} .

PROOF: Note that $\sum_{k=1}^{\infty} P(\delta_k) = I$ and $P(\delta_k)P(\delta_j) = 0$ if $k \neq j$. Let $u \in \mathcal{H}$. Then

$$\begin{aligned} \left\| \sum_{k=m+1}^n c_k P(\delta_k) u \right\|^2 &= \sum_{k=m+1}^n |c_k|^2 \|P(\delta_k) u\|^2 \leq M^2 \sum_{k=m+1}^n \|P(\delta_k) u\|^2 \\ &= M^2 \left[\left\| \sum_{k=1}^n P(\delta_k) u \right\|^2 - \left\| \sum_{k=1}^m P(\delta_k) u \right\|^2 \right] \rightarrow 0 \end{aligned}$$

as $n, m \rightarrow \infty$, since each of the sums on the right-hand side converges to $\|u\|^2$. Thus $\sum_{k=1}^{\infty} c_k P(\delta_k)$ converges. Furthermore

$$\left\| \sum_{k=1}^{\infty} c_k P(\delta_k) u \right\|^2 = \lim_{n \rightarrow \infty} \sum_{k=1}^n |c_k|^2 \|P(\delta_k) u\|^2 \leq M^2 \lim_{n \rightarrow \infty} \sum_{k=1}^n \|P(\delta_k) u\|^2 = M^2 \|u\|^2,$$

so the operator is bounded. Q.E.D.

Thus, the spectral integral exists for step functions. Note that the integral is independent of Δ , as follows from a standard argument in Riemann partition theory. For step functions f we have

$$\int_{-\infty}^{\infty} f(\lambda) dP_{\lambda} = \sum_k c_k P(\delta_k) \equiv f(A),$$

where $f(A)$ is defined by the expressions to the left.

The following theorem can be proved by simple verification:

Theorem 53 *Let f, f_1, f_2 be bounded step functions. Then*

1. $f(\lambda) \equiv 0 \implies f(A) = 0$
2. $f(\lambda) \equiv 1 \implies f(A) = I$
3. $f(\lambda) = a_1 f_1(\lambda) + a_2 f_2(\lambda) \implies f(A) = a_1 f_1(A) + a_2 f_2(A)$

4. $f(\lambda) = f_1(\lambda)f_2(\lambda) \implies f(A) = f_1(A)f_2(A)$
5. $\|f(A)\| \leq \max_{\lambda \in R} |f(\lambda)|$
6. $[f(A)]^* = \overline{f}(A)$ where $\overline{f}(\lambda) = \overline{f(\lambda)}$. If f is real then $F(A)$ is self-adjoint.
7. $f(A)cc\{P_\lambda\}$
8. $(f(A)u, v) = \int_{-\infty}^{\infty} f(\lambda)d(P_\lambda u, v)$ and $\|f(A)u\|^2 = \int_{-\infty}^{\infty} |f(\lambda)|^2 d\|P_\lambda u\|^2$
9. If $|f(\lambda) - g(\lambda)| < \epsilon$ for all λ then $\|f(A) - g(A)\| < \epsilon$.

Now let $f(\lambda)$ be bounded and uniformly continuous on $(-\infty, \infty)$. For each integer n let $\Delta_n = \{\delta_k^n\}$ be a partition of $(-\infty, \infty)$ into pairwise disjoint intervals, so that $|\Delta_n| \rightarrow 0$ as $n \rightarrow \infty$. Let $\lambda_k^n \in \delta_k^n$ and define a sequence of step functions $\{f_n(\lambda)\}$ by $f_n(\lambda) = \lambda_k^n$ if $\lambda \in \delta_k^n$. Then $f_n(\lambda) \rightarrow f(\lambda)$ uniformly on $(-\infty, \infty)$, so $\|f_n(A) - f_m(A)\| \leq \max_\lambda |f_n(\lambda) - f_m(\lambda)| \rightarrow 0$ as $n, m \rightarrow \infty$. from the last theorem we see that the operator sequence $\{f_n(A)\}$ is Cauchy in the operator norm.

Definition 28 For f uniformly continuous we define $f(A)$ by

$$f(A) = \lim_{n \rightarrow \infty} f_n(A) = \lim_{n \rightarrow \infty} \int_{-\infty}^{\infty} f_n(\lambda) dP_\lambda = \int_{-\infty}^{\infty} f(\lambda) dP_\lambda.$$

Corollary 10 Properties 1.-9. in the theorem above hold also for uniformly continuous functions on $(-\infty, \infty)$.

The above results can also be extended to piecewise continuous functions.

REMARK: We can justify the notation $f(A)$ as follows. Suppose A is a bounded symmetric operator and $\{P_\lambda\}$ is the spectral family of A . Then from our previous results, in particular $\lambda P_{\lambda\mu} \geq A \geq \mu P_{\lambda\mu}$, we have $A = \int \lambda dP_\lambda$, i.e., $A = f(A)$ where $f(\lambda) = \lambda$. Furthermore, if $m = \inf_{\|u\|=1} (Au, u)$, $M = \sup_{\|u\|=1} (Au, u)$ we have $mI \leq A \leq MI$ and $P_\lambda = 0$ if $\lambda < m$, $P_\lambda = I$ if $\lambda \geq M$. Thus $A = \int_a^b \lambda dP_\lambda$ for any $a < m$, $b > M$. Finally, if f is any function that is continuous on $[m, M]$ we can extend f to a function that is uniformly continuous on $(-\infty, \infty)$ and zero outside $[a, b]$. Thus we can write $f(A) = \int_a^b f(\lambda) dP_\lambda$, and the operator exists and is uniquely defined.

Theorem 54 (*Spectral Theorem for bounded self-adjoint operators.*) Let $f(\lambda) = a_n\lambda^n + \cdots + a_1\lambda + a_0$, with $a_n \neq 0$ be a polynomial in λ , so

$$f(A) = a_n A^n + \cdots + a_1 A + a_0 I.$$

Then $A^r = \int_{-\infty}^{\infty} \lambda^r dP_\lambda$, $r = 0, 1, \dots$, and $f(A) = \int_{-\infty}^{\infty} f(\lambda) dP_\lambda$.

Let B be a closed operator with resolvent set $\rho(B)$.

Lemma 18 *The resolvent set of B is open.*

PROOF: Let $\xi \in \rho(B)$. Thus $(B - \xi I)^{-1} \equiv R(\xi)$ exists and is bounded, with $\mathcal{D}_{R(\xi)} = \mathcal{H}$. Formally,

$$\begin{aligned} (B - \mu I)^{-1} &= [(B - \xi I) - (\mu - \xi)I]^{-1} = (B - \xi I)^{-1} [I - (\mu - \xi)R(\xi)]^{-1} \\ &= R(\xi) \left[I + (\mu - \xi)R(\xi) + (\mu - \xi)^2 R^2(\xi) + \cdots \right] \\ &= R(\xi) \sum_{n=0}^{\infty} (\mu - \xi)^n R^n(\xi). \end{aligned}$$

Note that this last series converges absolutely in the operator norm if $|\mu - \xi| < \frac{1}{\|R(\xi)\|}$. Therefore, $(B - \mu I)^{-1} = R(\mu)$ exists and is bounded if $|\mu - \xi| < \frac{1}{\|R(\xi)\|}$. Moreover,

$$\|R(\mu)\| \leq \frac{\|R(\xi)\|}{1 - |\mu - \xi| \cdot \|R(\xi)\|}.$$

Q.E.D.

Theorem 55 *Let A be bounded and symmetric, and λ a real number.*

1. *Suppose there exists $\epsilon > 0$ such that $P_\mu = P_\lambda$ for all μ such that $|\mu - \lambda| < \epsilon$. Then $\lambda \in \rho(A)$.*
2. *Suppose for **every** $\epsilon > 0$ there exist μ, ν such that $P_\mu - P_\nu > 0$ and $|\mu - \lambda| < \epsilon$, $|\nu - \lambda| < \epsilon$. Then λ belongs to the spectrum of A .*
3. *$P_{\lambda-0} \neq P_\lambda = P_{\lambda+0} \iff \lambda \in \sigma_P(A)$.*
4. *λ is a point of continuous increase of the spectral family $\{P_\mu\} \iff \lambda \in \sigma_C(A)$.*

PROOF:

1. Let

$$R(\lambda) = \int_{-\infty}^{+\infty} \frac{1}{\mu - \lambda} dP_\mu = \int_{-\infty}^{\lambda - \epsilon} \frac{1}{\mu - \lambda} dP_\mu + \int_{\lambda + \epsilon}^{+\infty} \frac{1}{\mu - \lambda} dP_\mu,$$

so $R(\lambda)$ exists. Now

$$(A - \lambda I)R(\lambda) = \int_{-\infty}^{+\infty} (\mu - \lambda) dP_\mu \int_{-\infty}^{+\infty} \frac{1}{\mu - \lambda} dP_\mu = \int_{-\infty}^{+\infty} dP_\mu = I.$$

Therefore $R(\lambda) = (A - \lambda I)^{-1}$. Furthermore, $\|R(\lambda)\|$ is bounded: $\|R(\lambda)\| \leq \epsilon^{-1}$.

2. Suppose $\lambda \in \rho(A)$. Then we can find $\mu_0 \in \rho(A)$ such that $|\mu_0 - \lambda| < \epsilon$, (say $\epsilon > \mu_0 - \lambda > 0$), and $P_{\mu_0} > P_\lambda$. Choose $v \neq \theta$ in the range of $P_{\mu_0} - P_\lambda$. Thus $v \in \mathcal{M}_{\mu_0} \cap \mathcal{M}_\lambda^\perp$. Now $P_\mu v = 0$ if $\mu \leq \lambda$ and $P_\mu v = v$ if $\mu \geq \mu_0$. Therefore,

$$(Av, Av) = \|Av\|^2 = \int_n^M \mu^2 d(P_\mu v, P_\mu v) = \int_\lambda^{\mu_0} \mu^2 d(P_\mu v, P_\mu v)$$

and

$$\|(A - \lambda I)v\|^2 = \int_\lambda^{\mu_0} (\mu - \lambda)^2 d(P_\mu v, P_\mu v) \leq (\mu_0 - \lambda)^2 \|v\|^2 < \epsilon^2 \|v\|^2.$$

It follows that $\|(A - \lambda I)^{-1}\| > \frac{1}{\epsilon}$ for ϵ arbitrary. Impossible! Therefore, λ belongs to the spectrum of A .

3. Let $\lambda > \mu$ and assume $P_{\lambda-0} \neq P_\lambda$. Then $\mu P_{\lambda\mu} \leq AP_{\lambda\mu} \leq \lambda P_{\lambda\mu}$. Now go to the limit as $\mu \rightarrow \lambda - 0$:

$$\lambda(P_\lambda - P_{\lambda-0}) \leq A(P_\lambda - P_{\lambda-0}) \leq \lambda(P_\lambda - P_{\lambda-0}).$$

Hence, $A(P_\lambda - P_{\lambda-0}) = \lambda(P_\lambda - P_{\lambda-0})$. Let v be a nonzero vector in $P_\lambda - P_{\lambda-0}$. Then $Av = \lambda v$, so $\lambda \in \sigma_P(A)$.

Conversely, suppose $\lambda \in \sigma_P(A)$ and that v is an eigenvector. Then

$$\|(A - \lambda I)v\|^2 = \int_{-\infty}^{\infty} |\mu - \lambda|^2 d(P_\mu v, P_\mu v) = 0,$$

so $\|P_\mu v\|^2$ is constant for $\mu > \lambda$, and for $\mu < \lambda$. But $P_\mu v = v$ for μ sufficiently large, and $P_\mu v = \theta$ for μ sufficiently small. Hence, $P_\mu v = v$ for $\mu > \lambda$ and $P_\mu v = \theta$ for $\mu < \lambda$. This implies that $P_{\lambda-0}v = \theta$, $P_{\lambda+0}v = P_\lambda v = v$. Therefore, $v \in \mathcal{M}_\lambda \cap \mathcal{M}_{\lambda-0}^\perp$. Q.E.D.

3.4.1 The spectral theorem for unbounded self-adjoint operators

In this section we begin to prove the analogs, for an unbounded self-adjoint operator A , of the properties of the spectral family that culminated in Theorem 54 for bounded self-adjoint operators. We start with an important special case in which we can easily transform the problem so that Theorem 54 applies.

Let A be self-adjoint and bounded below. Thus, A may be an unbounded operator, but there exists a finite real number a such that $(Au, u) \geq a(u, u)$ for all $u \in \mathcal{D}_A$, i.e., $A \geq aI$. Now set $B = A - (a-1)I$. Then $(Bu, u) \geq (u, u)$ for all $u \in \mathcal{D}_A$.

REMARKS:

1. B is self-adjoint
2. If $Bu = \theta$ then $u = \theta$, so B^{-1} exists.
3. $\mathcal{R}_B = \mathcal{H}$. PROOF: If $v \in \mathcal{R}_B^\perp$ then $(Bu, v) = 0$ for all $u \in \mathcal{D}_A$. This means that $v \in \mathcal{D}_{B^*}$ and $B^*v = Bv = \theta$, so $v = \theta$.

4. $\|B^{-1}\| \leq 1$. PROOF: Let $w \in \mathcal{R}_B$ with $w = Bu$. Then

$$\|B^{-1}w\|^2 = (B^{-1}w, B^{-1}w) = (u, u) \leq (Bu, u) = (w, B^{-1}w) \leq \|w\| \cdot \|B^{-1}w\|.$$

Hence $\|B^{-1}w\| \leq \|w\|$.

5. B^{-1} is self-adjoint. $\mathcal{D}_{B^{-1}} = \mathcal{R}_B = \mathcal{H}$.
6. B^{-1} is positive. PROOF: Let $w = Bu$. Then

$$(B^{-1}w, w) = (B^{-1}Bu, Bu) = (u, Bu) \geq (u, u) \geq 0.$$

It follows from these remarks that B^{-1} is self-adjoint and

$$0 \leq B^{-1} \leq I.$$

Therefore, from the spectral theorem for bounded self-adjoint operators, we see that there exists a spectral family $\{P_\lambda\}$ such that $B^{-1} = \int_0^1 \lambda dP_\lambda$.

Now (formally)

$$\int_0^1 \frac{1}{\lambda} dP_\lambda \int_0^1 \lambda dP_\lambda = \int_0^1 1 \cdot dP_\lambda = I$$

so $B = \int_0^1 \frac{1}{\lambda} dP_\lambda = A - (a-1)I$ and

$$A = \int_0^1 \left[(a-1) + \frac{1}{\lambda} \right] dP_\lambda = \int_a^\infty \mu dE_\mu, \quad (3.1)$$

where $\mu = (a-1) + 1/\lambda$, and

$$E_\mu = \begin{cases} I - P_{\frac{1}{\mu-a+1}-0}, & \mu \geq a \\ 0, & \mu < a. \end{cases}$$

DOES $B = \int_0^1 \frac{1}{\lambda} dP_\lambda$ MAKE SENSE? We need to study the behavior of the spectral family $\{P_\lambda\}$ as $\lambda \rightarrow 0$. To do this we set $P'_k = P_{\frac{1}{k}} - P_{\frac{1}{k+1}}$, $k = 1, 2, \dots$.

REMARKS:

1. $P'_k P'_\ell = 0$ if $k \neq \ell$.
2. The $\{P'_k\}$ are orthogonal projection operators.
3. $\sum_{k=1}^\infty P'_k = I$.
4. Set $\mathcal{M}_k = P'_k \mathcal{H}$. Then if $u \in \mathcal{H}$ we have the unique expansion

$$u = \sum_{k=1}^\infty u_k, \quad \text{where } u_k = P'_k u = P'_k u_k$$

and $(u_k, u_\ell) = 0$ for $k \neq \ell$.

Now if $v \in \mathcal{D}_B$ then $v = B^{-1}u$, $u \in \mathcal{H}$, and

$$v_k = P'_k B^{-1}u = B^{-1}P'_k u = B^{-1}u_k = \int_0^1 \lambda dP_\lambda (P_{\frac{1}{k}} - P_{\frac{1}{k+1}})u_k = \int_{\frac{1}{k+1}}^{\frac{1}{k}} \lambda dP_\lambda u_k.$$

It follows from this that

$$\int_{\frac{1}{k+1}}^{\frac{1}{k}} \frac{1}{\lambda} dP_\lambda = B P'_k$$

on \mathcal{H} . Since $Bv_k = BP'_k v$ we have

$$Bv = \sum_{k=1}^{\infty} Bv_k = \sum_{k=1}^{\infty} \int_{\frac{1}{k+1}}^{\frac{1}{k}} \frac{1}{\lambda} dP_{\lambda} v = \int_0^{\infty} \frac{1}{\lambda} dP_{\lambda} v.$$

Furthermore,

$$\|Bv\|^2 = \sum_{k=1}^{\infty} \int_{\frac{1}{k+1}}^{\frac{1}{k}} \frac{1}{\lambda^2} d\|P_{\lambda} v\|^2 = \int_0^{\infty} \frac{1}{\lambda^2} d\|P_{\lambda} v\|^2.$$

Indeed, one can show that $v \in \mathcal{D}_B$ if and only if this last integral is finite.

Hence, the spectral expansion (3.1) is established rigorously for all $v \in \mathcal{D}_A$.

Let T be a self-adjoint operator on \mathcal{H} with $\overline{\mathcal{D}_T} = \mathcal{H}$.

Lemma 19 *Let $B = I + T^2$, with $\mathcal{D}_B = \{u \in \mathcal{D}_T, Tu \in \mathcal{D}_T\}$. Then*

1. $\mathcal{D}_B = (T + iI)^{-1}(T - iI)^{-1}\mathcal{H}$, $\mathcal{R}_B = \mathcal{H}$ and B is symmetric on its domain.
2. $(Bu, u) \geq \|u\|^2$ for all $u \in \mathcal{D}_B$.
3. B^{-1} is self-adjoint and $0 < B^{-1} \leq I$.
4. Let $C = TB^{-1}$, $\mathcal{D}_C = \mathcal{H}$. Then C is bounded and symmetric, hence self-adjoint, and $\|C\| \leq 1$.

PROOF:

1. $Bu = (T + iI)(T - iI)u = (T - iI)(T + iI)u$ and, since T is self-adjoint $\pm i$ belongs to the resolvent set of T .
2. $(Bu, u) = (u, u) + (T^2u, u) = \|u\|^2 + \|Tu\|^2 \geq \|u\|^2$.
3. Obvious from the preceding proof.
4. Since

$$C = TB^{-1} = T(I + T^2)^{-1} = T(T + iI)^{-1}(T - iI)^{-1} = (T - iI)^{-1} - iB^{-1}$$

we have

$$C^* = (T + iI)^{-1} + iB^{-1} = (T + iI)^{-1} + i(T - iI)^{-1}(T + iI)^{-1}$$

$$= T(T - iI)^{-1}(T + iI)^{-1} = TB^{-1} = C.$$

Also for $v \in \mathcal{H}$ we have

$$\begin{aligned} \|Cv\|^2 &= (TB^{-1}v, TB^{-1}v) = (B^{-1}v, T^2B^{-1}v) \\ &= (B^{-1}v, [T^2 + I]B^{-1}v) - \|B^{-1}v\|^2 \\ &= (B^{-1}v, v) - \|B^{-1}v\|^2. \end{aligned}$$

Therefore,

$$\|Cv\|^2 + \|B^{-1}v\|^2 = (B^{-1}v, v) \leq (v, v) = \|v\|^2.$$

Q.E.D.

REMARKS:

1. Note that we have also shown that $B^{-1}T \subseteq TB^{-1}$.
2. The lemma is remarkable in the sense that it holds even though T^2 , hence B , may not be densely defined. Indeed, it could happen that $\mathcal{D}_B = \{\theta\}$. Nonetheless B^{-1} and C are globally defined, bounded and self-adjoint.

Now we can apply spectral techniques to the bounded self-adjoint operator B^{-1} in analogy to our earlier treatment of B^{-1} where $B = A - (a - 1)I$ was bounded below. By the spectral theorem for B^{-1} there exists a spectral family $\{F_\lambda\}$ such that

$$B^{-1} = \int_0^1 \lambda \, dF_\lambda.$$

Here it is easy to show that $F_0 = 0$. Now set $E_n = F_{\frac{1}{n}} - F_{\frac{1}{n+1}}$ for $n = 1, 2, \dots$. Then

$$\sum_{n=1}^{\infty} E_n = F_1 - F_0 = I.$$

Similarly if we define the subspaces $\mathcal{M}_n = E_n\mathcal{H}$, we have

$$\mathcal{H} = \sum_{n=1}^{\infty} \oplus \mathcal{M}_n.$$

Since $TB^{-1} \supseteq B^{-1}T$ where $TB^{-1} = C$ is bounded, then $TE_n \supseteq E_nT$, where TE_n is bounded. Hence $T\mathcal{M}_n \subseteq \mathcal{M}_n$.

Now set

$$s_n(\lambda) = \begin{cases} \frac{1}{\lambda} & \frac{1}{n+1} < \lambda \leq \frac{1}{n} \\ 0 & \text{otherwise,} \end{cases}$$

and let

$$S_n = \int_0^\infty s_n(\lambda) dF_\lambda = \int_{\frac{1}{n+1}}^{\frac{1}{n}} \frac{1}{\lambda} dF_\lambda.$$

Then

$$B^{-1}S_n = \int_{\frac{1}{n+1}}^{\frac{1}{n}} 1 dF_\lambda = E_n,$$

so

$$TE_n = TB^{-1}S_n = CS_n.$$

This shows that $T_n = TE_n$ is bounded and self-adjoint. Thus each T_n has a spectral resolution in terms of the spectral family $\{P_\mu^{(n)}\}$:

$$T_n = \int \mu dP_\mu^{(n)}, \quad n = 1, 2, \dots$$

Finally, set

$$P_\mu = \int_{n=1}^\infty P_\mu^{(n)} E_n, \quad E_n P_\mu = P_\mu E_n = P_\mu^{(n)}.$$

Then for any $u \in \mathcal{D}_T$ we have

$$Tu = \sum_{n=1}^\infty TE_n u = \sum_{n=1}^\infty \int \mu dP_\mu^{(n)} E_n u = \int_{-\infty}^\infty \mu dP_\mu u.$$

Here,

$$\mathcal{D}_T = \left\{ u \in \mathcal{H} : \|Tu\|^2 = \int_{-\infty}^\infty \mu^2 d\|P_\mu u\|^2 < \infty \right\}.$$

This establishes the spectral theorem for unbounded self-adjoint operators.

3.4.2 More on essentially self-adjoint operators

Recall that a symmetric operator A on \mathcal{H} is essentially self-adjoint if its closure \overline{A} is self-adjoint, i.e., if $\overline{A} = A^*$.

Theorem 56 *Let A be a symmetric operator. Then A is self-adjoint if and only if*

$$\mathcal{R}_{A+iI} = \mathcal{R}_{A-iI} = \mathcal{H},$$

i.e., $\pm i \in \rho(A)$.

PROOF: It is obvious that if A is self-adjoint, then $\pm i \in \rho(A)$. Conversely, suppose $\pm i \in \rho(A)$, and let $v \in \mathcal{D}_{A^*} \supseteq \mathcal{D}_A$. Then $(Au, v) = (u, A^*v)$, for all $u \in \mathcal{D}_A$, so

$$(Au + iu, v) = (Au, v) + (iu, v) = (u, A^*v - iv).$$

By our hypothesis, we can find $w \in \mathcal{D}_A$ such that $A^*v - iv = Aw - iw$, so

$$(u, A^*v - iv) = (u, Aw - iw) = (Au + iu, w).$$

Thus $v = w \in \mathcal{D}_A$. Hence $A = A^*$. Q.E.D.

Theorem 57 *The following are equivalent for a symmetric operator A .*

1. A is essentially self-adjoint.
2. $\overline{\mathcal{R}_{A+iI}} = \overline{\mathcal{R}_{A-iI}} = \mathcal{H}$.
3. $\mathcal{N}_{A^*+iI} = \mathcal{N}_{A^*-iI} = \{\theta\}$.

Lemma 20 *If A is symmetric then*

$$\mathcal{R}_{A+iI}^\perp = \mathcal{N}_{A^*-iI}, \quad \mathcal{R}_{A-iI}^\perp = \mathcal{N}_{A^*+iI}.$$

PROOF OF THEOREM: The equivalence of 2. and 3. follows from the lemma.

1. 1. \longrightarrow 3.: If A is essentially self-adjoint then $\overline{A} = A^*$ is self-adjoint. Hence $\mathcal{N}_{A^*\pm iI} = \{\theta\}$.
2. 3. \longrightarrow 1.: Consider $[u_1, u_2] \in \mathcal{H} \oplus \mathcal{H}$ with graph inner product

$$\langle [u_1, u_2], [v_1, v_2] \rangle = (u_1, v_1) + (u_2, v_2).$$

Recall that the graph of A is the subspace

$$\Gamma_A = \{[u, Au], u \in \mathcal{D}_A\},$$

and that $\Gamma_{\overline{A}}, \Gamma_{A^*}$ are closed subspaces with $\Gamma_{\overline{A}} \subseteq \Gamma_{A^*}$. Suppose $\Gamma_{\overline{A}} \neq \Gamma_{A^*}$. Then there exists a nonzero u such that $[u, A^*u] \in \Gamma_{A^*} \cap \Gamma_{\overline{A}}^\perp = \Gamma_{A^*} \cap \Gamma_A^\perp \implies (u, v) + (A^*u, Av) = 0$, for all $v \in \mathcal{D}_A$. Hence $A^*u \in \mathcal{D}_{A^*}$ and $(A^*)^2u = -u$. Thus $(A^* + iI)(A^* - iI)u = \theta$, or $u = \theta$. Impossible! Hence $\Gamma_{A^*} = \Gamma_{\overline{A}}$. Q.E.D.

Example 14 Let $\mathcal{H} = L_c^2(-\infty, \infty)$, $Au = -i\hbar u'$, and

$$\mathcal{D}_{A_1} = \{u(x) : u \in C^1(-\infty, \infty) \cap \mathcal{H}, Au \in \mathcal{H}\}.$$

Lemma 21 A_1 is essentially self-adjoint.

PROOF: From an earlier example, we know that A_1 is symmetric and

$$\mathcal{D}_{A_1^*} = \{u(x) : u \text{ absolutely continuous, } u, Au \in \mathcal{H}\}.$$

Solving the equation $(A_1^* + iI)u = \theta$ for $u \in \mathcal{D}_{A_1^*}$ we have $-\hbar u' + u = 0$, so $u = ae^{x/\hbar}$. However, since $u \in \mathcal{H}$ we must have $u \equiv 0$. Similarly, the equation $(A_1^* - iI)u = \theta$ for $u \in \mathcal{D}_{A_1^*}$ has only the solution $u \equiv 0$. Therefore, $A_1^* = \overline{A}$. Q.E.D.

Now we classify the spectra of the self-adjoint operator A_1^* .

1. $\sigma_P(A_1^*) = \emptyset$: Indeed if $A_1^*u = \lambda u$ then $u = ae^{i\lambda x/\hbar} \in \mathcal{H} \implies u = 0$.
2. $\sigma_C(A_1^*) = \mathbb{R}$, the real axis: For $v \in \mathcal{H}$ and λ real, the equation $(A_1^*u - \lambda)u = v$, or $-i\hbar u' - \lambda u = v$, has the general solution

$$u(x) = \frac{i}{\hbar} \int_{-\infty}^x e^{\frac{i\lambda}{\hbar}(x-t)} v(t) dt + ce^{\frac{i\lambda}{\hbar}x}.$$

As $x \rightarrow -\infty$ then for any $v \in \mathcal{H}$ we have $u(x) \rightarrow ce^{\frac{i\lambda}{\hbar}x}$, so u can't belong to \mathcal{H} unless $c = 0$. Thus the solution u is unique. However, for fixed real λ , unless v satisfies the condition $\int_{-\infty}^{\infty} e^{-\frac{i\lambda}{\hbar}t} v(t) dt = 0$, we have that $u(x) \rightarrow a \frac{i}{\hbar} e^{\frac{i\lambda}{\hbar}x}$ for nonzero a , so that $u \notin \mathcal{H}$. Clearly, $\lambda \notin \rho(A_1^*)$ and $\sigma_R(A_1^*) = \emptyset$ (since A_1^* is self-adjoint), so $\lambda \in \sigma_C(A_1^*)$.

Example 15 Here $\mathcal{H} = L_c^2[0, +\infty)$, $A = -iu'$ and

$$\mathcal{D}_A = \{u \in C^1[0, +\infty) \cap \mathcal{H} : u' \in \mathcal{H} \text{ and } u(0) = 0\}.$$

We have shown earlier that A is symmetric and

$$\mathcal{D}_{A^*} = \{u \in \mathcal{H} : u \text{ absolutely continuous, } u' \in \mathcal{H}\}.$$

Now

$$(A^* + iI)u = \theta \implies -iu' + iu = 0 \implies u(x) = ae^x.$$

If $u \in \mathcal{H}$ then $u \equiv 0$. However,

$$(A^* - iI)u = \theta \implies -iu' - iu = 0 \implies u(x) = ae^{-x}.$$

Note that $u \in \mathcal{H}$ for $a \neq 0$. Therefore, A is not an essentially self-adjoint operator. In fact, we will show later that A cannot be extended to a self-adjoint operator.

Example 16 *The Fourier Transform.* We describe, briefly, how the well known Fourier transform fits into the spectral theory of self-adjoint operators. Consider the interval $I = (-\infty, +\infty)$ and the Hilbert space $\mathcal{H} = L_c^2(I, 1)$. The operator A acts formally on this space via the differential operator $\tau = -i\frac{d}{dx}$. This is essentially the operator A_1 above, which we have shown is essentially self-adjoint. The equation $\tau u = \lambda u$ has the solution $u(x) = e^{i\lambda x}$ which is not in \mathcal{H} for any real λ . The spectrum of the self-adjoint operator \overline{A} is continuous and covers the real line. For any $u \in \mathcal{H}$ we define

$$g(y) = \frac{1}{\sqrt{2\pi}} \lim_{n \rightarrow \infty} \int_{-n}^n e^{-iyx} u(x) dx = Tu(y).$$

The basic properties of the Fourier transform on $L_c^2(I, 1)$ are that

$$u(x) = \frac{1}{\sqrt{2\pi}} \lim_{n \rightarrow \infty} \int_{-n}^n e^{iyx} g(y) dy, \text{ a.e.}$$

and

$$\int_{-\infty}^{\infty} |u(x)|^2 dx = \int_{-\infty}^{\infty} |g(y)|^2 dy.$$

We define the spectral projection operators E_λ by

$$E_\lambda u(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\lambda} e^{iyx} g(y) dy = \frac{1}{2\pi} \int_{-\infty}^{\lambda} \int_{-\infty}^{\infty} e^{iy(x-t)} f(t) dt dy,$$

so $dE_\lambda u(x) = \frac{1}{\sqrt{2\pi}} e^{i\lambda x} g(\lambda) d\lambda$ and

$$\overline{A}u = \int_{-\infty}^{\infty} \lambda dE_\lambda u(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \lambda e^{i\lambda x} g(\lambda) d\lambda.$$

The following results give some sufficient conditions for a symmetric operator to be essentially self-adjoint.

Theorem 58 *Suppose*

1. A is symmetric.
2. $\overline{\mathcal{R}_A} = \mathcal{H}$.
3. $\|Au\| \geq a\|u\|$, for all $u \in \mathcal{D}_A$. Here, $a > 0$.

Then A is essentially self-adjoint.

PROOF: By 3. A^{-1} exists and $\|A^{-1}\| \leq \frac{1}{a}$. Since A is symmetric, it follows that A^{-1} is symmetric, hence self-adjoint. Now suppose $(A^* + iI)v = \theta$. Then, for all $u \in \mathcal{D}_A$, we have

$$0 = (u, [A^* + iI]v) = (Au, v) - (iu, v) = (w - iA^{-1}w, v),$$

where $u = A^{-1}w$. Choose a sequence $\{w_n\}$ in \mathcal{R}_A such that $w_n \rightarrow v$ as $n \rightarrow \infty$. Then $A^{-1}w_n \rightarrow \overline{A^{-1}v}$ so

$$(v - i\overline{A^{-1}v}, v) = 0 \implies \|v\|^2 = i(\overline{A^{-1}v}, v) = 0,$$

since the left-hand side is real and the right-hand side is imaginary. Thus $v = \theta$. A similar proof shows that if $(A^* - iI)v = \theta$, then $v = \theta$. Q.E.D.

Corollary 11 *If A is symmetric operator, $\overline{\mathcal{R}_A} = \mathcal{H}$, and A^{-1} exists and is bounded, then A is essentially self-adjoint.*

Corollary 12 *If A is a symmetric ordinary Sturm-Liouville operator then A is essentially self-adjoint.*

PROOF: Choose a real number λ , not an eigenvalue of A . Then $(A - \lambda I)^{-1}$ exists and is bounded. Hence $\overline{\mathcal{R}_{A-\lambda I}} = \mathcal{H}$, so $A - \lambda I$ is essentially self-adjoint. This implies that A is essentially self-adjoint. Q.E.D.

3.5 A first look at deficiency indices

Definition 29 *Let A be a symmetric operator. The positive and negative deficiency indices of A are given, respectively, by*

$$\mathcal{D}_+(A) = \dim \mathcal{R}_{A+iI}^\perp = \dim \mathcal{N}_{A^*-iI},$$

$$\mathcal{D}_-(A) = \dim \mathcal{R}_{A-iI}^\perp = \dim \mathcal{N}_{A^*+iI}.$$

Here it may be that one or both of the deficiency indices are infinite. Note that A is essentially self-adjoint $\iff \mathcal{D}_+(A) = \mathcal{D}_-(A) = 0$.

PREVIEW OF COMING ATTRACTIONS: A can be extended to a self-adjoint operator $\iff \mathcal{D}_+(A) = \mathcal{D}_-(A)$.

What is the significance of the complex numbers $\pm i$? Answer: convenience.

Let B be a linear operator with $\overline{\mathcal{D}}_B = \mathcal{H}$.

Definition 30 *The complex number λ is a **point of regular type** of B if there exists a positive number $k(\lambda)$ such that $\|(B - \lambda I)u\| \geq k\|u\|$ for all $u \in \mathcal{D}_B$, i.e., if and only if $(B - \lambda I)^{-1}$ exists and is bounded.*

Note that it isn't required that $(B - \lambda I)^{-1}$ be densely defined. Now let $\text{Reg}(B)$ be the set of points of regular type for B .

Lemma 22 *$\text{Reg}(B)$ is an open set in the complex plane.*

PROOF: Suppose λ_0 is a point of regular type, and λ is a complex number such that $|\lambda - \lambda_0| \leq \frac{1}{2}k(\lambda_0) = \delta$. Then

$$\begin{aligned} \|(B - \lambda I)u\| + |\lambda - \lambda_0| \cdot \|u\| &\geq \|(B - \lambda_0 I)u\| \\ \implies \|(B - \lambda I)u\| &\geq [k(\lambda_0) - \frac{1}{2}k(\lambda_0)]\|u\| = \frac{1}{2}k(\lambda_0)\|u\|. \end{aligned}$$

Q.E.D.

Note that if B is symmetric and λ is not real, then $\|(B - \lambda I)u\| \geq |\text{Im } \lambda| \cdot \|u\|$, so λ is a point of regular type for B . It follows that the points of nonregular type for a symmetric operator must form a closed subset of the real line. We will show that if A is symmetric then $\dim \mathcal{R}_{A-\lambda I}^\perp$ is constant on any arcwise connected subset of $\text{Reg}(A)$. This will show that $\dim \mathcal{R}_{A-\lambda I}^\perp$ is constant on the upper half plane. Thus i is chosen only for convenience.

To prove this result we have to introduce some machinery. Let $U : \mathcal{H} \longrightarrow \mathcal{H}$ be a linear operator.

Definition 31 *U is an **isometric transformation** if*

1. $\mathcal{D}_U = \mathcal{H}$
2. $(Uu, Uv) = (u, v)$, for all $u, v \in \mathcal{H}$, i.e., $U^*U = I$.

If also $\mathcal{R}_U = \mathcal{H}$ then U is a **unitary transformation** and also $UU^* = I$, so $U^* = U^{-1}$.

REMARKS:

1. If \mathcal{H} is finite dimensional, then every isometry is unitary.
2. If \mathcal{H} is infinite dimensional then an isometric transformations may not be unitary. For example, let $\{e_n\}$ be an ON basis for \mathcal{H} . Then the linear transformation defined by $Ue_n = e_{n+1}$, $n = 1, 2, \dots$ is an isometry but not unitary.

Theorem 59 *Let \mathcal{M} and \mathcal{N} be closed subspaces of the Hilbert space \mathcal{H} , with corresponding orthogonal projection operators P, Q , respectfully. If $\|P - Q\| < 1$ then \mathcal{M} can be mapped linearly and isometrically onto \mathcal{N} . In particular, $\dim \mathcal{M} = \dim \mathcal{N}$.*

PROOF: If $\|P - Q\| < 1$ then $\|P(Q - P)P\| < 1$, so the symmetric operator

$$A \equiv I + P(Q - P)P \geq aI > 0,$$

where $a > 0$. Therefore the operators A^{-1} and $(A^{-1})^{\frac{1}{2}} = A^{-\frac{1}{2}}$ exist and are bounded, positive and symmetric.

Consider the operators $U = QA^{-\frac{1}{2}}P$ and $U^* = PA^{-\frac{1}{2}}Q$. Now $P \subset \subset A \implies P \subset \subset A^{-\frac{1}{2}}$, so

$$\begin{aligned} U^*U &= PA^{-\frac{1}{2}}QQA^{-\frac{1}{2}}P = A^{-\frac{1}{2}}PQQPA^{-\frac{1}{2}} \\ &= A^{-\frac{1}{2}}PQPA^{-\frac{1}{2}} = A^{-\frac{1}{2}}[P + P(Q - P)P]A^{-\frac{1}{2}} \\ &= A^{-\frac{1}{2}}PAA^{-\frac{1}{2}} = PA^{-\frac{1}{2}}AA^{-\frac{1}{2}} = P. \end{aligned}$$

Clearly, $U : \mathcal{M} \rightarrow \mathcal{N}$. I claim that this map is onto. First of all, $U\mathcal{M}$ is closed in \mathcal{N} . Now suppose there is a $v \in \mathcal{N}$ such that $v \perp U\mathcal{M}$. Then

$$(v, Um) = (v, QA^{-\frac{1}{2}}Pm) = 0,$$

for all $m \in \mathcal{H}$ so $U^*v = \theta$. But $U^*v = PA^{-\frac{1}{2}}Qv = \theta$. Thus

$$PQv = A^{\frac{1}{2}}A^{-\frac{1}{2}}PQv = A^{\frac{1}{2}}PA^{-\frac{1}{2}}Qv = A^{\frac{1}{2}}U^*v = \theta.$$

This implies $(Q - P)Qv = Qv$. However, since $\|Q - P\| < 1$ we must have $Qv = \theta$. Since $v \in \mathcal{N}$ this means that $v = \theta$, so U is onto. Q.E.D.

Let $P' = E - P$, $Q' = E - Q$ where P, Q are orthogonal projection operators.

Lemma 23 *If $\|Q'P\| \leq \frac{1}{2}$ and $\|P'Q\| \leq \frac{1}{2}$ then $\|P - Q\| < 1$.*

PROOF: For any nonzero $u \in \mathcal{H}$

$$P - Q = PQ' - P'Q, \quad \|P'Qu\|^2 = \|P'QQu\|^2 \leq \frac{1}{4}\|Qu\|^2,$$

$$\|PQ'u\|^2 = (PQ'u, PQ'u) = (Q'PQ'u, Q'u) \leq \frac{1}{2}\|Q'u\|^2,$$

so

$$\|(P - Q)u\|^2 = \|PQ'Q'u\|^2 + \|P'QQu\|^2 \leq \frac{1}{2}\|Q'u\|^2 + \frac{1}{4}\|Qu\|^2 < \|u\|^2.$$

Q.E.D.

Theorem 60 *Let Γ be an arcwise connected subset of $\text{Reg}(A)$. Then $\dim \mathcal{R}_{A-\lambda E}^\perp$ is the same for all $\lambda \in \Gamma$.*

PROOF: Let P_λ be the orthogonal projection operator on the space $\mathcal{R}_{A-\lambda E}^\perp$. By the Heine-Borel theorem, it is enough to show that for each $\lambda_0 \in \Gamma$ there is a $\delta(\lambda_0) > 0$ such that $\|P_\lambda - P_{\lambda_0}\| < 1$ for $|\lambda - \lambda_0| < \delta$. Let $\lambda_0 \in \Gamma$ and let $0 < \delta(\lambda_0) \leq \frac{1}{3}k(\lambda_0)$. Now

$$k(\lambda_0)\|u\| \leq \|(A - \lambda_0 E)u\| \leq \|(A - \lambda E)u\| + |(\lambda - \lambda_0)| \cdot \|u\|$$

for all $u \in \mathcal{D}_A$. Thus if $|\lambda - \lambda_0| \leq \delta$ then

$$\|(A - \lambda E)u\| \geq \frac{2}{3}k(\lambda_0)\|u\|.$$

Therefore, if $|\lambda - \lambda_0| \leq \delta$ and $v \in \mathcal{R}_{A-\lambda E}^\perp$ with $\|v\| = 1$, we have

$$\begin{aligned} \|P'_{\lambda_0} v\| &= \sup_{u \in \mathcal{D}_A} \frac{|(v, (A - \lambda_0 E)u)|}{\|(A - \lambda_0 E)u\|} = \sup_{u \in \mathcal{D}_A} \frac{|(v, (A - \lambda E)u + (\lambda - \lambda_0)u)|}{\|(A - \lambda_0 E)u\|} \\ &= \sup_{u \in \mathcal{D}_A} \frac{|(\lambda - \lambda_0)(v, u)|}{\|(A - \lambda_0 E)u\|} \leq \sup_{u \in \mathcal{D}_A} \frac{\frac{1}{3}k(\lambda_0)\|v\| \cdot \|u\|}{\frac{2}{3}k(\lambda_0)\|u\|} = \frac{1}{2}. \end{aligned}$$

Therefore, $\|(E - P_{\lambda_0})v\| \leq \frac{1}{2}$ for unit vector $v \in \mathcal{R}_{A-\lambda E}^\perp$. Similarly $\|(E - P_{\lambda_0})w\| \leq \frac{1}{2}$ for unit vector $w \in \mathcal{R}_{A-\lambda_0 E}^\perp$. Thus, the theorem is implied by the preceding lemma. Q.E.D.

Corollary 13 *If A is symmetric and λ is a complex number with $\text{Im } \lambda > 0$, then $\dim \mathcal{R}_{A+\lambda E}^\perp = \mathcal{D}_+(A)$ and $\dim \mathcal{R}_{A+\bar{\lambda} E}^\perp = \mathcal{D}_-(A)$.*

Corollary 14 *If A is symmetric, closed and bounded below, then $\mathcal{D}_+(A) = \mathcal{D}_-(A)$.*

Corollary 15 *If A is symmetric and there is a real λ such that $\lambda \in \text{Reg } (A)$, then $\mathcal{D}_+(A) = \mathcal{D}_-(A)$.*

3.6 Essential self-adjointness of generalized Sturm-Liouville operators

In this section we will determine the essential self-adjointness of a family of Sturm-Liouville operators in R_n similar to that which was introduced in Section 1.3.2. Now, however, we will consider only the case of partial differential operators in n variables that act on functions defined on the full n -dimensional Euclidean space R_n . That is, there is no boundary, though there is a weight function $k(x)$. We denote points in R_n by $x = (x_1, \dots, x_n)$. Our Hilbert space is

$$\mathcal{H} = \left\{ u(x), \text{ real valued} : \int_{R_n} |u(x)|^2 k(x) dx < \infty \right\} = L_c^2\{R_n, k\}$$

$$(u, v) = \int_{R_n} u(x)v(x)k(x) dx, \quad u, v \in \mathcal{H}.$$

Formally, the Sturm-Liouville operator is

$$Au = \frac{1}{k(x)} \left[- \sum_{\ell, j=1}^n (p_{\ell j}(x) u_{x_j})_{x_\ell} + i \sum_{j=1}^n p_j(x) u_{x_j} + i \sum_{j=1}^n (p_j(x))_{x_j} u + q(x) u \right]. \quad (3.2)$$

This formal operator enables us to define three operators, A_1, A_2, A_3 with domains

$$\mathcal{D}_{A_1} = \left\{ u \in \overset{\circ}{C}^\infty(R_3) \right\},$$

$$\mathcal{D}_{A_2} = \left\{ u \in \overset{\circ}{C}^2(R_3) \right\},$$

$$\mathcal{D}_{A_3} = \left\{ u \in C^2(R_3) : u \in \mathcal{H} \text{ and } Au \in \mathcal{H} \right\},$$

respectively. We require

1. $p_{\ell j}(x), k(x), q(x)$ real and $p_{\ell j} = p_{j\ell}$
2. $p_{\ell j}(x) \in C^3(R_n), p_j(x) \in C^2(R_n), \quad k, q \in C^1(R_n)$
3. $k > 0$ for all $x \in R_n$
4. $\sum_{\ell, j=1}^n p_{\ell j}(x) \xi_\ell \overline{\xi_j} \geq \rho(x) \sum_{j=1}^n |\xi_j|^2$ for all $x \in R_n$ and arbitrary complex ξ_j . Here $\rho(x) > 0$ for all $x \in R_n$.

Recall that the S-L operators A_1, A_2, A_3 are symmetric. Furthermore,

$$\mathcal{D}_{A_1} \subset \mathcal{D}_{A_2} \subset \mathcal{D}_{A_3}$$

and $\overline{\mathcal{D}_{A_1}} = \mathcal{H}$.

To prove the essential self-adjointness of these operators we need a technical (and deep) lemma. Let G be an open, simply connected subset of R_n , and let D be the differential operator

$$D = - \sum_{j, \ell=1}^n a_{j\ell}(x) u_{x_j x_\ell} + \sum_{j=1}^n a_j(x) u_{x_j} + a(x) u.$$

Here,

$$\mathcal{D}_D = \left\{ u(x) : u \in \overset{\circ}{C}^\infty(G) \right\},$$

and we require

1. $a_{\ell j}(x), a_j(x), a(x)$ complex and $a_{\ell j} = a_{j\ell}$
2. $a_{\ell j}(x) \in C^3(G), a_j(x) \in C^2(G), \quad a(x) \in C^1(G)$
3. $\sum_{\ell, j=1}^n a_{\ell j}(x) \xi_\ell \overline{\xi_j} \geq \rho(x) \sum_{j=1}^n |\xi_j|^2$ for all $x \in G$ and arbitrary complex ξ_j . Here $\rho(x) > 0$ for all $x \in G$.

Lemma 24 (*Hermann Weyl*) *Let $\eta(x) \in C^1(G)$ and suppose $w(x)$ is locally integrable in G . If*

$$\int_G w(x) \overline{Du(x)} \, dx = \int_G \eta(x) \overline{u(x)} \, dx$$

*holds for all $u \in \mathcal{D}_D$ then $w(x) = \tilde{w}(x)$, a.e., where $\tilde{w} \in C^2(G)$. Furthermore, $D^*w = \eta$, a.e., where D^* is the formal adjoint of D .*

Theorem 61 *The operators A_1, A_2, A_3 , defined above, are essentially self adjoint.*

PROOF: We will show that $\mathcal{D}_+(A_1) = \mathcal{D}_-(A_1) = 0$. Since $A_3^* \subseteq A_2^* \subseteq A_1^*$, the theorem will follow. Suppose $v \in \mathcal{D}_{A_1}$ and $A_1^*v = iv$. Then

$$([A_1^* - iE]v, u) = 0, \quad \text{for all } u \in \mathcal{D}_{A_1} = \overset{\circ}{C}^\infty(R_n)$$

$$\implies (v, [A_1 + iE]u) = 0, \quad \text{for all } u \in \overset{\circ}{C}^\infty(R_n).$$

Note: v is locally integrable in R_n since

$$\int_B |v| \, dx = \int_B |v| \sqrt{k} \left(\frac{1}{\sqrt{k}} \right) dx \leq \sqrt{\int_B |v|^2 k \, dx} \int_B \frac{1}{k} dx < \infty,$$

where B is any compact set.

It follows from the Weyl lemma for the case $\eta \equiv 0$ that we can assume $v \in C^2(R_n)$. Thus $Av = iv$, and $v \in \mathcal{D}_{A_3}$. Since A_3 is symmetric, we must have $v = \theta$. Thus $\mathcal{D}_+(A_1) = 0$. A similar proof gives $\mathcal{D}_-(A_1) = 0$. Q.E.D.

Corollary 16 *Let $\lambda \in \sigma_P(\overline{A_3})$ and suppose there is a nonzero v such that $\overline{A_3}v = \lambda v$. Then, by redefining v on a set of measure zero if necessary, we can assume $v \in \mathcal{D}_{A_3}$, $A_3v = \lambda v$.*

PROOF: $([A_3^* - \lambda E]v, u) = 0$ for all $u \in \mathcal{D}_{A_1}$ implies from the Weyl lemma that $v \in C^2(R_n)$. Thus $v \in \mathcal{D}_A$. Q.E.D.

In Chapter 4 we give a detailed proof of the Weyl lemma for second-order ordinary differential operators. The verification for partial differential operators is more challenging, and we merely sketch a proof of the Weyl lemma for the case $Du = -\Delta_n u + a(x)u$. (More details can be found in Hellwig.) We need to show that if

$$\int_G w(x)[- \Delta_n u(x) + a(x)u(x)] \, dx = \int_G \eta(x)u(x) \, dx$$

for some $\eta \in C^1(G)$ and all $u \in \overset{\circ}{C}^\infty(G)$ then $w \in C^2(G)$.

Fix a point $x_0 \in G$ and let K_1 be a ball centered about x_0 such that $\overline{K_1} \subset G$. Let K_2 be a ball centered at x_0 such that $\overline{K_2} \subset K_1$. Let $\rho(x) \in \overset{\circ}{C}^\infty(K_1)$

such that $\rho(x) \equiv 1$ for all $x \in K_2$. Let $s(x, y) = s(y, x)$ be the fundamental solution of $\Delta_n u = 0$:

$$s(x, y) = \begin{cases} \frac{1}{(n-2)\omega_n} |x - y|^{2-n}, & n > 2 \\ -\frac{1}{2\pi} \ln |x - y|, & n = 2. \end{cases}$$

Suppose $w \in C^2(G)$ and set $\eta(x) = -\Delta_n w(x) + a(x)w(x)$. From Green's formula,

$$\int_{K_1} w(y) \Delta_n^y [\rho(y) s(x, y)] dy - \int_{K_1} \rho(y) s(x, y) \Delta_n^y w(y) dy = w(x)$$

if $x \in K_2$, where Δ_n^y signifies that Δ_n is acting on the y coordinates. Thus we have

$$w(x) = \int_{K_1} w(y) \Delta_n^y [\rho(y) s(x, y)] dy + \int_{K_1} \rho(y) s(x, y) [\eta(y) - a(y)w(y)] dy. \quad (3.3)$$

However, for the Weyl lemma we can only assume that $w(x)$ is locally integrable. The Green's formula computation suggests that we define a function $v(x)$ by the integrals

$$v(x) = \int_{K_1} w(y) \Delta_n^y [\rho(y) s(x, y)] dy + \int_{K_1} \rho(y) s(x, y) [\eta(y) - a(y)w(y)] dy.$$

Note by inspection that $v \in C^2(K_2)$. If we can show that for all $u \in \overset{\circ}{C}^\infty(K_2)$

$$\int_{K_2} v(y) u(y) dy = \int_{K_2} w(y) u(y) dy - \int_{K_1} w(x) [D\Psi(x) - \eta(x)\Psi(x)] dx \quad (3.4)$$

where

$$\Psi(x) = \rho(x) \int_{K_2} s(y, x) u(y) dy,$$

and $D\Psi(x) - \eta(x)\Psi(x) = 0$ for $x \in K_1$, it will follow that

$$\int_{K_2} u(y) [v(y) - w(y)] dy = 0$$

so that $v(y) = w(y)$, a.e. in K_2 . This will imply that (3.3) holds.

We have

$$\int_{K_2} v(y) u(y) dy = \int_{K_1} w(x) \left[\int_{K_2} u(y) \Delta_n^x [\rho(x) s(y, x)] dy \right] dx$$

$$\begin{aligned}
& + \int_{K_1} \left[\rho(x) [\eta(x) - a(x)w(x)] \, dy \int_{K_2} u(y)s(x, y) \, dy \right] dx \\
& = \int_{K_1-K_2} w(x) \left[\Delta_n^x \rho(x) \int_{K_2} u(y)s(y, x) \, dy \right] dx + \cdots.
\end{aligned}$$

Note that

$$u(x) = -\Delta_n^x \int_{K_2} s(y, x)u(y)dy, \quad u \in \overset{o}{C}^\infty(K_2)$$

and set $\Psi(x) = \rho(x) \int_{K_2} u(y)s(x, y)dy$. Then we find

$$\begin{aligned}
& \int_{K_2} u(y)[v(y) - w(y)] \, dy = - \int_{K_2} w(y)u(y)dy \\
& + \int_{K_1-K_2} w(x)\Delta_n^x \Psi(x)dx + \int_{K_1} [\eta(x) - a(x)w(x)]\Psi(x)dx \\
& = - \int_{K_1} w(x) [D\Psi(x) - \eta(x)\Psi(x)] \, dx = 0.
\end{aligned}$$

Q.E.D.

3.7 B-bounded operators and their applications

Definition 32 Let B, C be operators on the Hilbert space \mathcal{H} with $\mathcal{D}_B \subseteq \mathcal{D}_C$, $\overline{\mathcal{D}_B} = \mathcal{H}$. We say that C is **B -bounded** if there exist real constants δ, ϵ , with $0 \leq \epsilon < 1$ and such that

$$\|Cu\| \leq \epsilon \|Bu\| + \delta \|u\|$$

for all $u \in \mathcal{D}_B$.

Note that any bounded operator C is automatically bounded with respect to any other operator B . The main interest is in cases where C is an unbounded but B -bounded operator.

A principal result for such operators is

Theorem 62 Suppose B, C are operators on \mathcal{H} with $\mathcal{D}_B \subseteq \mathcal{D}_C$, $\overline{\mathcal{D}_B} = \mathcal{H}$. If

1. B is essentially self-adjoint

2. C is symmetric

3. C is B -bounded.

Then $B + C$ is essentially self-adjoint and $\mathcal{D}_{B+C} = \mathcal{D}_B$.

PROOF: The basic strategy behind the proof is to show that there exists a complex number λ with $\text{Im } \lambda \neq 0$ such that both $(B + C + \lambda E)\mathcal{D}_B$ and $(B + C + \bar{\lambda}E)\mathcal{D}_B$ are dense in \mathcal{D}_B , so that the deficiency indices of $B + C$ are both zero. Clearly, $B + C$ is symmetric in \mathcal{H} . Since B is essentially self-adjoint it follows that $(B + ikE)\mathcal{D}_B$ is dense in \mathcal{H} for all real $k \neq 0$, and that $(B + ikE)^{-1}$ exists and is bounded. Indeed $\|(B + ikE)u\|^2 = \|Bu\|^2 + k^2\|u\|^2$ for $u \in \mathcal{D}_B$ so $\|(B + ikE)^{-1}\| \leq \frac{1}{|k|}$. We will show that there exists a real $k \neq 0$ such that $(B + C \pm ikE)\mathcal{D}_B$ is dense in \mathcal{H} .

Note that (formally)

$$(B + C + ikE)\mathcal{D}_B = \left(C(B + ikE)^{-1} + E \right) (B + ikE)\mathcal{D}_B$$

and, since C is B -bounded,

$$\|C(B + ikE)^{-1}u\| \leq \epsilon \|B(B + ikE)^{-1}u\| + \delta \|(B + ikE)^{-1}u\|.$$

Therefore,

$$\|C(B + ikE)^{-1}\| \leq \epsilon + \frac{\delta}{|k|}.$$

Now choose $|k|$ so large that $\epsilon + \frac{\delta}{|k|} < 1$. This means that the operator $A = C(B + ikE)^{-1}$ is bounded with norm $\|A\| < 1$. But this in turn means that the operator

$$(E + A)^{-1} = \sum_{j=0}^{\infty} (-1)^j A^j$$

exists and is bounded. Here,

$$\mathcal{R}_{E+A} = \mathcal{D}_{(E+A)^{-1}} = \mathcal{D}_A = \mathcal{R}_{B+ikE}.$$

Therefore,

$$\left(C(B + ikE)^{-1} + E \right) (B + ikE)\mathcal{D}_B = (B + C + ikE)\mathcal{D}_B$$

is dense in \mathcal{H} . Q.E.D.

Corollary 17 *Replace requirement 1. in theorem 62 by*

1. *B is self-adjoint.*

Then $C + B$ is self-adjoint.

Corollary 18 *Suppose*

1. *B is essentially self-adjoint*
2. *C is symmetric and $\mathcal{D}_C \supseteq \mathcal{D}_B$*
3. *$\|Cu\|^2 \leq \rho_1(u, Bu) + \rho_2\|u\|^2$ for some $\rho_1, \rho_2 \geq 0$ and all $u \in \mathcal{D}_B$.*

Then $C + B$ is essentially self-adjoint.

PROOF:

$$\begin{aligned} \|C(B + ikE)^{-1}u\|^2 &\leq \rho_1(B + ikE)^{-1}u, B(B + ikE)^{-1}u + \rho_2\|(B + ikE)^{-1}u\|^2 \\ &\leq \rho_1\|(B + ikE)^{-1}u\| \cdot \|B(B + ikE)^{-1}u\| + \rho_2\|(B + ikE)^{-1}u\|^2 \\ &\leq \left(\frac{\rho_1}{|k|} \|B(B + ikE)^{-1}\| + \frac{\rho_2}{|k|^2} \right) \|u\|^2. \end{aligned}$$

Therefore, by choosing $|k|$ large enough, we have $\|C(B + ikE)^{-1}\| < 1$. From the proof of Theorem 62 it follows that $(B + C \pm ikE)\mathcal{D}_B$ is dense in \mathcal{H} . Q.E.D.

We will apply these results to essentially self-adjoint operators introduced in Section 3.6. Recall that the Hilbert space is

$$\mathcal{H} = \left\{ u(x), \text{ real valued} : \int_{R_n} |u(x)|^2 k(x) dx < \infty \right\} = L_c^2\{R_n, k\},$$

and the formal Sturm-Liouville operator is

$$Au = \frac{1}{k(x)} \left[- \sum_{\ell, j=1}^n (p_{\ell j}(x) u_{x_j})_{x_\ell} + i \sum_{j=1}^n p_j(x) u_{x_j} + i \sum_{j=1}^n (p_j(x))_{x_j} u + q(x) u \right]. \quad (3.5)$$

Here,

1. $p_{\ell j}(x), k(x), q(x)$ real and $p_{\ell j} = p_{j\ell}$

2. $p_{\ell j}(x) \in C^3(R_n)$, $p_j(x) \in C^2(R_n)$, $k, q \in C^1(R_n)$
3. $k > 0$ for all $x \in R_n$
4. $\sum_{\ell,j=1}^n p_{\ell j}(x) \xi_{\ell} \overline{\xi_j} \geq \rho(x) \sum_{j=1}^n |\xi_j|^2$ for all $x \in R_n$ and arbitrary complex ξ_j . Here $\rho(x) > 0$ for all $x \in R_n$.

The essentially self-adjoint operators A_1, A_2 have domains

$$\mathcal{D}_{A_1} = \left\{ u \in \overset{\circ}{C}^{\infty}(R_3) \right\},$$

$$\mathcal{D}_{A_2} = \left\{ u \in \overset{\circ}{C}^2(R_3) \right\},$$

respectively.

Theorem 63 *The operators A_1, A_2 remain essentially self-adjoint if q satisfies the weaker condition $q(x) \in C^0(R_n)$.*

PROOF: Suppose $q \in C^0(R_n)$. Clearly there exists some $\tilde{q}(x) \in C^1(R_n)$ such that $|q(x) - \tilde{q}(x)| \leq k(x)$ for all $x \in R_n$. Let \tilde{A}_j , $j = 1, 2$ be the symmetric operators corresponding to the potential function $\tilde{q}(x)$, and A_j , $j = 1, 2$ be the symmetric operators corresponding to the potential function $q(x)$. Then the \tilde{A}_j are essentially self-adjoint. Define the operator C by

$$Cu(x) = \left(\frac{q(x) - \tilde{q}(x)}{k(x)} \right) u(x).$$

The $A_j u = \tilde{A}_j u + Cu$, C are symmetric with $\mathcal{D}_B \subseteq \tilde{\mathcal{D}}_{\tilde{A}_j}$ and $\|Cu\| \leq \|u\|$. Since C is a bounded operator, it is trivially \tilde{A}_j -bounded. Thus by Theorem 62 the operators A_j are essentially self-adjoint. Q.E.D.

A deeper result is the following.

Theorem 64 *Suppose $q(x)$ is a real potential in R_n and a finite positive number M such that*

$$\int_{|y-x| \leq R} \frac{q^2(x)}{|x-y|^{n-4+\alpha}} dy \leq M$$

for all $x \in R_n$, all $R \in (0, 1)$ and some α with $0 < \alpha < 4$. Define the formal operator A by

$$Au(x) = -\Delta_n u(x) + q(x)u(x).$$

Then A_1 and A_2 are essentially self-adjoint.

SKETCH OF PROOF: The theorem follows from the inequality

$$||q(x)u(x)|| \leq K_1 R^{\alpha/2} M^{1/2} ||\Delta_n u(x)|| + K_2 R^{(\alpha-4)/2} M^{1/2} ||u(x)|| \quad (3.6)$$

where K_1, K_2 are constants and $u \in \mathcal{D}_{A_1}$ or $u \in \mathcal{D}_{A_2}$. If we set $Bu = -\Delta_n u$ and $Cu = q(x)u$ we see that C is symmetric, B is essentially self-adjoint and there exist constants ϵ, δ such that

$$||Cu|| \leq \epsilon ||Bu|| + \delta ||u||.$$

We can require $0 < \epsilon < 1$ if we choose R sufficiently small. This shows that C is B -bounded, so that $B + C$ is essentially self-adjoint. Thus the theorem follows once we show that (3.6) holds. We will indicate the proof of the inequality shortly.

Theorem 64 shows that the operators A_1 and A_2 can be essentially self-adjoint even when the potential $q(x)$ has a singularity in R_n . Indeed, we have the following estimate.

Theorem 65 *Let $b(x) = \rho^{-\delta}(x)$, where $\rho^2(x) = \sum_{j=1}^m x_j^2$, $1 \leq m \leq n$ and $\delta \geq 0$. If $\alpha > 0$, $2\delta < 4 - \alpha \leq m$ then for all $x \in R_n$, $n \geq 2$ we have*

$$\int_{|y-x| \leq R} \frac{b^2(x)}{|x-y|^{n-4+\alpha}} dy \leq M$$

for all $0 < R < 1$.

SKETCH OF PROOF: This follows from introducing spherical coordinates r, θ_j in R_n . In these coordinates $dy \sim r^{n-1} dr d\omega$ where $d\omega$ is the area measure on the unit sphere in R_n . The maximum possible singularity of the integral occurs at $x = y$, and we can evaluate this case by passing to spherical coordinates and see that the integral converges as indicated by the statement of the theorem. Q.E.D.

To indicate the proof of the inequality (3.6) in Theorem 64 we will review and extend some results about the operator A_2 with $q \equiv 0$, i.e. (restricting to the important case $n = 3$ for simplicity)

$$A_2 = -\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2} - \frac{\partial^2}{\partial x_3^2} = -\Delta_3,$$

where

$$\mathcal{H} = L^2(R_3), \quad \mathcal{D}_{A_2} = \overset{o}{C}^\infty(R_3).$$

Then A_2 is symmetric,

$$A_2 \subseteq A_2^*$$

and $A_2^* = \overline{A_2}$ is self-adjoint and A_2 is essentially self-adjoint. (The analogous statements are also true for A_1 .)

Recall some of the steps in the construction of $\overline{A_2}$. The Fourier transform

$$\hat{u}(y) = \mathcal{F}u(y) \equiv \frac{1}{(2\pi)^{\frac{3}{2}}} \lim_{r \rightarrow \infty} \int \int \int_{|x| \leq r} e^{-ix \cdot y} u(x) dx,$$

where $x = (x_1, x_2, x_3)$, $y = (y_1, y_2, y_3)$ is a unitary mapping of \mathcal{H} onto $\hat{\mathcal{H}} = L^2(R_3)$ (in the y coordinates), i.e., the map is 1-1, onto and preserves inner product. Now if $u \in \mathcal{D}_{A_2}$ then

$$\hat{A}u(y) = -\frac{1}{(2\pi)^{\frac{3}{2}}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-ix \cdot y} \Delta_3 u(x) dx = |y|^2 \hat{u}(y).$$

Now let K be the operator with maximal domain that multiplies by $|y|^2$ in $\hat{\mathcal{H}}$:

$$\mathcal{D}_K = \{ \hat{v} \in \hat{\mathcal{H}} : |y|^2 \hat{v}(y) \in \hat{\mathcal{H}} \}.$$

Clearly, $K = K^*$. Let \tilde{A} be the operator on \mathcal{H} defined by $A = \mathcal{F}^{-1} K \mathcal{F}$. (Note that $\mathcal{F}^{-1} = \mathcal{F}^*$ since \mathcal{F} is unitary. So $(\tilde{A}u, v) = (\mathcal{F}^{-1} K \mathcal{F}u, v) = (K \mathcal{F}u, \mathcal{F}v) = (\hat{K} \hat{u}, \hat{v})$, where (\cdot, \cdot) is the inner product on $\hat{\mathcal{H}}$.) We see that \tilde{A} is an extension of A_2 . Further, $\tilde{A} = A^*$, since $K = K^*$. Thus A_2 (as well as A_1) has a self-adjoint extension. We have already shown that, in fact, $\tilde{A} = \overline{A_1 A_2}$.

Now if $u \in \mathcal{D}_{\tilde{A}}$ then

$$\begin{aligned} |u(x)| &= \left| \frac{1}{(2\pi)^{\frac{3}{2}}} \int \int \int e^{ix \cdot y} \hat{u}(y) dy \right| \leq \frac{1}{(2\pi)^{\frac{3}{2}}} \int \int \int |\hat{u}(y)| dy \\ &\leq \frac{1}{(2\pi)^{\frac{3}{2}}} \int \int \int \frac{1}{|y|^2 + \alpha^2} \cdot (|y|^2 + \alpha^2) |\hat{u}(y)| dy \\ &\leq \frac{1}{(2\pi)^{\frac{3}{2}}} \sqrt{\int \int \int \frac{dy}{(|y|^2 + \alpha^2)^2}} \sqrt{\int \int \int (|y|^2 + \alpha^2)^2 |\hat{u}(y)|^2 dy} \end{aligned}$$

for all $\alpha > 0$. The first integral in the last inequality can be evaluated explicitly, and we find

$$|u(x)| \leq \frac{\pi}{(2\pi)^{\frac{3}{2}} \alpha^{1/2}} \|(\tilde{A} + \alpha^2)u\| \leq \frac{\pi}{(2\pi)^{\frac{3}{2}}} (\alpha^{-1/2} \|(\tilde{A}u)\| + \alpha^{3/2} \|u\|) \quad (3.7)$$

for all $\alpha > 0$. This shows in particular that $u(x)$ is bounded and continuous if $u \in \mathcal{D}_{\tilde{A}}$. Note that (3.7) is the verification of (3.6) in the case $n = 3$. The proof for general n is similar.

To make clearer how Theorem 64 can be applied, we will look more carefully at the case $n = 3$. Suppose q is locally square integrable and that

$$q(x) = q_0(x) + q_1(x)$$

where q_0 is a bounded measurable function in R_3 and $q_1 \in L^2(R_3)$.

NOTE: A physically important example is the Coulomb potential

$$q(x) = \frac{1}{r}, \quad r = \sqrt{x_1^2 + x_2^2 + x_3^2}.$$

Here q is locally square integrable and we can take

$$q_1(x) = \begin{cases} 0, & r \leq 1 \\ \frac{1}{r}, & r > 1, \end{cases} \quad q_2(x) = \begin{cases} \frac{1}{r}, & 0 < r \leq 1 \\ 0, & r > 1. \end{cases}$$

Let Q be the operator defined by multiplication by $q(x)$ and let

$$Q_1 u(x) = q_1(x)u(x), \quad \mathcal{D}_{Q_1} = \left\{ u \in L^2(R_3) : q_1 u \in L^2(R_3) \right\},$$

$$Q_0 u(x) = q_0(x)u(x), \quad \mathcal{D}_{Q_0} = L^2(R_3).$$

Then $Q = Q_0 + Q_1$ and $\mathcal{D}_Q = \mathcal{D}_{Q_1}$. Now consider the operator

$$H = \tilde{A} + Q = \tilde{A} + Q_0 + Q_1,$$

where \tilde{A} is self-adjoint and Q is symmetric. Recall that if $u \in \mathcal{D}_{\tilde{A}}$ then $u(x)$ is bounded, hence $u \in \mathcal{D}_Q$. Let $\mathcal{D}_H = \mathcal{D}_{\tilde{A}}$.

Theorem 66 *H is self-adjoint and $A_1 + Q$ (with $\mathcal{D}_{A_1+Q} = \mathcal{D}_{A_1}$), is essentially self-adjoint.*

PROOF:

$$u \in \mathcal{D}_{\tilde{A}} \implies \|Q_1 u\| \leq \|q_1\| \sup |u(x)| \leq K \|q_1\| (\alpha^{-1/2} \|\tilde{A}u\| + \alpha^{3/2} \|u\|).$$

Also, $\|Q_0 u\| \leq \|u\| \sup |q_0(x)|$. Thus

$$\|Qu\| \leq \|Q_1 u\| + \|Q_0 u\| \leq \frac{K}{\alpha^{1/2}} \|q_1\| \cdot \|\tilde{A}u\| + [K\alpha^{3/2} \|q_1\| + \sup |q_0(x)|] \cdot \|u\|.$$

Choose α so large that $K \|q_1\| / \alpha^{1/2} < 1$. Then Q is \tilde{A} -bounded. Q.E.D.

3.8 The graph approach to extensions of symmetric operators

We now continue the development of the operator graph approach to linear operators that was introduced in Section 1.3.1. Here we will be interested in the possible ways that a symmetric closed operator can be extended to a self-adjoint operator. Recall that if A is a linear operator on the Hilbert space \mathcal{H} , with dense domain, the **graph** $\Gamma(A)$ of A is the set of all ordered pairs $[u, Au] \in \mathcal{H} \oplus \mathcal{H}$ with $u \in \mathcal{D}_A$. If we assume that A is symmetric, then $A \subseteq A^*$ and $\Gamma_{A^*} \supseteq \Gamma_A$. Thus we can regard Γ_A as a subspace of the graph Hilbert space Γ_{A^*} with graph inner product

$$\langle u, v \rangle = (u, v) + (A^*u, A^*v), \quad u, v \in \mathcal{D}_A.$$

A is closed if and only if Γ_A is a closed subspace of Γ_{A^*} . Recall also that if B is symmetric and $B \supseteq A$ then

$$A \subseteq B \subseteq B^* \subseteq A^*.$$

(In the following we will, for convenience, often employ the identification $v \leftrightarrow [v, A^*v]$ between elements $v \in \mathcal{D}_{A^*}$ and elements $[v, A^*v] \in \Gamma_{A^*}$.)

Definition 33

$$\mathcal{D}_+ = \{u \in \mathcal{D}_{A^*} : A^*u = iu\}, \quad \dim \mathcal{D}_+ = D_+(A),$$

$$\mathcal{D}_- = \{u \in \mathcal{D}_{A^*} : A^*u = -iu\}, \quad \dim \mathcal{D}_- = D_-(A),$$

Here, $\mathcal{D}_+, \mathcal{D}_-$ are called the **positive and negative deficiency subspaces** corresponding to A .

Theorem 67 $\mathcal{D}_{\overline{A}}, \mathcal{D}_+, \mathcal{D}_-$ are mutually orthogonal closed linear subspaces in \mathcal{D}_{A^*} (with respect to the inner product $\langle \cdot, \cdot \rangle$) and

$$\mathcal{D}_{A^*} = \mathcal{D}_{\overline{A}} \oplus \mathcal{D}_+ \oplus \mathcal{D}_-.$$

PROOF:

1. $\mathcal{D}_+ \perp \mathcal{D}_-$: Let $u_+ \in \mathcal{D}_+, u_- \in \mathcal{D}_-$. Then

$$\begin{aligned} \langle u_+, u_- \rangle &= (u_+, u_-) + (A^*u_+, A^*u_-) = (u_+, u_-) + (iu_+, -iu_-) \\ &= (u_+, u_-) - (u_+, u_-) = 0. \end{aligned}$$

2. $\mathcal{D}_+ \perp \mathcal{D}_{\bar{A}}$: Let $u_+ \in \mathcal{D}_+$, $u \in \mathcal{D}_{\bar{A}}$. Then

$$\begin{aligned} \langle u, u_+ \rangle &= (u, u_+) + (A^*u, A^*u_+) = (u, u_+) - i(\bar{A}u, u_+) \\ &= (u, u_+) - i(u, A^*u_+) = (u, u_+) - (u, u_+) = 0. \end{aligned}$$

Similarly, $\mathcal{D}_- \perp \mathcal{D}_{\bar{A}}$.

3. If $v \perp \mathcal{D}_{\bar{A}}, \mathcal{D}_+, \mathcal{D}_-$ then $v = \theta$: If $u \in \mathcal{D}_{\bar{A}}$ then

$$(\langle u, v \rangle = 0 = (u, v) + (A^*u, A^*v) \implies (u, v) = -(A^*u, A^*v) \implies A^*v \in \mathcal{D}_{A^*},$$

and $A^*A^*v = -v$. Thus

$$(A^* + iE)(A^* - iE)v = \theta \implies (A^* - iE)v \in \mathcal{D}_-.$$

For any $u_- \in \mathcal{D}_-$ we have

$$(u_-, [A^* - iE]v) = (u_-, A^*v) + i(u_-, v) = i(A^*u_-, A^*v) + i(u_-, v) = i \langle u_-, v \rangle = 0.$$

Therefore $[A^* - iE]v = \theta$, so $v \in \mathcal{D}_+$. But $v \perp \mathcal{D}_+$. Hence $v = \theta$.

Q.E.D.

REMARK: Let

$$P_+ = -\frac{i}{2}(A^* + iE), \quad P_- = \frac{i}{2}(A^* - iE).$$

Then

$$1. P_+ + P_- = E.$$

$$2. P_+P_- = P_-P_+ = 0.$$

3.

$$P_+^2 = -\frac{1}{4}(A^* + iE)^2 = -\frac{1}{4}(A^*A^* + 2iA^* - E) = -\frac{i}{2}(A^* + iE) = P_+.$$

Similarly, $P_-^2 = P_-$.

$$4. P_+v = v \implies A^*v = iv \text{ and } P_-v = v \implies A^*v = -iv.$$

$$5. \langle P_{\pm}u, v \rangle = \langle u, P_{\pm}v \rangle \text{ for all } u, v \in \mathcal{D}_{A^*}.$$

Thus, P_{\pm} are orthogonal self-adjoint projection operators on \mathcal{D}_{A^*} , commuting with A^* . Also P_+ projects onto \mathcal{D}_+ and P_- projects onto \mathcal{D}_- .

Let B be a closed symmetric extension of the symmetric operator A . The following observations are pertinent:

1.

$$\mathcal{D}_{\overline{A}} \subseteq \mathcal{D}_B \subseteq \mathcal{D}_{\overline{A}} \oplus \mathcal{D}_+ \oplus \mathcal{D}_- = \mathcal{D}_{A^*}$$

2. If u_+ is a nonzero element of \mathcal{D}_+ then $u_+ \notin \mathcal{D}_B$. Indeed, if $u_+ \in \mathcal{D}_B$ then (Bu_+, u_+) would be a real number. However,

$$(Bu_+, u_+) = (iu_+, u_+) = i\|u_+\|^2 \neq 0$$

is not real. Similarly, a nonzero element of u_- of \mathcal{D}_- cannot belong to \mathcal{D}_B .

3. Which elements of $\mathcal{D}_{\overline{A}} \oplus \mathcal{D}_+ \oplus \mathcal{D}_- = \mathcal{D}_{A^*}$ do belong to \mathcal{D}_B ? If $v \in \mathcal{D}_B$ then it can be expressed uniquely in the form

$$v = u + u_+ + u_-, \quad u \in \mathcal{D}_{\overline{A}}, \quad u_+ \in \mathcal{D}_+, \quad u_- \in \mathcal{D}_-.$$

Let

$$\mathcal{S}_+ = \{u_+ \in \mathcal{D}_+ : v = u + u_+ + u_- \text{ for some } v \in \mathcal{D}_B\}.$$

Then there exists a 1-1 map $C : \mathcal{S}_+ \rightarrow \mathcal{D}_-$ such that $\mathcal{D}_B = \mathcal{D}_{\overline{A}} \oplus \mathcal{S}$, where

$$\mathcal{S} = \{u_+ + Cu_+ : u_+ \in \mathcal{S}_+\}.$$

Indeed, if both $u_+ + u_-$ and $u_+ + u'_-$ belong to \mathcal{D}_B then $u_- - u'_- \in \mathcal{D}_B \cap \mathcal{D}_-$, which implies $u_- - u'_- = \theta$. Thus the map C is 1-1.

Lemma 25 *If A_1 is a closed symmetric extension of A then there exists an isometric (i.e., inner product preserving) map C of a closed subspace \mathcal{D}_C of \mathcal{D}_+ onto a subspace \mathcal{R}_C of \mathcal{D}_- such that $\mathcal{D}_{A_1} = \mathcal{D}_{\overline{A}} \oplus \mathcal{S}$, where*

$$\mathcal{S} = \{u_+ + Cu_+ : u_+ \in \mathcal{D}_C\}.$$

Conversely, if C is such an isometric operator from the closed subspace $\mathcal{D}_C \subseteq \mathcal{D}_+$ to $\mathcal{R}_C \subseteq \mathcal{D}_-$ then the restriction of A^ to $\mathcal{D}_{\overline{A}} \oplus \mathcal{S}$ is a closed symmetric extension of A .*

PROOF: Let $a, b \in \mathcal{D}_{\overline{A}} \oplus \mathcal{S}$ so that

$$a = u + u_+ + Cu_+, \quad b = v + v_+ + Cv_+.$$

Then

$$\begin{aligned} (A_1 a, b) &= (A_1 u + iu_+ - iCu_+, v + v_+ + Cv_+) = \\ &= (A_1 u, v) + (A_1 u, v_+) + (A_1 u, Cv_+) + i(u_+, v) + i(u_+, v_+) \\ &\quad + i(u_+, Cv_+) - i(Cu_+, v) - i(Cu_+, v_+) - i(Cu_+, Cv_+) \\ &= i(u_+, v_+) - i(Cu_+, Cv_+), \\ (a, A_1 b) &= (u + u_+ + Cu_+, A_1 v + iv_+ - iCv_+) = \\ &= (u, A_1 v) + (u_+, A_1 v) + (Cu_+, A_1 v) - i(u, v_+) - i(u_+, v_+) \\ &\quad - i(Cu_+, v_+) + i(u, Cv_+) - i(u_+, Cv_+) + i(Cu_+, Cv_+) \\ &= -i(u_+, v_+) + i(Cu_+, Cv_+). \end{aligned}$$

Hence

$$(A_1 a, b) - (a, A_1 b) = 2i [(u_+, v_+) - (Cu_+, Cv_+)].$$

Thus A_1 is symmetric if and only if C is isometric. Note that $\langle u_+, u_+ \rangle = 2\langle u_+, u_+ \rangle$ and $\langle v_+, v_+ \rangle = 2\langle v_+, v_+ \rangle$. Note further that if A_1 is symmetric then \mathcal{S} must be a closed subspace of \mathcal{D}_{A^*} , in the graph norm. Since C is isometric, it follows that $\mathcal{S}_+ = \mathcal{D}_C$ must also be closed (in both the graph and the usual $\|\cdot\|$ norm). Q.E.D.

Recall that

$$\overline{A} \subseteq A_1 \subseteq A_1^* \subseteq A^*.$$

Lemma 26 *Let C be an isometric map of a closed subspace \mathcal{D}_C of $\text{cal } \mathcal{D}_+$ onto a subspace \mathcal{R}_C of \mathcal{D}_- , and let A_1 be the resulting closed symmetric extension of A . Then $\mathcal{D}_{A_1^*}$ is a closed subspace of \mathcal{D}_{A^*} . let $\mathcal{D}_{\pm}(A_1)$ be the deficiency subspaces of A_1 with decomposition*

$$\mathcal{D}_{A_1^*} = \mathcal{D}_{A_1} \oplus \mathcal{D}_+(A_1) \oplus \mathcal{D}_-(A_1).$$

Then

$$\mathcal{D}_+(A_1) = \{u \in \mathcal{D}_+(A) : \langle u, \mathcal{D}_C \rangle = 0\}, \quad \mathcal{D}_-(A_1) = \{u \in \mathcal{D}_-(A) : \langle u, \mathcal{R}_C \rangle = 0\}. \quad (3.8)$$

PROOF: Clearly $\mathcal{D}_+(A_1) \subseteq \mathcal{D}_+(A)$ and $\mathcal{D}_-(A_1) \subseteq \mathcal{D}_-(A)$. The only part of the lemma remaining to be proved is the characterization (3.8).

1. $u \in \mathcal{D}_+(A_1) \longrightarrow \langle u, \mathcal{D}_C \rangle = 0$: Let $v \in \mathcal{D}_C \subseteq \mathcal{D}_+(A)$. Then $v + Cv \in \mathcal{D}_{A_1}$ implies $u \perp (v + Cv)$ in the graph inner product. Hence

$$\langle u, v + Cv \rangle = 0 = \langle u, v \rangle + \langle u, Cv \rangle = \langle u, v \rangle,$$

since $u \in \mathcal{D}_+$, $Cv \in \mathcal{D}_-$. Similarly $u \in \mathcal{D}_- \implies \langle u, \mathcal{R}_C \rangle = 0$.

2. $u \in \mathcal{D}_+(A)$, $\langle u, \mathcal{D}_C \rangle = 0 \implies u \in \mathcal{D}_+(A_1)$: Here we must show $u \in \mathcal{D}_{A_1}^*$. For this it is enough to show that $(A_1 v, u) = (v, A^*, u)$ for all $v \in \mathcal{D}_{A_1}$. Now

$$\begin{aligned} (A_1 v, u) &= (Aa + ia_+ - iCa_+, u) = (Aa, u) + i(a_+, u) - i(Ca_+, u) \\ &= (a, A^*u) + i(a_+, u) - i(Ca_+, u) = -i(a, u) - i(Ca_+, u). \end{aligned}$$

Similarly,

$$(v, A^*u) = (a + a_+ + Ca_+, iu) = -i(a, u) - i(Ca_+, u).$$

The proof of the statement involving \mathcal{R}_C is similar. Q.E.D.

Theorem 68 *If C is an isometric map of all of \mathcal{D}_+ onto all of \mathcal{D}_- then the restriction A_1 of A^* to $\mathcal{D}_{A_1} \oplus \mathcal{S}$, $\mathcal{S} = \{u + Cu : u \in \mathcal{D}_+\}$ is self-adjoint. Conversely, if A_1 is a self-adjoint extension of A , then there exists a unique isometric map C such that A_1 is obtained as above.*

PROOF: If C maps \mathcal{D}_+ onto \mathcal{D}_- then from Lemma 26

$$\mathcal{D}_{A_1^*} = \mathcal{D}_{A_1} \oplus \{\theta\} \oplus \{\theta\}$$

so $A_1 = A_1^*$. Conversely, if $A_1 = A_1^*$ then

$$\mathcal{D}_+(A_1) = \mathcal{D}_-(A_1) = \{\theta\} \implies \mathcal{D}_C = \mathcal{D}_+, \mathcal{R}_C = \mathcal{D}_-.$$

Q.E.D.

Corollary 19 *A symmetric operator A has self-adjoint extensions if and only if $\dim \mathcal{D}_+ = \dim \mathcal{D}_-$. If this is the case, the possible self-adjoint extensions of A are in 1-1 correspondence with isometric maps C of $\mathcal{D}_+ = \mathcal{D}_C$ onto $\mathcal{D}_- = \mathcal{R}_C$.*

Definition 34 Let \mathcal{M}, \mathcal{N} be vector spaces with $\mathcal{M} \subseteq \mathcal{N}$. We say that \mathcal{M} is of **co-dimension** m in \mathcal{N} if $\mathcal{N} = \mathcal{M} \oplus \mathcal{K}$ where $\dim \mathcal{K} = m$.

Corollary 20 \mathcal{D}_A is of co-dimension $D_+(A) + D_-(A)$ in \mathcal{D}_{A^*} .

Corollary 21 Suppose $D_+(A) = D_-(A) = m$. A symmetric extension A_1 of A is self-adjoint if and only if the co-dimension of \mathcal{D}_A in \mathcal{D}_{A_1} is m .

EXAMPLE: Let

$$A = i \frac{d}{dx}, \quad \mathcal{H} = L_2^c\{[0, 1]\},$$

$$\mathcal{D}_A = \{u(x) : u \text{ absolutely continuous, } Au \in \mathcal{H}, \quad u(0) = u(1) = 0\}.$$

Here, A is symmetric and closed. Further,

$$\mathcal{D}_{A^*} = \{u(x) : u \text{ absolutely continuous, } Au \in \mathcal{H}\}.$$

We will compute \mathcal{D}_\pm for this case. If $A^*u = iu$ then $u(x) = ce^x$. Since $\int_0^1 e^{2x} dx = (e^2 - 1)/2$ we see that $D_+ = 1$ and $\{u_1(x) = \sqrt{\frac{2}{e^2-1}}e^x\}$ in an ON basis for \mathcal{D}_+ . Similarly, $D_- = 1$ and $\{v_1(x) = \sqrt{\frac{2e^2}{e^2-1}}e^{-x}\}$ in an ON basis for \mathcal{D}_- . Define the linear transformation $C_\theta : \mathcal{D}_+ \longrightarrow \mathcal{D}_-$ by

$$C_\theta u_1 = e^{i\theta} v_1, \quad 0 \leq \theta < 2\pi.$$

We see that the possible self-adjoint extensions of A are A_θ , where

$$\mathcal{D}_{A_\theta} = \left\{ v(x) = u(x) + \alpha(e^x + e^{i\theta+1-x}) : u \in \mathcal{D}_A, \alpha \in \mathbb{C} \right\}.$$

Here,

$$A_\theta v(x) = iu'(x) + i\alpha(e^x - e^{i\theta+1-x}), \quad u(0) = u(1) = 0.$$

To characterize the domain of A_θ in a simpler fashion, note that if $v \in \mathcal{D}_{A_\theta}$ then

$$v(0) = \alpha(1 + e^{i\theta+1}), \quad v(1) = \alpha(e + e^{i\theta}),$$

so

$$\frac{v(0)}{v(1)} = \frac{1 + e^{1+i\theta}}{1 + e^{1-i\theta}} e^{-i\theta} = \beta_\theta$$

where $|\beta_\theta| = 1$. Thus $v \in \mathcal{D}_{A_\theta}$ if and only if $v \in \mathcal{D}_{A^*}$ and v satisfies the **boundary condition**

$$B(v) = v(0) - \beta_\theta v(1) = 0, \quad |\beta_\theta| = 1, \quad e^{i\theta} = \frac{\beta_\theta e - 1}{e - \beta_\theta}.$$

REMARK: We can consider $B(v)$ as a bounded linear functional on \mathcal{D}_{A^*} (with respect to the graph inner product). Indeed, we can find a $w_\theta \in \mathcal{D}_{A^*}$ such that $\langle w_\theta, \mathcal{D}_{A_\theta} \rangle = 0$ and normalize it so that $B(v) = \langle w_\theta, v \rangle$. Thus $v \in \mathcal{D}_{A_\theta}$ if and only if $B(v) = \langle w_\theta, v \rangle = 0$. We will exploit this point of view in the next chapter.

We conclude this section with a result that illustrates the wide variety of possible spectra for the self-adjoint extensions of a symmetric operator A with $D_+ = D_- > 0$.

Theorem 69 *Let A be a symmetric operator with deficiency indices $D_+ = D_- = m > 0$ and let λ be a real number such that $\lambda \in \text{Reg}(A)$. Then there exists a self-adjoint extension \tilde{A} of A such that $\lambda \in \sigma_P(\tilde{A})$ with multiplicity m .*

PROOF: Let $\mathcal{D}_\lambda = \{u \in \mathcal{H} : A^*u = \lambda u\}$. From Theorem 60 we know that $\dim \mathcal{D}_\lambda = D_+ = D_- = m$. Let

$$\mathcal{D}_{\tilde{A}} = \mathcal{D}_A \oplus \mathcal{D}_\lambda \subseteq \mathcal{D}_{A^*},$$

(we know that this sum is direct, since $\lambda \notin \sigma_P(A)$), and let \tilde{A} be the restriction of A^* to $\mathcal{D}_{\tilde{A}}$.

We show that \tilde{A} is symmetric. For any $u, v \in \mathcal{D}_{\tilde{A}}$ we have the unique decompositions $u = u_0 + u_\lambda$, $v = v_0 + v_\lambda$ where $u_0, v_0 \in \mathcal{D}_A$ and $u_\lambda, v_\lambda \in \mathcal{D}_\lambda$. Then

$$\begin{aligned} (\tilde{A}u, v) &= (Au_0 + \lambda u_\lambda, v_0 + v_\lambda) \\ &= (Au_0, v_0) + (A^*u_\lambda, v_0) + \lambda(u_\lambda, v_\lambda) + (Au_0, v_\lambda) \\ &= (Au_0, v_0) + (u_\lambda, Av_0) + \lambda(u_\lambda, v_\lambda) + (Au_0, v_\lambda), \end{aligned}$$

and

$$\begin{aligned} (u, \tilde{A}v) &= (u_0 + u_\lambda, Av_0 + A^*v_\lambda) \\ &= (u_0, Av_0) + (u_\lambda, Av_0) + (u_0, A^*v_\lambda) + (u_\lambda, A^*v_\lambda) \\ &= (Au_0, v_0) + (u_\lambda, Av_0) + (Au_0, v_\lambda) + \lambda(u_\lambda, v_\lambda), \end{aligned}$$

so $(\tilde{A}u, v) = (u, \tilde{A}v)$. Further \tilde{A} is self-adjoint because the co-dimension of \mathcal{D}_A in $\mathcal{D}_{\tilde{A}}$ is m . Q.E.D.

3.8.1 Symmetric operators bounded below

In this section we show that if A is symmetric and bounded below by the real number a then we can directly construct a certain self-adjoint extension \tilde{A} of A , called the Friedrichs extension, that is also bounded below by a .

We first consider the case that $a > 0$.

Theorem 70 *let A be a symmetric, strictly positive operator with lower bound $a > 0$. Then there exists a self-adjoint operator \tilde{A} such that*

1. $\tilde{A} \supseteq A$
2. \tilde{A}^{-1} exists and is bounded in \mathcal{H}
3. a is the greatest lower bound of \tilde{A} .

Note that the equation $\tilde{A}u = v$ can always be solved for $v \in \mathcal{H}$.

PROOF: We will embed \mathcal{D}_A in a new Hilbert space \mathcal{F} . We first introduce a new inner product $(u, v)' = (Au, v)$, defined for all $u, v \in \mathcal{D}_A$. The new norm is $\|u\|' = \sqrt{(u, u)'} = \text{sqrt}(Au, u)$. Note that

$$(\|u\|')^2 = (Au, u) \geq a(u, u) = a\|u\|^2.$$

Thus $\|u\| \leq \frac{1}{\sqrt{a}}\|u\|'$. We see that \mathcal{D}_A with inner product $(\cdot, \cdot)'$ is a pre-Hilbert space \mathcal{D}'_A . We can complete this space to get a (unique) Hilbert space \mathcal{F} since that (with respect to the norm $\|\cdot\|'$) \mathcal{D}'_A is dense in \mathcal{F} .

REMARKS:

1. Since $\|u - v\| \leq \frac{1}{\sqrt{a}}\|u - v\|'$, every Cauchy sequence in \mathcal{D}_A (with respect to $\|\cdot\|'$) is a Cauchy sequence with respect to $\|\cdot\|$.
2. Suppose $\{u_n : u_n \in \mathcal{D}_A\}$ is a Cauchy sequence with respect to $\|\cdot\|'$ and $u_n \xrightarrow{\prime} u^* \in \mathcal{F}$. Then also $u_n \rightarrow v \in \mathcal{H}$ in the $\|\cdot\|$ norm. However,

$$\|u_n - u^*\| \leq \frac{1}{\sqrt{a}}\|u_n - u^*\|' \rightarrow 0$$

as $n \rightarrow \infty$. Thus $v = u^*$.

3. Suppose $\{u_n : u_n \in \mathcal{D}_A\}$ is a Cauchy sequence in \mathcal{D}'_A such that $\lim_{n \rightarrow \infty} \|u_n\|' \neq 0$. Then $u_n \longrightarrow' v^* \in \mathcal{F}$ with $v^* \neq \theta$ and, also $u_n \longrightarrow v \in \mathcal{H}$. Can $v = \theta$? No, because if $v = \theta$ then

$$(u, v^*)' = \lim_{n \rightarrow \infty} (u, u_n)' = \lim_{n \rightarrow \infty} (Au, u_n) = (Au, v) = 0$$

for all $u \in \mathcal{D}_A$, which implies $v^* = \theta$, a contradiction.

4. It follows that we can assign to each $v^* \in \mathcal{F}$ a unique $v \in \mathcal{H}$ and this correspondence is linear.
5. The correspondence

$$\begin{array}{ccc} \mathcal{F} & \longrightarrow & \mathcal{H} \\ v^* & \longrightarrow & v \end{array}$$

of \mathcal{F} into \mathcal{H} is 1-1 and $u \longrightarrow u$ for $u \in \mathcal{D}_A$. Therefore, we can identify \mathcal{F} with a dense subspace \mathcal{H}_0 of \mathcal{H} .

6. For $u \in \mathcal{H}_0$, $v \in \mathcal{H}$ we have

$$|(u, v)| \leq \|u\| \cdot \|v\| \leq \frac{1}{\sqrt{a}} \|v\| \cdot \|u\|'.$$

Therefore $L_v(u) = (u, v)$ is a bounded linear functional on $\mathcal{H}_0 \cong \mathcal{F}$. From the Riesz representation theorem, there exists a unique $w \in \mathcal{H}_0$ such that

$$L_v(u) = (u, v) = (u, w)'.$$

Denote this correspondence $v \longrightarrow w$ by $w = Bv$. Clearly, B is a linear operator with domain \mathcal{H} and range in \mathcal{H}_0 . If $Bv = \theta$ then $(u, v) = 0$ for all $u \in \mathcal{H}_0$ which implies $v = \theta$. Therefore B is 1-1. Set $\tilde{A} = B_1$. Then $\mathcal{D}_{\tilde{A}} \subseteq \mathcal{H}_0$ and $\mathcal{R}_{\tilde{A}} = \mathcal{H}$.

7. We show that B is bounded and symmetric in \mathcal{H} . Note that $(u, v) = (u, Bv)'$ for $u \in \mathcal{H}_0$, $v \in \mathcal{H}$. Define $v_0 \in \mathcal{H}$ by $u = Bv_0$.

SYMMETRY:

$$\begin{aligned} (Bv_0, v) &= (u, v) = (u, Bv)' = (Bv_0, Bv)' = \overline{(Bv, Bv_0)'} \\ &= \overline{(Bv, v_0)} = (v_0, Bv). \end{aligned}$$

BOUNDEDNESS:

$$|L_v(u)| = |(u, w)'| \leq \|u\|' \cdot \|w\|'$$

for a unique $w \in \mathcal{H}_0$. Here, $\|w\|'$ is the best bound. Aso,

$$|L_v(u)| = |(u, v)| \leq \|u\| \cdot \|v\| \leq \frac{1}{\sqrt{a}} \|u\|' \cdot \|v\|.$$

Therefore

$$\frac{\|v\|}{\sqrt{a}} \geq \|w\|' \geq \sqrt{a}\|w\| \implies \frac{\|v\|}{\sqrt{a}} \geq \|Bv\|' \geq \sqrt{a}\|Bv\|.$$

This proves that $\|B\| \leq 1/a$.

8. \tilde{A} is self-adjoint.

9. \tilde{A} is an extension of A . Indeed for $u, v \in \mathcal{D}_A \subseteq \mathcal{H}_0 \subseteq \mathcal{H}$ we have

$$(u, BAv)' = (u, Av) = (Au, v) = (u, v)'$$

so $BAv = v$. Hence $\tilde{A}^{-1}Av = v$ for all $v \in \mathcal{D}_A \implies v \in \mathcal{R}_{\tilde{A}^{-1}} = \mathcal{D}_{\tilde{A}}$
 $\implies v \in \mathcal{D}_{\tilde{A}}$. Therefore $Av = \tilde{A}v$ for all $v \in \mathcal{D}_A$.

10. \tilde{A} is bounded below by a . For suppose $u \in \mathcal{D}_{\tilde{A}}$, $\tilde{A}u = v$, $Bv = u$.
Then

$$(\tilde{A}u, u) = (u, \tilde{A}u) = (Bv, v) = (Bv, Bv)' = (\|Bv\|')^2 \geq a\|Bv\|^2 = a\|u\|^2.$$

Q.E.D.

Corollary 22 *If A is symmetric and bounded below by a real number a then there exists a self-adjoint operator \tilde{A} such that*

1. $\tilde{A} \supseteq A$
2. \tilde{A} is bounded below by a .

PROOF: We need consider only the case $a \leq 0$. Set $C = A + (1 - a)E$. Then C is symmetric and bounded below by 1. The preceding theorem implies that C has a self-adjoint extension \tilde{C} bounded below by 1. Set $\tilde{A} = \tilde{C} - (1 - a)E$.
Q.E.D.

Chapter 4

Spectral Theory for Second-order Ordinary Differential Operators

In this chapter we will apply the general spectral theory for self-adjoint operators to the physically relevant case where the eigenvalue equations are second-order ODEs. We will work out the explicit details of the spectral expansions for a number of important examples. Since the deficiency subspaces for a second-order symmetric OD operator are of dimension at most 2, we can give a rather complete analysis of the self-adjoint extensions. This is in contrast to the case of partial differential operators where the deficiency subspaces may be infinite-dimensional.

4.1 The setting for the second-order ODE eigenvalue problem

Definition 35 *Let I be an interval on the real line, either $[\ell, m]$, or $[\ell, m)$, or $(\ell, m]$ or (ℓ, m) , where $\ell = -\infty$ and $m = \infty$ are also allowed. A **formal second-order ordinary differential operator** τ on I is an expression*

$$\tau = a_2(x) \frac{d^2}{dx^2} + a_1(x) \frac{d}{dx} + a_0(x), \quad a_j(x) \in C^2(I).$$

Here the a_j are complex-valued functions and $a_2(x) \neq 0$ for any $x \in I$.

Definition 36

$$H^2(I) = \left\{ f \in C^1(I) : f' \text{ absolutely continuous on each compact sub-interval of } I \right\}$$

Theorem 71 *Let g be complex-valued, measurable and locally integrable on I , let c_0, c_1 be complex numbers and $x_0 \in I$. Then there exists a unique $f \in H^2(I)$ such that*

1. $\tau f = g$,
2. $f(x_0) = c_0, \quad f'(x_0) = c_1$.

PROOF: From the definition of $H^2(I)$ there is no loss of generality in the proof by assuming I is closed and bounded. Our original equation $\tau f = g$ is equivalent to the first-order system

$$\begin{aligned} \frac{df_0}{dx}(x) &= f_1(x) \\ \frac{df_1}{dx}(x) + \frac{a_1(x)}{a_2(x)}f_1(x) + \frac{a_0(x)}{a_2(x)}f_0(x) &= \frac{g(x)}{a_2(x)}. \end{aligned} \tag{4.1}$$

Now let

$$\begin{aligned} \mathbf{f}(x) &= \begin{bmatrix} f_0(x) \\ f_1(x) \end{bmatrix}, \quad \mathbf{g}(x) = \begin{bmatrix} 0 \\ \frac{g(x)}{a_2(x)} \end{bmatrix}, \\ \mathcal{A}(x) &= \begin{bmatrix} 0 & 1 \\ \frac{a_0(x)}{a_2(x)} & \frac{a_1(x)}{a_2(x)} \end{bmatrix}. \end{aligned}$$

Then system (4.1) and the initial conditions can be written in the matrix form

$$\mathbf{f}'(x) = \mathcal{A}(x)\mathbf{f}(x) + \mathbf{g}(x), \quad \mathbf{f}(x_0) = \begin{bmatrix} c_0 \\ c_1 \end{bmatrix}. \tag{4.2}$$

By the Fundamental Theorem of Calculus (generalized to L^1), this is in turn equivalent to the matrix integral system

$$\mathbf{f}(x) + \int_{x_0}^x \mathcal{A}(y)\mathbf{f}(y) dy = \int_{x_0}^x \mathbf{g}(y) dy + \mathbf{f}(x_0), \tag{4.3}$$

or

$$\mathbf{f}(x) + \int_{x_0}^x \mathcal{A}(y)\mathbf{f}(y) dy = \mathbf{k}(x)$$

where $\mathbf{k}(x) = \int_{x_0}^x \mathbf{g}(y) dy + \mathbf{f}(x_0)$. Finally, if we define the matrix integral operator A on vectors

$$\mathbf{h}(x) = \begin{bmatrix} h_0(x) \\ h_1(x) \end{bmatrix}$$

by

$$A\mathbf{h}(x) = \int_{x_0}^x \mathcal{A}(y)\mathbf{h}(y) dy$$

the system takes the form

$$(E + A)\mathbf{f} = \mathbf{k}, \quad (4.4)$$

where $E\mathbf{h}(x) = \mathbf{h}(x)$.

Now (4.4) is a Volterra equation of the second kind and always has a unique solution. Formally, the solution can be written as

$$\mathbf{f} = (E + A)^{-1}\mathbf{k} = \mathbf{k} - A\mathbf{k} + A^2\mathbf{k} - \cdots + (-1)^n A^n \mathbf{k} + \cdots.$$

In fact

$$(E + A)^{-1}\mathbf{k} = \sum_{n=0}^{\infty} (-1)^n A^n \mathbf{k}$$

converges uniformly and absolutely on I to a vector-valued function that is the solution to our problem. To show this we will make use of the matrix norm $|\mathcal{A}(y)|$ and the vector space norm $|\mathbf{h}(y)| = \sqrt{|h_0(y)|^2 + |h_1(y)|^2}$, each evaluated for a fixed y , and the associated Banach space norm on vector-valued functions $\|\mathbf{h}\| = \int_I |\mathbf{h}(y)| dy$. (We need the standard property $|\mathcal{A}(y)\mathbf{h}(y)| \leq |\mathcal{A}(y)| \cdot |\mathbf{h}(y)|$.) Let $a = \sup_{y \in I} |\mathcal{A}(y)|$. Then

$$|A\mathbf{k}(x)| = \left| \int_{x_0}^x \mathcal{A}(y)\mathbf{k}(y) dy \right| \leq \int_{x_0}^x |\mathcal{A}(y)\mathbf{k}(y)| dy \leq a \int_{x_0}^x |\mathbf{k}(y)| dy$$

$$\leq a \int_I |\mathbf{k}(y)| dy = a \|\mathbf{k}\|,$$

$$|A^2\mathbf{k}(x)| = \left| \int_{x_0}^x \mathcal{A}(y)A\mathbf{k}(y) dy \right| \leq a \int_{x_0}^x a \|\mathbf{k}\| dy = a^2 \|\mathbf{k}\| (x - x_0),$$

$$|A^3\mathbf{k}(x)| = \left| \int_{x_0}^x \mathcal{A}(y)A^2\mathbf{k}(y) dy \right| \leq a \int_{x_0}^x a^2 \|\mathbf{k}\| (y - x_0) dy = a^3 \|\mathbf{k}\| \frac{(x - x_0)^2}{2},$$

$\dots,$

$$|A^n\mathbf{k}(x)| = \left| \int_{x_0}^x \mathcal{A}(y)A^n\mathbf{k}(y) dy \right| \leq a^n \|\mathbf{k}\| \frac{(x - x_0)^{n-1}}{(n-1)!},$$

...

Thus,

$$\left| \sum_{n=n_0}^{n_1} (-1)^n A^n \mathbf{k}(x) \right| \leq \sum_{n=n_0}^{n_1} a^n \|\mathbf{k}\| \frac{(x-x_0)^{n-1}}{(n-1)!}$$

and the right-hand side converges uniformly in I . Q.E.D.

Corollary 23 *If $g \in C^0(I)$ then $f \in C^2(I)$.*

Now we define a basic (minimal) symmetric operator A_0 related to a (formally symmetric) operator τ . The possible self-adjoint operators related to τ will be extensions of A_0 .

ASSUMPTIONS:

$$\tau u(x) = \frac{1}{k(x)} ([-p(x)u'(x)]' + q(x)u(x)), \quad \mathcal{H} = L_c^2(\{\ell, m\}, k), \quad (4.5)$$

and

1. $I = \{\ell, m\}$ an interval on the real line
2. $p, p', q, k \in C^0(I)$ and real
3. $p(x) > 0, k(x) > 0$ in I .

The operators A_0, A_1 are determined by

$$\mathcal{D}_{A_0} = \left\{ u : u \in \overset{o}{C}^2(I) \right\}, \quad A_0 u = \tau u, \quad u \in \mathcal{D}_{A_0}, \quad (4.6)$$

$$\mathcal{D}_{A_1} = \left\{ u \in \mathcal{H} : u \in H^2(I) \text{ and } \tau u \in \mathcal{H} \right\}, \quad A_1 u = \tau u, \quad u \in \mathcal{D}_{A_1}, \quad (4.7)$$

Here, we have chosen τ in the most general form so that it will be formally symmetric, i.e., it will be symmetric if all of the boundary terms vanish in the integration by parts. This is exactly what occurs for the minimal operator A_0 .

Theorem 72 *A_0 is symmetric and $A_0^* = A_1$.*

The first statement in the theorem is easy, but the second relies on the Weyl lemma, which we will prove in detail.

Lemma 27 (Weyl) *Let v be a measurable complex-valued function on I such that v is square integrable over every compact subinterval of I . Suppose*

$$\int_I v(y) \overline{\tau u(y)} k(y) dy = (v, \tau u) = 0$$

for all $u \in \mathcal{D}_{A_0}$, i.e., $u \in \overset{o}{C}^2(I)$. Then (after modification on a set of measure zero) $v \in C^2(I)$ and $\tau v = 0$.

PROOF: There is no loss of generality in assuming the I is compact. Let Σ be the set of all solutions σ of the equation $\tau\sigma = 0$, $\sigma \in C^2(I)$. From Theorem 71 it follows that $\dim \Sigma = 2$, so that Σ is a closed subspace of \mathcal{H} . The Weyl lemma will follow from a string of three subordinate lemmas.

Lemma 28 *If $w \in \mathcal{H}$, $w \perp \Sigma$ then $(w, v) = 0$.*

REMARK: Lemma 28 shows that

$$v \in (\Sigma^\perp)^\perp = \overline{\Sigma} = \Sigma,$$

since Σ is closed.

Lemma 29 *$\mathcal{D}_{A_0} \cap \Sigma^\perp$ is dense in Σ^\perp .*

Lemma 30 *If $g \in \mathcal{D}_{A_0}$ and $g \perp \Sigma$ then $(g, v) = 0$.*

REMARK: Lemmas 29 and 30 prove lemma 28.

PROOF OF LEMMA 29: \mathcal{D}_{A_0} is dense in \mathcal{H} . let σ_1, σ_2 be an ON basis for Σ and choose $\phi_1, \phi_2 \in \mathcal{D}_{A_0}$ such that the 2×2 matrix $\{B_{ij} = (\phi_i, \sigma_j)\}$ is nonsingular.

Let $h \in \Sigma^\perp$. Choose a Cauchy sequence $\{h_n\}$ in \mathcal{D}_{A_0} such that $h_n \rightarrow h$. We will construct a sequence $\{k_n\}$ in $\mathcal{D}_{A_0} \cap \Sigma^\perp$ such that $k_n \rightarrow h$. Write $k_n = h_n - \sum_{\ell=1}^2 \alpha_{n\ell} \phi_\ell$ and choose $\{\alpha_{n\ell}\}$ such that $(k_n, \sigma_j) = 0$, $j = 1, 2$. This gives 2 equations in 2 unknowns for each n . The solution is

$$k_n = h_n - \sum_{i,j=1}^2 (B^{-1})_{ij} (h_n, \sigma_i) \phi_j \in \mathcal{D}_{A_0} \cap \Sigma^\perp.$$

Indeed,

$$(k_n, \sigma_1) = (h_n, \sigma_1) - \sum_{i,j} (B^{-1})_{ij} B_{j1}(h_n, \sigma_1) = 0,$$

with a similar result for (k_n, σ_2) . Now

$$k_n \longrightarrow_{n \rightarrow \infty} h - \sum (B^{-1})_{ij} (h, \phi_i) \phi_j = h.$$

Q.E.D.

PROOF OF LEMMA 30. If $g \in \mathcal{D}_{A_0} \cap \Sigma^\perp$ then $(g, v) = 0$. If there exists a $w \in \mathcal{D}_{A_0}$ such that $\tau w = g$ Then

$$(v, g) = \int_I v \bar{g} k(x) dx = \int_I v \overline{\tau w} k(x) dx = 0.$$

We can prove the lemma if we can find w . recall that we can assume without loss of generality that $I = [\ell, m]$. From Theorem 71 there exists a unique solution w of $\tau w = g$ such that $w(\ell) = w'(ell) = 0$. We must verify that $w \in \mathcal{D}_{A_0}$. Clearly $w \in C^2(I)$. Then foe all $\sigma \in \Sigma$ (the nullspace of τ) we have

$$\begin{aligned} 0 &= \int_\ell^m (\tau \sigma) \bar{w} k dx = \int_\ell^m \sigma \overline{\tau w} k dx + p(m)(\sigma(m) \overline{w'(m)} - \sigma'(m) \overline{w(m)}) \\ &= p(m)(\sigma(m) \overline{w'(m)} - \sigma'(m) \overline{w(m)}). \end{aligned}$$

Since $p(m) \neq 0$ and $\sigma(m), \sigma'(m)$ are arbitrary, we must have $w(m) = w'(m) = 0$, so $w \in \mathcal{D}_{A_0}$. Q.E.D.

PROOF OF THEOREM 72: We must show $A_0^* = A_1$.

1. $A_1 \subseteq A_0^*$: If $w \in \mathcal{D}_{A_1}$ then for all $u \in \mathcal{D}_{A_0}$ we have

$$\int_I (\tau u) \bar{w} k dx = \int_I u \overline{\tau w} k dx$$

so $w \in \mathcal{D}_{A_0^*}$ with $A_0^* w = \tau w$.

2. $A_0^* \subseteq A_1$: Let $f \in \mathcal{D}_{A_0^*}$ with $A_0^* f = g$. Then $(A_0 u, f) = (u, A_0^* f) = (u, g)$ for all $u \in \mathcal{D}_{A_0}$. From Theorem 71 there is a $f_0 \in H^2(I)$ such that $\tau f_0 = g$. Therefore

$$\int_I (\tau u) \bar{f} k dx = (u, g) = \int_I u \overline{\tau f_0} k dx = \int_I (\tau u) \bar{f}_0 k dx$$

for all $u \in \mathcal{D}_{A_0}$. This implies

$$\int_I (f_0 - f) \overline{\tau u} k \, dx = 0$$

for all $u \in \mathcal{D}_{A_0}$. Therefore (by the Weyl Lemma) $f_0 - f = h \in C^2(I)$ and $\tau(f_0 - f) = 0$.

This means that $f \in H^2(I)$ and $\tau f = \tau f_0$. We conclude that $f \in \mathcal{D}_{A_1}$ and $A_0^* f = A_1 f = \tau f$. Q.E.D.

At this point we know that

$$A_0^* = A_1, \quad \mathcal{D}_{A_1} = \mathcal{D}_{\overline{A_0}} \oplus \mathcal{D}_+ \oplus \mathcal{D}_-$$

where

$$\mathcal{D}_\pm = \{u \in \mathcal{D}_{A_1} : \tau u = \pm iu\},$$

and \mathcal{D}_\pm consists of C^2 functions. Recall that $D_\pm = \dim \mathcal{D}_\pm$.

Corollary 24 $D_+ \leq 2, D_- \leq 2$.

Corollary 25 *If $I = [\ell, m]$ is closed and bounded then every solution of $\tau u = \pm iu$ is in \mathcal{D}_{A_1} . Thus in this case $D_+ = D_- = 2$ and A_0 has infinitely many self-adjoint extensions.*

Corollary 26 *Since the coefficients of τ are real, we have $D_+ = D_-$ in all cases. This means that A_0 always has self-adjoint extensions.*

PROOF: The solutions of $\tau u = iu$ are complex conjugates of the solutions of $\tau u = -iu$. Indeed, $\mathcal{D}_- = \{\overline{u(x)} : u(x) \in \mathcal{D}_+\}$. Therefore A_0 has deficiency indices $D_+ = D_- = 0, 1, 2$. Q.E.D.

We know that

$$\mathcal{D}_{A_1} = \mathcal{D}_{\overline{A_0}} \oplus \mathcal{D}_+ \oplus \mathcal{D}_-$$

where \mathcal{D}_{A_1} has co-dimension $2d$ in \mathcal{D}_{A_1} and $D_+ = D_- = d = 0, 1, 2$. Further, any self-adjoint extension A of A_0 takes the form

$$\mathcal{D}_A = \mathcal{D}_{\overline{A_0}} \oplus \mathcal{S}, \quad \mathcal{S} = \{u + Cu : u \in \mathcal{D}_+\}$$

where C is an isometry of \mathcal{D}_+ onto \mathcal{D}_- , $\mathcal{D}_{\overline{A_0}}$ has co-dimension d in \mathcal{D}_A and \mathcal{D}_A has co-dimension d in \mathcal{D}_{A_1} . Now we describe a convenient method for specifying A . Let

$$\mathcal{S}^\perp = \{v \in \mathcal{D}_{A_1} : \langle v, \mathcal{D}_A \rangle = 0\}.$$

Clearly, $\dim \mathcal{S}^\perp = d$ and $\mathcal{S}^\perp \subseteq \mathcal{D}_+ \oplus \mathcal{D}_-$.

Lemma 31 $\mathcal{S}^\perp = \{u - Cu : u \in \mathcal{D}_+\}$.

PROOF: Let $\mathcal{M} = \{v - Cv : u \in \mathcal{D}_+\}$. Then if $u, v \in \mathcal{D}_+$ we have

$$\begin{aligned} \langle u + Cu, v - Cv \rangle &= \langle u, v \rangle + \langle Cu, -Cv \rangle = \langle u, v \rangle - \langle Cu, Cv \rangle \\ &= \langle u, v \rangle - \langle u, v \rangle = 0. \end{aligned}$$

Thus $\mathcal{M} \subseteq \mathcal{S}^\perp$. However, $\dim \mathcal{M} = d = \dim \mathcal{S}^\perp$, so $\mathcal{M} = \mathcal{S}^\perp$. Q.E.D.

Let v_1, \dots, v_d be an ON basis for \mathcal{S}^\perp , with respect to the graph inner product. Then $\mathcal{D}_A = \{u \in \mathcal{D}_{A_1} : \langle u, \mathcal{S}^\perp \rangle = 0, \text{ i.e.,}$

$$\mathcal{D}_A = \{u \in \mathcal{D}_{A_1} : \langle u, v_j \rangle = 0, \quad j = 1, \dots, d\}.$$

We call each of the conditions $\langle u, v_j \rangle = 0$ a **boundary condition** for A , and we characterize \mathcal{D}_A by these boundary conditions.

4.2 The theory of boundary values

Definition 37 *A boundary value for tau on I is a bounded linear functional B on the Hilbert space \mathcal{D}_{A_1} that vanishes on \mathcal{D}_{A_0} (and therefore on $\mathcal{D}_{A_0}^\perp$).*

REMARK: B is a boundary value for $\tau \iff$ there exists a unique $v \in \mathcal{D}_+ \oplus \mathcal{D}_-$ such that $B(u) = \langle u, v \rangle$, for all $u \in \mathcal{D}_{A_1}$.

Suppose $I = \{\ell, m\}$.

Definition 38 *B is a boundary value at ℓ if B vanishes on all functions in \mathcal{D}_{A_1} that are zero in a neighborhood of ℓ .*

There is a similar definition for a boundary value at m .

Theorem 73 *Let B_1, \dots, B_d be d linearly independent boundary values on I such that*

$$(A_1 u, v) = (u, A_1 v)$$

for all $u, v \in \mathcal{J}$, where

$$\mathcal{J} = \{u \in \mathcal{D}_{A_1} : B_k(u) = 0, \quad k = 1, \dots, d\}.$$

Then the restriction of A_1 to \mathcal{J} is self-adjoint.

We can be more specific concerning the form of boundary values for ODEs. If B is a boundary value for τ on I then, from the general theory, there exists a $v \in \mathcal{D}_+ \oplus \mathcal{D}_- \subseteq C^2(I)$ such that $B(u) = \langle u, v \rangle$, for all $u \in \mathcal{D}_{A_1}$. Now since

$$B(u) = (u, v) + (A_1 u, A_1 v) = 0$$

for all $u \in \mathcal{D}_{A_0}$, we have $A_1 v \in \mathcal{D}_{A_1}$ and $A_1 A_1 v = -v$, i.e., $\tau \tau v = -v$. Let $\tilde{v} = -\tau v$, so $\tau \tilde{v} = v$. Then for any $u \in \mathcal{D}_{A_1}$ we have

$$\begin{aligned} B(u) &= (u, \tau \tilde{v}) - (\tau u, \tilde{v}) = \lim_{r \rightarrow \ell, s \rightarrow m} \int_r^s (u \overline{\tau \tilde{v}} - (\tau u) \overline{\tilde{v}}) dx. \\ &= \lim_{x \rightarrow m} \rho(x) \left(u(x) \overline{\tilde{v}'(x)} - u'(x) \overline{\tilde{v}(x)} \right) - \lim_{x \rightarrow \ell} \rho(x) \left(u(x) \overline{\tilde{v}'(x)} - u'(x) \overline{\tilde{v}(x)} \right) \\ &= [u, \tilde{v}]_m - [u, \tilde{v}]_\ell \end{aligned}$$

where the symbols $[u, \tilde{v}]_m$, $[u, \tilde{v}]_\ell$ are defined by the obvious limits.

Lemma 32

$$u \in \mathcal{D}_{\overline{A_0}} \iff [u, w]_m = [u, w]_\ell = 0$$

for all $w \in \mathcal{D}_{A_1}$.

PROOF:

1. \Leftarrow : Easy.
2. \Rightarrow : If $u \in \mathcal{D}_{\overline{A_0}}$ we have $(\overline{A_0} u, w) = (u, A_1 w)$ for all $w \in \mathcal{D}_{A_1} = \mathcal{D}_{\overline{A_0}}$. Thus $\int_I (\tau u) \overline{w} k \, dx = \int_I u \overline{\tau w} k \, dx$ so

$$[u, w]_\ell - [u, w]_m = 0,$$

for all $w \in \mathcal{D}_{A_1}$. Now let $s \in C^2(I)$ with compact support such that $s \equiv 0$ for x in a neighborhood of $x = \ell$ and $s \equiv 1$ in a neighborhood of $x = m$. Then $sw \in \mathcal{D}_{A_1}$ and $[u, sw]_\ell = 0$, $[u, sw]_m = [u, w]_m$. Thus if $u \in \mathcal{D}_{\overline{A_0}}$ we must have $0 = [u, sw]_\ell - [u, sw]_m = -[u, w]_m$. Similarly $[u, w]_\ell = 0$.

Q.E.D.

REMARKS:

1. If, say, $m \in I$, i.e., $I = \{\ell, m\}$, then

$$[u, \tilde{v}]_m = \rho(m) \left(u(m) \overline{\tilde{v}'(m)} - u'(m) \overline{\tilde{v}(m)} \right) = a_1 u(m) + a_2 u'(m).$$

2. If $B(u) = \langle u, v \rangle$ is a boundary value at, say, m then $[u, \tilde{v}]_\ell = 0$ for all $u \in \mathcal{D}_{A_1}$. PROOF: Let $s \in C^2(I)$ with compact support and such that $s \equiv 0$ in a neighborhood of m and $s \equiv 1$ in a neighborhood of ℓ . Now for $u \in \mathcal{D}_{A_1}$ we have also that $su, (1-s)u \in \mathcal{D}_{A_1}$ and $u = su + (1-s)u$. Since B is a boundary value at m we have

$$\begin{aligned} B(u) &= B(su) + B((1-s)u) = B((1-s)u) \\ &= [(1-s)u, \tilde{v}]_m - [(1-s)u, \tilde{v}]_\ell = [(1-s)u, \tilde{v}]_m. \end{aligned}$$

Q.E.D.

Theorem 74 *The space M of boundary values is $2d$ -dimensional and is the direct sum of the subspaces M_ℓ, M_m of boundary values at ℓ and m : $M = M_\ell \oplus M_m$.*

PROOF: Choose $s_1, s_2 \in C^2(I)$ such that each function has compact support on the real line and

1. $s_1 + s_2 \equiv 1$ on I
2. $s_1 \equiv 0$ in a neighborhood of m
3. $s_2 \equiv 0$ in a neighborhood of ℓ .

Let B be a boundary value: $B(u) = \langle u, v \rangle$, for all $u \in \mathcal{D}_{A_1}$. Here, $v = u_+ + u_- \in \mathcal{D}_+ \oplus \mathcal{D}_-$. Recall that $\tilde{v} = -Cv = -i(u_+ - u_-) \in \mathcal{D}_+ + \mathcal{D}_-$. Now $\tilde{v} = s_1 \tilde{v} + s_2 \tilde{v}$. Since $\mathcal{D}_{A_1} = \mathcal{D}_{\overline{A_0}} \oplus \mathcal{D}_+ \oplus \mathcal{D}_-$, we have the unique decompositions

$$s_1 \tilde{v} = u_1 + \tilde{v}_1, \quad s_2 \tilde{v} = u_2 + \tilde{v}_2, \quad u_1, u_2 \in \mathcal{D}_{\overline{A_0}}, \quad \tilde{v}_1, \tilde{v}_2 \in \mathcal{D}_+ + \mathcal{D}_-.$$

Then

$$\tilde{v} - \tilde{v}_1 - \tilde{v}_2 = u_1 + u_2$$

where the left-hand side belongs to $\mathcal{D}_+ + \mathcal{D}_-$ and the right-hand side belongs to $\mathcal{D}_{\overline{A_0}}$. Therefore, $u_1 = -u_2$, $\tilde{v} = \tilde{v}_1 + \tilde{v}_2$, and the last equality holds if and only if $v = v_1 + v_2$. Therefore

$$B(u) = \langle u, v \rangle = \langle u, v_1 \rangle + \langle u, v_2 \rangle = B_1(u) + B_2(u).$$

I claim that B_1 is a boundary value at ℓ . Indeed,

$$B_1(u) = \langle u, v_1 \rangle = [u, \tilde{v}_1]_m - [u, \tilde{v}_1]_\ell$$

and $\tilde{v}_1 = s_1 \tilde{v} - u_1$, where $u_1 \in \mathcal{D}_{\overline{A_0}}$. Now for all $u \in \mathcal{D}_{A_1}$ we have

$$[u, \tilde{v}_1]_m = [u, s_1 \tilde{v}]_m - [u, u_1]_m = 0 - 0 = 0,$$

so $B_1(u) = [u, -\tilde{v}_1]_\ell$. Similarly, B_2 is a boundary value at m . This decomposition is unique, because if $B \in M_\ell \cap M_m$ then $B(u) = [u, \tilde{v}]_m - [u, \tilde{v}]_\ell = 0 - 0 = 0$. Q.E.D.

REMARKS:

1. The most general boundary value at m is of the form

$$B_m(u) = [u, \tilde{v}]_m, \quad \tilde{v} \in \mathcal{D}_+ \oplus \mathcal{D}_-.$$

Similarly the most general boundary value at ℓ is of the form $B_\ell(u) = [u, \tilde{v}]_\ell$.

2. If $v_0 \in \mathcal{D}_{\overline{A_0}}$ then $v_0(\ell) = v'_0(\ell) = v_0(m) = v'_0(m) = 0$.
3. Suppose $I = [\ell, m]$, i.e., $\ell \in I$. Then

$$[u, g]_\ell = \rho(\ell) \left(u(\ell) \overline{g'(\ell)} - u'(\ell) \overline{g(\ell)} \right).$$

4. Clearly there exists a $v \in \mathcal{D}_{A_1}$ such that

$$v(\ell) = \frac{-1}{\rho(\ell)}, \quad v'(\ell) = 0.$$

Write $v = v_0 + g$ where $v_0 \in \mathcal{D}_{\overline{A_0}}$, $g \in \mathcal{D}_+ \oplus \mathcal{D}_-$. Then

$$g(\ell) = \frac{-1}{\rho(\ell)}, \quad g'(\ell) = 0,$$

so $[u, g]_\ell = u'(\ell)$ for $u \in \mathcal{D}_{A_1}$. Hence $u'(\ell) = 0$ is a boundary condition at ℓ

5. Similarly we can find $g \in \mathcal{D}_+ \oplus \mathcal{D}_-$ such that

$$g(\ell) = 0, \quad g'(\ell) = \frac{1}{\rho(\ell)}.$$

Then $[u, g]_\ell = u(\ell)$ for $u \in \mathcal{D}_{A_1}$. Hence $u(\ell) = 0$ is a boundary condition at ℓ

6. It follows that $B_1(u) = u(\ell)$, $B_2(u) = u'(\ell)$ form a basis for the boundary conditions at the fixed endpoint ℓ . Thus a fixed endpoint always has two linearly independent boundary conditions.

Lemma 33 *Let $I = \{\ell, m\}$ and $\ell < c < m$. Let τ' be the restriction of τ to $I' \setminus \{\ell, c\}$. Then τ and τ' have the same number of linearly independent boundary values at ℓ .*

PROOF: Let \mathcal{D}'_{A_1} be the restriction of \mathcal{D}_{A_1} to I' . Every boundary value of τ at ℓ is of the form $B(u) = [u, v]_\ell$, $v \in \mathcal{D}_+ \oplus \mathcal{D}_-$. Let \hat{v} be the restriction of v to I' . Then $\hat{v} \in \mathcal{D}'_+ \oplus \mathcal{D}'_-$ and $[u, \hat{v}]_\ell = [u, v]_\ell$ is a boundary value of τ' at ℓ .

Conversely, if $\hat{w} \in \mathcal{D}'_+ \oplus \mathcal{D}'_-$ we can extend \hat{w} to a function $w \in \mathcal{D}_{A_1}$ on I , not unique. Write $w = v_0 + v$ where $v_0 \in \mathcal{D}_{A_0}$, $v \in \mathcal{D}_+ \oplus \mathcal{D}_-$. Then

$$[u, v]_\ell = [u, v_0 + v]_\ell = [u, w]_\ell = [u, \hat{w}]_\ell$$

is a boundary value of τ at ℓ . Q.E.D.

Corollary 27 *There are at most 2 boundary values at ℓ .*

PROOF: In general τ can have at most 4 boundary values. There are exactly 2 boundary values at any interior fixed point c . Hence there can be at most 2 independent boundary values at ℓ . Q.E.D.

4.2.1 Limit point and limit circle conditions

Let $I = \{\ell, m\}$ with $c \in (\ell, m)$. Thus I can be decomposed into the subintervals $I' = \{\ell, c\}$, $I'' = [c, m\}$ that have only the point c in common. Let τ', τ'' be the restriction of τ on I to I', I'' , respectively. Let d, d', d'' be the number of linearly independent solutions of $(\tau - i)u = 0$ in $L_2(I), L_2(I'), L_2(I'')$, respectively. Note that $d' = d_\ell$ is the number of linearly independent solutions of $(\tau - i)u = 0$ square integrable near ℓ , and $d'' = d_m$ is the number of linearly

independent solutions of $(\tau - i)u = 0$ square integrable near m . Finally let b_ℓ, b_m be the number of linearly independent boundary values of τ near ℓ and near m , respectively. From the last corollary we have

$$2d = \dim (\mathcal{D}_+ \oplus \mathcal{D}_-) = b_\ell + b_m,$$

$$2d' = \dim (\mathcal{D}'_+ \oplus \mathcal{D}'_-) = b_\ell + 2,$$

$$2d'' = \dim (\mathcal{D}''_+ \oplus \mathcal{D}''_-) = 2 + b_m.$$

Now since $d' = d_\ell = 1$ or 2 we see that $b_\ell = 0$ or 2 , and since $d'' = d_m = 1$ or 2 we must have $b_m = 0$ or 2 . it follows that there are 4 cases:

Case	d_ℓ	d_m	b_ℓ	b_m
i)	2	2	2	2
ii)	1	2	0	2
iii)	2	1	2	0
iv)	1	1	0	0

(4.8)

Definition 39 *If $d_\ell = 1$ we say that τ is in the **limit point** case at $x = \ell$. If $d_\ell = 2$ we say that τ is in the **limit circle** case at $x = \ell$. There are similar definitions for $x = m$.*

The reasons for this point/circle terminology will be made clear shortly.

We see from table (4.8) that $\overline{A_0}$ is self-adjoint if and only if the limit point case holds at both ℓ and m (case iv).

For the remaining three cases let's first review how we can use boundary conditions to determine any self-adjoint extension of A_0 . Each such extension has domain $\mathcal{D}_A = \mathcal{D}_{\overline{A_0}} \oplus \mathcal{S}$ where $\mathcal{S} = \{u + Cu : u \in \mathcal{D}_+\}$ where $C : \mathcal{D}_+ \longrightarrow \mathcal{D}_-$ is an isometry. Let v_1, \dots, v_d be an ON basis for \mathcal{D}_+ and $\overline{v_1}, \dots, \overline{v_d}$ an ON basis for \mathcal{D}_- . Then a basis for \mathcal{S} is the set

$$w_j = (v_j + \sum_{k=1}^d c_{k,j} \overline{v_k}), \quad j = 1, \dots, d,$$

where $\{c_{k,j}\}$ is a $d \times d$ unitary matrix. Also, $\mathcal{S}^\perp = \{u - Cu : u \in \mathcal{D}_+\}$ has the basis

$$w_j^\perp = (v_j - \sum_{k=1}^d c_{k,j} \overline{v_k}), \quad j = 1, \dots, d.$$

Therefore the boundary values defining A can be taken as

$$B'_j(u) = \langle u, w_j^\perp \rangle = [u, \tilde{w}_j^\perp]_m - [u, \tilde{w}_j^\perp]_\ell$$

where $w_j^\perp = -i(v_j + \sum_{k=1}^d c_{k,j} \overline{v_k}) = -iw_j$. We conclude that the boundary values

$$B_j(u) = [u, w_j]_m - [u, w_j]_\ell, \quad j = 1, \dots, d$$

determine \mathcal{D}_A .

There is a second way of obtaining the same result. As before A is a self-adjoint extension with domain $\mathcal{D}_A = \mathcal{D}_{\overline{A_0}} \oplus \mathcal{S}$ and $\{w_1, \dots, w_d\}$ is a basis for \mathcal{S} . Therefore

$$\mathcal{D}_A = \left\{ u + \sum_{j=1}^d a_j w_j : u \in \mathcal{D}_{\overline{A_0}}, a_j \in \mathbf{C} \right\},$$

and

$$z \in \mathcal{D}_A \iff (Av, z) = (v, A_1^* z) \iff [v, z]_\ell^m = 0$$

for all $v \in \mathcal{D}_A$. Here the boundary condition $[v, z]_\ell^m$ is determined by

$$(Av, z) = \int_I (\tau v) \overline{z} k \, dx = [v, z]_\ell^m + \int_I v \overline{\tau z} k \, dx = (v, Az).$$

However,

$$[v, z]_\ell^m = \sum_j \overline{a_j} [w_j, z]_\ell^m = 0 \iff [w_j, z]_\ell^m = 0, \quad j = 1, \dots, d.$$

Case i): limit circle - limit circle. Here $d = 2$ and w_1, w_2 form a basis for \mathcal{S} . Then

$$\mathcal{D}_A = \{u \in \mathcal{D}_{A_1} : B_j(u) = [u, w_j]_m - [u, w_j]_\ell \equiv [u, w_j]_\ell^m = 0\}.$$

Note that

$$[w_j, w_k]_\ell^m = 0, \quad j, k = 1, 2. \quad (4.9)$$

Now suppose $I = [\ell, m]$ and set

$$w_j(\ell) = -\frac{\overline{b_j}}{p(\ell)}, \quad w_j(m) = \frac{\overline{d_j}}{p(m)},$$

$$w'_j(\ell) = \frac{\overline{a_j}}{p(\ell)}, \quad w'_j(m) = -\frac{\overline{c_j}}{p(m)}, \quad j = 1, 2.$$

Then

$$\mathcal{D}_A = \{u \in \mathcal{D}_{A_1} : B_j(u) = a_j u(\ell) + b_j u'(\ell) + c_j u(m) + d_j u'(m) = 0, \quad j = 1, 2\},$$

where, from (4.9),

$$\frac{\overline{b_j} a_k - \overline{a_j} b_k}{p(\ell)} + \frac{-\overline{d_j} c_k + \overline{c_j} d_k}{p(m)} = 0, \quad j, k = 1, 2. \quad (4.10)$$

Conversely, it can be shown that any two linearly independent boundary values B_1, B_2 satisfying (4.10) define a self-adjoint extension of A_0 .

Case ii): limit point - limit circle. Here $d = 1$. Let $\{u_+\}$ be a basis for \mathcal{D}_+ . Then

$$\mathcal{S} = \{\alpha(u_+ + e^{i\theta} \overline{u_+}) : \alpha \in \mathbf{C}\}, \quad \mathcal{D}_A = \{u + \alpha(u_+ + e^{i\theta} \overline{u_+}) : u \in \mathcal{D}_{A_0}, \alpha \in \mathbf{C}\}.$$

The element $w = (u_+ + e^{i\theta} \overline{u_+})$ forms a basis for \mathcal{S} so we have

$$\mathcal{D}_A = \{v \in \mathcal{D}_{A_1} : B(v) = [v, m]_m = 0\}.$$

(Note that $[v, m]_\ell$ is always zero since there are no boundary values at ℓ .)
Therefore,

$$B(v) = \lim_{x \rightarrow m} p(x)(v(x) \overline{w'(x)} - v'(x) \overline{w(x)}).$$

A special case of this condition occurs when $m \in I$. Then we have

$$B(v) = p(m)(v(m) \overline{w'(m)} - v'(m) \overline{w(m)})$$

where

$$w(m) = u_+(m) + e^{i\theta} \overline{u_+(m)} = e^{i\theta/2} (e^{-i\theta/2} u_+(m) + e^{i\theta/2} \overline{u_+(m)}),$$

$$w'(m) = u'_+(m) + e^{i\theta} \overline{u'_+(m)} = e^{i\theta/2} (e^{-i\theta/2} u'_+(m) + e^{i\theta/2} \overline{u'_+(m)}).$$

Therefore we can write the boundary condition in the form

$$B(v) = av(m) + bv'(m) \quad (4.11)$$

with a, b real and $a^2 + b^2 \neq 0$. Conversely, it is easy to show that the set

$$\mathcal{T} = \{v \in \mathcal{D}_{A_1} : av(m) + bv'(m) = 0\}$$

defines a self-adjoint extension of A_0 for any a, b real and $a^2 + b^2 \neq 0$.

Case iii): limit circle - limit point. Here $d = 1$. This is a simple transposition of case ii).

Suppose

$$I = \{\ell, m\}, \quad \tau u = \frac{1}{k(x)} (-(pu')' + qu), \quad \mathcal{H} = L_c^2(k, I).$$

Theorem 75 (*Weyl's first theorem*) Let $\lambda_0 \in C$, $\ell < c < m$. If $\int_C^m |u(x)|^2 k(x) dx < \infty$ for all solutions u of $\tau u = \lambda_0 u$ in $[c, m\}$, then $\int_c^m |v(x)|^2 k(x) dx < \infty$ for all solutions v of $\tau v - \lambda v$ in $[c, m\}$, where λ is any complex number. This means that τ is limit circle at m . Similar remarks hold for $\{\ell, c\}$.

NOTE: This means that there are exactly two possibilities at m :

1. There are 2 independent square integrable solutions of $\tau u = \lambda_0 u$ in $[c, m\} \implies \tau$ is limit circle at m .
2. There are 0 or 1 independent square integrable solutions of $\tau u = \lambda_0 u$ in $[c, m\} \implies \tau$ is limit point at m .

Example 17

$$\tau u = \frac{1}{x^2} ((x^2 u')'), \quad I = (0, \infty), \quad c \in (0, \infty),$$

i.e., $k(x) = x^2$, $p(x) = x^2$, $q(x) = 0$. The equation $\tau u = \lambda u$ becomes

$$u'' + \frac{2}{x} u' = \lambda u.$$

Take the case $\lambda = 0$. The trial solution $u = x^\alpha$ is an actual solution if $\alpha(\alpha + 1) = 0$. Thus there are solutions $u_1(x) = x^{-1}$, $u_2(x) = 1$. Now $\int_0^c |u_j(x)|^2 x^2 dx < \infty$ for $j = 1, 2$, so τ is limit circle at 1. However $\int_c^\infty |u_j(x)|^2 x^2 dx$ diverges for $j = 1, 2$ so τ is limit point at $+\infty$. Thus the deficiency indices are 1, 1.

Before proceeding with the proof of the theorem, let us recall some facts about the Wronskian of two solutions $u_1(x), u_2(x)$ of $\tau u - \lambda u = 0$, where $\tau u = \frac{1}{k(x)} (-(pu')' + qu)$:

$$W(x) = \begin{vmatrix} u_1(x) & u_2(x) \\ u_1'(x) & u_2'(x) \end{vmatrix}.$$

The basic result is that $p(x)W(x) \equiv \text{constant}$. Let

$$[u, v](x) = p(x) \left(u(x)\overline{v'(x)} - u'(x)\overline{v(x)} \right),$$

so that a boundary value at m can be written in the form $[u, v]_m = \lim_{x \rightarrow m} [u, v](x)$. Then we have $p(x)W(x) = [u_1, \overline{u_2}](x)$.

PROOF OF THEOREM 75: Let $I' = [c, m]$. Suppose u, v are linearly independent solutions of $\tau z = \lambda_0 z$ in $L_c^0(I', k)$. Let $\lambda \in C$ and let w be any solution of $\tau w = \lambda w$ on $I' \rightarrow \tau w - \lambda_0 w = (\lambda - \lambda_0)w$. Normalize u, v so that $[u, \overline{v}](x) \equiv 1 = p(x)W(x)$. Then by variation of parameters

$$w(x) = c_1 u(x) + c_2 v(x) + (\lambda - \lambda_0) \int_{x_1}^x k(t) (u(x)v(t) - u(t)v(x)) w(t) dt$$

for $c \leq x_1 < m$. Let

$$\|w\|_{x_1}^{x_2} = \int_{x_1}^{x_2} |w(t)|^2 k(t) dt$$

for fixed x_1, x_2 and choose K so that $\sup_{x_1 < x_2} (\|u\|_{x_1}^{x_2} \cdot \|v\|_{x_1}^{x_2}) = K$. By the Schwarz inequality

$$\begin{aligned} \left| \int_{x_1}^{x_2} (u(x)v(t) - u(t)v(x)) k(t) w(t) dt \right| &\leq K \|w\|_{x_1}^{x_2} (|u(x)| + |v(x)|), \quad x_1 \leq x \leq x_2 \\ \implies |w(x)| &\leq |c_1| \cdot |u(x)| + |c_2| \cdot |v(x)| + |\lambda - \lambda_0| \cdot K \cdot \|w\|_{x_1}^{x_2} (|u(x)| + |v(x)|) \\ \implies \|w\|_{x_1}^{x_2} &\leq (|c_1| + |c_2|)K + 2|\lambda - \lambda_0| \cdot K^2 \cdot \|w\|_{x_1}^{x_2}. \end{aligned}$$

Now choose x_1 so large that $|\lambda - \lambda_0| K^2 < 1/4$. Then $\|w\|_{x_1}^{x_2} \leq 2(|c_1| + |c_2|)K$, independent of x_2 . Thus

$$\int_{x_1}^m |w(t)|^2 k(t) dt < \infty \implies w \in L_c^2(I', k).$$

Q.E.D.

We return to the case of the general τ operator defined on the interval $I = \{\ell, m\}$. Choose $c \in (\ell, m)$ and set $I' = [c, m]$. Now, fix α , $0 \leq \alpha < \pi$. Then there is a unique basis of solution $\phi(x, \lambda), \psi(x, \lambda)$ of $\tau u = \lambda u$ in I' such that

$$\begin{aligned} \phi(c, \lambda) &= \sin \alpha, & p(c)\phi'(c, \lambda) &= -\cos \alpha, \\ \psi(c, \lambda) &= \cos \alpha, & p(c)\psi'(c, \lambda) &= -\sin \alpha. \end{aligned}$$

REMARK: ϕ, ψ are entire functions of the complex variable λ for fixed x , and ϕ, ψ are linearly independent. In fact

$$p(c)W(c) = p(c) \begin{vmatrix} \phi(c) & \psi(c) \\ \phi'(c) & \psi'(c) \end{vmatrix} = 1 = [\phi, \overline{\psi}](c).$$

Therefore $[\phi, \overline{\psi}](x) \equiv 1$.

Define the boundary values B_1, B_2 at c by

$$B_1(u) = \cos \alpha u(c) + \sin \alpha p(c)u'(c), \quad B_2(u) = \sin \alpha u(c) - \cos \alpha p(c)u'(c),$$

so that $B_1(\phi) = B_2(\psi) = 0$. Now choose $b \in (c, m)$ and consider the boundary value B_3 at b defined by

$$B_3(u) = \cos \beta u(b) + \sin \beta p(b)u'(c),$$

for some fixed β such that $0 \leq \beta < \pi$.

REMARK: Every solution v of $\tau v = \lambda v$ on I' (except ψ) can be written in the form $v = \phi + M\psi$, up to a constant multiple.

1. What must M be so that $B_3(v) = 0$?

SOLUTION: Since $B_3(v) = B_3(\phi) + MB_3(\psi) = 0$, we have

$$M(b, \lambda, \beta) = -\frac{B_3(\phi)}{B_3(\psi)} = -\frac{\cot \beta \phi(b, \lambda) + p(b)\phi'(b, \lambda)}{\cot \beta \psi(b, \lambda) + p(b)\psi'(b, \lambda)}. \quad (4.12)$$

Note that $M(b, \lambda, \beta)$ is meromorphic in λ (i.e., it is analytic in the λ -plane except for isolated poles) and it is real for real λ .

2. For fixed λ, β what are all values of M such that v satisfies a real boundary condition at b ?

SOLUTION: For a real boundary condition we have $0 \leq \beta < \pi$ so that $\cot \beta$ runs over all real numbers (and ∞). We have

$$M = -\frac{\cot \beta A + B}{\cot \beta C + D}, \quad \cot \beta = -\frac{MD + B}{MC + A},$$

where

$$A = \phi(b, \lambda), \quad B = p(b)\phi'(b, \lambda), \quad C = \psi(b, \lambda), \quad D = p(b)\psi'(b, \lambda).$$

NOTE: Since $[u, v](x) = p(x)(u(x)\overline{v'(x)} - u'(x)\overline{v(x)})$ and $p(x)W(x) = [u, \overline{v}](x)$ we have

$$[\phi, \psi](b) = A\overline{D} - B\overline{C}, \quad [\psi, \psi](b) = C\overline{D} - D\overline{C},$$

$$[\phi, \overline{\psi}](b) = 1, \quad [\phi, \phi](b) = A\overline{B} - B\overline{A}.$$

The possible solutions M form a circle C_b in the complex M -plane. Indeed since $\cot \beta$ is required only to be real, we see that the equation of C_b is

$$\frac{MD + B}{MC + A} = \frac{\overline{MD} + \overline{B}}{\overline{MC} + \overline{A}}$$

or

$$(MD + B)(\overline{MC} + \overline{A}) - (MC + A)(\overline{MD} + \overline{B}) = 0. \quad (4.13)$$

This last equation can be written in the standard form

$$\left| M - \frac{A\overline{D} - B\overline{C}}{\overline{C}D - C\overline{D}} \right|^2 = \left(\frac{|AD - BC|}{|\overline{C}D - C\overline{D}|} \right)^2. \quad (4.14)$$

If we denote by M_b and r_b the center and the radius of the circle C_b , respectively, we see that

$$M_b = \frac{A\overline{D} - B\overline{C}}{\overline{C}D - C\overline{D}} = -\frac{[\phi, \psi](b)}{[\psi, \psi](b)},$$

$$r_b = \frac{|AD - BC|}{|\overline{C}D - C\overline{D}|} = \left| \frac{[\phi, \overline{\psi}](b)}{[\psi, \psi](b)} \right| = \frac{1}{|[\psi, \psi](b)|},$$

since $[\phi, \overline{\psi}](b) = 1$.

Recalling that $v = \phi + M\psi$, we see from (4.13) that another way to write the equation of C_b is $[v, v](b) = 0$. Indeed:

$$[v, v](b) = [\phi, \phi] + \overline{M}[\phi, \psi] + M[\psi, \phi] + |M|^2[\psi, \psi] = 0.$$

3. An inequality for the interior of C_b :

$$\frac{[v, v](b)}{[\psi, \psi](b)} < 0.$$

4. An integral representation for C_b . As before, let $v = \phi + M\psi$ and suppose $\text{Im } \lambda \neq 0$. Then integration by parts yields

$$\int_c^b (\tau v) \bar{v} k \, dx - \int_c^b v \overline{\tau v} k \, dx = [v, v](b) - [v, v](c),$$

so

$$2i \, \text{Im } \lambda \int_c^b |v|^2 k \, dx = [v, v](b) - [v, v](c).$$

For the special case $v = \psi$ we have

$$2i \, \text{Im } \lambda \int_c^b |\psi|^2 k \, dx = [\psi, \psi](b)$$

since $[\psi, \psi](c) = 0$. (Note that in general, $[v, v](c) = -2i \, \text{Im } M$.) Therefore the equation for C_b can be written as

$$\int_c^b |v|^2 k \, dx = \frac{\text{Im } M}{\text{Im } \lambda} \quad (4.15)$$

and the inequality for the interior of C_b is

$$\int_c^b |v|^2 k \, dx < \frac{\text{Im } M}{\text{Im } \lambda} \quad (4.16)$$

5. It follows from (4.15) and (4.16) that if $b_1 > b_2$ then the circle C_{b_1} is contained in the interior of C_{b_2} .

It follows that there are exactly two possibilities as $b \rightarrow m$:

CASE 1: C_b shrinks to a point M_∞ , i.e., $r_b \rightarrow 0$ and $M_b \rightarrow M_\infty$ as $b \rightarrow m$. Then $v_0 = \phi + M_\infty \psi$ has the property

$$\int_c^m |v_0|^2 k \, dx = \frac{\text{Im } M_\infty}{\text{Im } \lambda} < \infty,$$

whereas since $r_b \rightarrow 0$ as $b \rightarrow m$ we have $|\psi, \psi](b)| \rightarrow \infty$, so

$$\int_c^m |\psi|^2 k \, dx = \infty.$$

Thus the only square integrable solutions of $\tau v = \lambda v$ are constant multiples of v_0 where $[v_0, v_0]_m = 0$. **This is the limit point case.**

CASE 2: C_b shrinks to a circle C_∞ with radius $r_\infty = \lim_{b \rightarrow m} r_b > 0$ and center $M_\infty = \lim_{b \rightarrow m} M_b$. Then

$$r_\infty = \frac{1}{|[\psi, \psi]_m|} > 0, \quad M_\infty = -\frac{[\phi, \psi]_m}{[\psi, \psi]_m}.$$

Now since $v = \phi + M\psi$ we see that if M belongs to the interior or the boundary of C_∞ then

$$\int_c^b |v_0|^2 k \, dx = \frac{\operatorname{Im} M_\infty}{\operatorname{Im} \lambda}$$

for all b , so

$$\int_c^m |v_0|^2 k \, dx = \frac{\operatorname{Im} M_\infty}{\operatorname{Im} \lambda} \leq \infty,$$

and v is square integrable near m . Similarly, we know that ψ is square integrable near m . Thus we can conclude that all solutions of $\tau v = \lambda v$ are square integrable near m . **This is the limit circle case.**

Lemma 34 *Let $v = \phi + M\psi$. Then M is on the boundary of C_∞*

$$\iff [v, v]_m = 0 \iff \int_c^m |v_0|^2 k \, dx = \frac{\operatorname{Im} M_\infty}{\operatorname{Im} \lambda}.$$

PROOF:

$$\begin{aligned} [v, v](b) &= |M|^2[\psi, \psi](b) + M[\psi, \phi](b) + \overline{M}[\phi, \psi](b) + [\phi, \phi](b) \\ &= [\psi, \psi](b) (|M - M_b|^2 - r_b^2). \end{aligned}$$

Q.E.D.

4.3 Qualitative theory of the deficiency index

We begin with a technical result and refer to Hellwig for the proof.

Theorem 76 *Let $I = \{\ell, \infty\}$, $\tau u = \frac{d^2}{dx^2}u + q(x)u$. Suppose there exist constants $\alpha_1, \alpha_2 > 0$ and a function $M(x) > 0$ such that*

1. $M(x), M'(x)$ are continuous on the interval $x_0 \leq x < \infty$ for some finite x_0 .

2.

$$q(x) \geq -\alpha_1 M(x), \quad |M'(x)M^{-3/2}(x)| \leq \alpha_2$$

for $x_0 \leq x < \infty$.

3.

$$\int_{x_0}^{\infty} \frac{1}{\sqrt{M(x)}} dx = \infty.$$

Then the limit point case occurs at $x = \infty$.

Corollary 28 *If $q(x) \geq -kx^2$ then $x = \infty$ is limit point.*

PROOF: Set $M(x) \equiv 1$ and $x_0 > 0$ in the theorem. Q.E.D.

Corollary 29 *$-u'' + q(x)u$ is limit point at $x = \infty$ if $q(x) \geq 0$ for all x .*

REMARKS:

1. Suppose we have the limit point case at m . Then M_∞ is independent of β . Therefore we can set $\beta = 0$ for convenience and obtain

$$M_\infty = \lim_{b \rightarrow m} M(\beta, b, \lambda) = \lim_{b \rightarrow m} M(0, b, \lambda) = - \lim_{b \rightarrow m} \frac{\phi(b\lambda)}{\psi(b, \lambda)}.$$

2. $M_\infty(\lambda)$ is an analytic function of λ for $\text{Im } \lambda > 0$ and for $\text{Im } \lambda < 0$. Further $\text{Im } M_\infty > 0$ for $\text{Im } \lambda > 0$ and if $M_\infty(\lambda)$ has zeros or poles on the real axis, they are all simple.

PROOF: For fixed b the center and radius of C_b are continuous functions of λ for $\text{Im } \lambda > 0$, and the circles are nested as b increases. Therefore if λ is restricted to a bounded set Γ in the upper half plane the functions $M(\lambda, b, \beta)$ are analytic in λ and uniformly bounded as $b \rightarrow m$. Thus the functions $M(\lambda, b, \beta)$ are equicontinuous so $M_b \rightarrow M_\infty$ uniformly. The uniform limit of a sequence of analytic functions is analytic. The rest follows from the identity

$$\int_c^m |v_0|^2 k dx = \frac{\text{Im } M_\infty}{\text{Im } \lambda}.$$

Q.E.D.

Recall that $I = \{\ell, m\}$.

Theorem 77 *Let A be a self-adjoint operator obtained from τ by imposition of separated boundary conditions. Suppose $\text{Im } \lambda \neq 0$. Then there is exactly one solution $u(x, \lambda)$ of $(\tau - \lambda)u = 0$, square integrable at ℓ and satisfying the boundary conditions at ℓ , and exactly one solution $v(x, \lambda)$ of $(\tau - \lambda)v = 0$, square integrable at m and satisfying the boundary conditions at m . Further u and v are linearly independent.*

PROOF: Since $\text{Im } \lambda \neq 0$ and A is self-adjoint, λ doesn't belong to the spectrum of A . We break the proof up into cases, depending on the boundary conditions at ℓ and at m :

1. limit point - limit point. Then there is exactly one square integrable solution u at ℓ and one square integrable solution v at m and no boundary conditions.
2. limit point - limit circle. There must be one boundary condition B at m , none at ℓ . There is exactly one solution u at ℓ , square integrable. All solutions at m are square integrable and there exists a square integrable solution v at m such that $B(v) = 0$. If there are two linearly independent solutions at m satisfying the boundary conditions then $v \in \mathcal{H}$ and $B(v) = 0$, so $v \in \mathcal{D}_A$ and v is an eigenvector of A with eigenvalue λ . Impossible!
3. limit circle - limit point. Same proof as case 2.
4. limit circle - limit circle. The proof is similar to case 2, but boundary conditions have to be applied at both endpoints.

Q.E.D.

Corollary 30 *The conclusions of the theorem hold in the limit circle - limit circle case if λ is real but not an eigenvalue.*

PROOF: This follows from Weyl's first theorem. Q.E.D.

Let A be a self-adjoint operator on $I = \{\ell, m\}$, defined by separated boundary conditions. Suppose τ is limit circle at m , and let $B(w) = 0$ be the boundary condition at m corresponding to A . The following remarks are pertinent:

1. There exists a $v \in \mathcal{D}_+ \oplus \mathcal{D}_-$ such that

$$B(w) = [w, v]_m = \langle w, \tilde{v} \rangle.$$

2. Suppose $w_1, w_2 \in \mathcal{D}_{A_1}$ such that $w_1 \equiv w_2 \equiv 0$ in a neighborhood of ℓ . Then

$$(\tau w_1, w_2) - (w_1, \tau w_2) = [w_1, w_2]_m - [w_1, w_2]_\ell = [w_1, w_2]_m$$

since $[w_1, w_2]_\ell = 0$. Therefore $B(w_1) = B(w_2) = 0$ so $w_1, w_2 \in \mathcal{D}_A$, which implies $[w_1, w_2]_m = 0$.

3. If $w_1, w_2 \in \mathcal{D}_{A_1}$ and $B(w_1) = B(w_2) = 0$ then $[w_1, w_2]_m = 0$.
4. Let $\text{Im } \lambda \neq 0$. By the theorem, there exists exactly one solution u of $(\tau - \lambda)u = 0$ which is square integrable near m and satisfies $B(u) = 0 = [u, v]_m$.
5. From comment 3, if $B(w) = 0$ then $[w, u]_m = 0$. In particular, $[u, u]_m = 0$ implies $u = \phi + M(\lambda)\psi$ where $M(\lambda)$ lies on the unit circle.
6. We have shown that $B(w) = [w, v]_m = 0 \implies [w, u]_m = 0$. Now u defines a nonzero boundary value $B_1(w) = [w, u]_m = \langle w, \tilde{v}_1 \rangle$ on \mathcal{D}_{A_1} with $v_1 \in \mathcal{D}_+ \oplus \mathcal{D}_-$. We have shown that $\langle w, \tilde{v} \rangle = 0$ implies $\langle w, \tilde{v}_1 \rangle = 0$, so $\tilde{v} = \alpha \tilde{v}_1$, $\alpha \in C$. Therefore, the boundary condition $B(w) = 0$ is equivalent to the boundary condition $B_1(w) = [w, u]_m = 0$.

CONCLUSION: All separated boundary conditions defining self-adjoint operators are of the form

$$B(w) = [w, u]_m = 0$$

where

$$[u, u]_m = 0, \quad u = \phi + \tilde{M}\psi, \quad \tau u = \lambda u,$$

and \tilde{M} lies on the boundary of the limit circle.

- 7.

$$B(\bar{u}) = [\bar{u}, u]_m = \overline{p(x)W(x)} = 0.$$

Therefore, if $w \in \mathcal{D}_A$ and $B(w) = 0$ then $0 = [\bar{u}, w]_m = -[\bar{w}, u]_m$. It follows that if $B(w) = 0$ then $B(\bar{w}) = 0$, i.e., if $w \in \mathcal{D}_A$ then $\bar{w} \in \mathcal{D}_A$. We say that the boundary condition B is **real**.

4.3.1 Separated boundary conditions in the limit circle - limit circle case

Again let $I = \{\ell, m\}$ and choose $c \in (\ell, m)$. Let $\text{Im } \lambda \neq 0$ and $\phi\psi$ be a basis for solutions of $(\tau - \lambda)u = 0$ as before. Denote by C_∞ the limit circle at m and $C_{-\infty}$ the limit circle at ℓ . Let

$$u_1 = \phi + \tilde{M}_1\psi, \quad \tilde{M}_1 \in C_{-\infty},$$

$$u_2 = \phi + \tilde{M}_2\psi, \quad \tilde{M}_2 \in C_\infty.$$

Note that $u_1, u_2 \neq 0$ must be linearly independent, since if $u_1 = u_2$ then

$$\int_\ell^m |u_1|^2 k \, dx = [u, u]_m - [u, u]_\ell = 0,$$

which is impossible. Let

$$\mathcal{D}_A = \{w \in \mathcal{D}_{A_1} : [w, u_1]_\ell = 0, [w, u_2]_m = 0\}.$$

Define $Aw = \tau w$ for $w \in \mathcal{D}_A$. We will show that A is symmetric, hence self-adjoint. To do this we first solve the equation $(A - \lambda E)u = f$ for $u \in \mathcal{D}_A$ where f is any element of $\mathcal{H} = L_c^2(I, k)$.

Normalize u_1, u_2 so that $[u_1, \bar{u}_2](x) = p(x)W(x) \equiv 1$. Then, using the method of variation of parameters to solve the second order ODE we find

$$u(x) = au_1(x) + bu_2(x) + \int_\ell^x (u_1(x)u_2(t) - u_2(x)u_1(t)) f(t)k(t)dt.$$

Differentiating once we have

$$u'(x) = au_1'(x) + bu_2'(x) + \int_\ell^x (u_1'(x)u_2(t) - u_2'(x)u_1(t)) f(t)k(t)dt.$$

From these expressions we see that

$$[u, u_1]_\ell = b[u_2, u_1]_\ell = 0$$

for $u \in \mathcal{D}_A$.

Lemma 35 $[u_2, u_1]_\ell \neq 0, [u_2, u_1]_m \neq 0$.

PROOF: It is straightforward to verify the identity

$$[u_1, u_1](x) [u_2, u_2](x) - |[u_1, u_2](x)|^2 = |[u_1, \overline{u_2}](x)|^2.$$

However, $[u_1, \overline{u_2}](x) = 1$ for all x . Since $[u_1, u_1](x) \rightarrow 0$ as $x \rightarrow \ell$ and $[u_2, u_2](x) \rightarrow 0$ as $x \rightarrow m$ it follows that $[u_2, u_1]_\ell \neq 0$, $[u_2, u_1]_m \neq 0$. Q.E.D

Since $[u_2, u_1]_\ell \neq 0$ we must have $b = 0$. Similarly the boundary condition for u at $x = m$ gives

$$[u, u_2]_m = a[u_1, u_2]_m + [u_1, u_2]_m \int_\ell^m u_2(t) f(t) k(t) dt = 0$$

where $[u_1, u_2]_m = 1$. Thus we can solve for a and finally obtain the result

$$u(x) = \int_\ell^m g(x, t; \lambda) f(t) k(t) dt = Gf,$$

where

$$g(x, t; \lambda) = \begin{cases} -u_2(x)u_1(t) & \ell < x < t < m \\ -u_1(x)u_2(t) & \ell < t < x < m. \end{cases}$$

Note that $u \in \mathcal{D}_A$ and

$$\int_\ell^m \int_\ell^m |g(x, t, \lambda)|^2 dx dt < \infty,$$

i.e., G is a Hilbert-Schmidt operator, which implies that G is completely continuous, but not symmetric. We conclude that $G = (A - \lambda E)^{-1}$ is a bounded operator with $\mathcal{D}_G = \mathcal{H}$ and $\mathcal{R}_G = \mathcal{D}_A$.

REMARKS:

1. A is symmetric, hence self-adjoint. Indeed, if $v_1, v_2 \in \mathcal{D}_A$ there are $f_1, f_2 \in \mathcal{H}$ such that $v_1 = Gf_1$, $v_2 = Gf_2$. Thus

$$[v_1, v_2]_m = [Gf_1, Gf_2]_m = 0, \quad [v_1, v - 2]_\ell = [Gf_1, Gf_2]_\ell = 0,$$

by explicit computation. Therefore

$$(Av_1, v_2) - (v_1, Av_2) = [v_1, v_2]_m - [v_1, v_2]_\ell = 0.$$

Q.E.D.

2. There exists a real number λ_0 that is **not** an eigenvalue of A . Indeed, A and $G = (A - \lambda E)^{-1}$ have the same eigenvalues. But G is completely continuous so it has only a countable number of eigenvalues. Thus there must exist a real number λ_0 that is not an eigenvalue of G . Q.E.D.
3. Repeating the same construction as above, but for the real number λ_0 rather than the complex number λ with $\text{Im } \lambda \neq 0$ we can obtain a function

$$g(x, t, \lambda_0) = \begin{cases} -v_2(x)v_1(t) & t < x \\ -v_1(x)v_2(t) & x < t \end{cases}$$

such that

$$[v_1, u_1]_\ell = [v_2, u_2]_m = 0, \quad (\tau - \lambda_0)v_j = 0, \quad j = 1, 2,$$

so that the associated operator $(A - \lambda_0)^{-1}$ is a symmetric (since λ_0 is real), completely continuous Hilbert-Schmidt operator. Thus A has a countably infinite number of eigenvalues λ_n such that $\lambda_n \rightarrow \infty$ as $n \rightarrow \infty$ (no finite limit point) and corresponding ON eigenvectors ϕ_n that form a basis for \mathcal{H} . Thus

$$A\phi_n = \lambda_n\phi_n, \quad n = 1, 2, \dots,$$

and for every $u \in \mathcal{H}$ we have

$$u = \sum_{n=1}^{\infty} (u, \phi_n) \phi_n.$$

If $u \in \mathcal{D}_A$ then the series

$$u(x) = \sum_{n=1}^{\infty} (u, \phi_n) \phi_n(x).$$

converges uniformly in any bounded subinterval of I .

EXAMPLE: The Legendre equation

$$\tau u = -[(1 - x^2)u']', \quad I = (-1, 1).$$

Here, $p(x) = 1 - x^2$, $k(x) = 1$ and the eigenvalue equation is $\tau u = \lambda u$. let us solve the equation $\tau u = 0$, i.e., $\lambda = 0$. If we can show that all solutions of

this equation are square integrable, it will follow that this is the limit circle - limit circle case. The equation to solve is

$$-(1-x^2)u'' + 2xu' = 0.$$

Set $v = u'$. Then the equation is

$$v' = \frac{2x}{1-x^2}v \implies \frac{dv}{v} = \left(\frac{1}{1-x} - \frac{1}{1+x} \right) dx,$$

so

$$\ln u' = -\ln|1-x| - \ln|1+x| + \ln c$$

or $u' = c/(1-x^2)$. Thus the general solution is

$$u(x) = c_1 \ln \left(\frac{1+x}{1-x} \right) + c_2.$$

A basis for the solution space is

$$u_1(x) = 1, \quad u_2(x) = \ln \left(\frac{1+x}{1-x} \right).$$

Both these solutions are square integrable in I , so by Weyl's first theorem, this is the limit circle - limit circle case.

Now let us solve the general equation $\tau u = \lambda u$. We will try a power series solution $u(x) = \sum_{n=0}^{\infty} a_n x^n$. Substituting into the differential equation we find

$$-(1-x^2) \sum n(n-1)a_n x^{n-2} + 2x \sum n a_n x^{n-1} - \lambda \sum a_n x^n = 0.$$

Equating coefficients of x^n on both sides of this identity we obtain the conditions

$$-(n+2)(n+1)a_{n+2} + n(n-1)a_n + 2na_n - \lambda a_n = 0, n = 0, 1, \dots,$$

or

$$a_{n+2} = \frac{(n+1)n - \lambda}{(n+2)(n+1)} a_n.$$

1. One solution is obtained by setting $a_0 = 1, a_1 = 0$. We see that this is an even solution and contains only even powers of x . By the ratio test, the series converges for $|x| < 1$. We denote this solution as $u_1(x, \lambda)$.

2. The second solution is obtained by setting $a_0 = 0, a_1 = 1$. This solution contains only odd powers of x . By the ratio test, the series converges for $|x| < 1$. We denote this solution as $u_2(x, \lambda)$.

We assume that u_1, u_2 are normalized such that $\|u_j\| = 1, j = 1, 2$.

Note that one of these solutions is a polynomial in x if and only if $\lambda = k(k+1), k = 0, 1, 2, \dots$. Now let's look for solutions of the form $\sum b_n(x-1)^n$, i.e., solutions expanded about $x = 1$. The result is as follows: There are solutions

$$P_\mu(x) = \sum_{n=0}^{\infty} c_n \left(\frac{1-x}{2}\right)^n$$

where

$$c_0 = 1, \quad c_n = \frac{(\mu+1)(\mu+2) \cdots (\mu+k) \cdot (-\mu)(-\mu+1) \cdots (-\mu+k-1)}{(n!)^2}$$

and $\lambda = \mu(\mu+1)$. The series converges for $|x-1| < 2$. Note that

$$P_\mu(1) = 1, \quad P'_\mu(1) = \frac{\mu(\mu+1)}{2}.$$

It can be shown that there is an independent solution that behaves like $\ln(\frac{1-x}{1+x})$ near $x = 1$, i.e., has logarithmic behavior. Similarly, near $x = -1$ there is the solution $P_\mu(-x)$ and an independent solution that acts like $\ln(\frac{1+x}{1-x})$.

The following facts can be obtained from special function theory:

1. $P_\mu(x), P_\mu(-x)$ are linearly independent unless μ is an integer.

- 2.

$$\lim_{x \rightarrow -1+0} \frac{P_\mu(x)}{\ln(\frac{1-x}{1+x})} = -\frac{\sin \pi\mu}{\pi},$$

- 3.

$$\lim_{x \rightarrow -1+0} (1-x^2)P'_\mu(x) \frac{\sin \pi\mu}{\pi},$$

- 4.

$$P_\mu(x) = P_{-\mu-1}(x).$$

Thus, if μ is not an integer, we have

$$u_1(x, \lambda) = A_\mu (P_\mu(x) + P_\mu(-x)), \quad u_2(x, \lambda) = B_\mu (P_\mu(x) - P_\mu(-x)),$$

where $A_\mu, B_\mu > 0$.

From these results we can write down an explicit basis for the boundary values at $x = 1$ and $x = -1$:

$$B_1(w) = [w, 1]_1 = \lim_{x \rightarrow +1} (x^2 - 1)w'(x), \quad B_2(w) = [w, 1]_{-1} = \lim_{x \rightarrow -1} (x^2 - 1)w'(x),$$

$$B_3(w) = [w, \ln(\frac{1+x}{1-x})]_1 = \lim_{x \rightarrow +1} (1 - x^2) \left(w(x) \frac{2}{1 - x^2} - \ln(\frac{1+x}{1-x}) w'(x) \right),$$

$$B_4(w) = [w, \ln(\frac{1+x}{1-x})]_{-1} = \lim_{x \rightarrow -1} (1 - x^2) \left(w(x) \frac{2}{1 - x^2} - \ln(\frac{1+x}{1-x}) w'(x) \right).$$

What does \mathcal{D}_{A_1} look like? Note that $B_1(\ln \frac{1+x}{1-x}) = B_2(\ln \frac{1+x}{1-x}) = 2$. let $f \in \mathcal{R}_{A_1}$ where

$$\mathcal{D}_{A_1} = \{u : \tau u = f, f \in L_c^2(I, 1)\}.$$

By the method of variation of parameters we have the general solution

$$\begin{aligned} u &= c_1 + c_2 \ln(\frac{1+x}{1-x}) + \int_{-1}^x \frac{1}{2} [\ln(\frac{1+t}{1-t}) - \ln(\frac{1+x}{1-x})] f(t) dt \\ &= [c_1 + \frac{1}{2} \int_{-1}^x \ln(\frac{1+t}{1-t}) f(t) dt] + \ln(\frac{1+x}{1-x}) [c_2 - \frac{1}{2} \int_{-1}^x f(t) dt]. \end{aligned}$$

Note that $u \in \mathcal{H}$ and

$$u'(x) = \frac{2}{1 - x^2} [c_2 - \frac{1}{2} \int_{-1}^x f(t) dt].$$

Thus, $B_1(u) = B_2(u) = 0 \iff c_2 = \int_{-1}^1 f(t) dt = 0 \iff u(x)$ is bounded at -1 and $+1$.

Let

$$\mathcal{D}_A = \{u \in \mathcal{D}_{A_1} : B_1(u) = B_2(u) = 0\}$$

and $Au = \tau u$, for all $u \in \mathcal{D}_A$. Then A is symmetric because for $u, v \in \mathcal{D}_A$ we have

$$(Au, v) - (u, Av) = \left[(1 - x^2) (u(x) \overline{v'(x)} - \overline{v(x)} u'(x)) \right]_{-1}^1 = 0.$$

Note:

$$[u, \bar{v}](x) = \frac{1}{2}[u, 1](x) \overline{[v, \ln \frac{1+x}{1-x}]}(x) - \frac{1}{2}\overline{[v, 1]}(x) [u, \ln \frac{1+x}{1-x}](x).$$

The normalized eigenvectors of A are

$$v_n(x) = \sqrt{n + \frac{1}{2}} P_n(x), \quad \lambda_n = n(n+1), \quad n = 0, 1, 2, \dots$$

where the $P_n(x)$ are the Legendre polynomials. (A simple expression for these polynomials is $P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n$.) If $u \in \mathcal{D}_A$ then $u(x) = \sum_{n=0}^{\infty} (u, v_n) v_n(x)$ and the series converges uniformly on $[-1, 1]$.

To describe the general self-adjoint extension we need to consider the case $\lambda = \mu(\mu + 1) = i$. Thus

$$u_1(x, i) = A_\mu(P_\mu(x) + P_\mu(-x)), \quad u_2(x, i) = B_\mu(P_\mu(x) - P_\mu(-x)).$$

Each self-adjoint extension is defined by a 2×2 unitary matrix $\theta = (\theta_{jk})$. The domain for the self-adjoint operator A_θ is

$$\mathcal{D}_{A_\theta} = \mathcal{D}_{A_0} \oplus \mathcal{S}.$$

A basis for \mathcal{S} is

$$w_1(x) = u_1(x, i) + \theta_{11} \overline{u_1(x, i)} + \theta_{12} \overline{u_2(x, i)},$$

$$w_2(x) = u_2(x, i) + \theta_{21} \overline{u_1(x, i)} + \theta_{22} \overline{u_2(x, i)}.$$

The boundary conditions describing A_θ are

$$B_1(u) = [u, w_1]_{-1}^1 = 0, \quad B_2(u) = [u, w_2]_{-1}^1 = 0.$$

Then particular extension \mathcal{D}_A is the case

$$\theta = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

See the book of Akheiser and Glazman for more details.

Example 18 *Bessel's equation. Before proceeding with our theoretical development we look at Bessel's equation*

$$-(xu')' + \frac{\nu^2}{x^2}u - \lambda xu = 0, \quad \nu \geq 0$$

as an important example of one equation that leads to several very distinct spectral problems. Here the formal differential operator action is

$$\tau u = -\frac{(xu')'}{x} + \frac{\nu^2}{x^2}u.$$

Thus, in terms of our usual notation, $k(x) = x$, $p(x) = x$, $q(x) = \nu^2/x^2$. Since $x = 0$ is a singular point for this operator we must choose our interval I such that it does not contain $x = 0$ as an interior point. There are essentially three distinct cases:

Case 1: $I_1 = (0, b)$, $b > 0$.

Case 2: $I_2 = (0, +\infty)$.

Case 3: $I_3 = (b, +\infty)$, $b > 0$.

To determine the nature of the conditions at the boundary points we set $\lambda = 0$ in the eigenvalue equation $\tau u = \lambda u$:

$$-xu'' - u' + \frac{\nu^2 u}{x} = 0.$$

Substituting a trial solution $u = x^n$ into this equation we find the condition

$$-n(n-1) - n + \nu^2 = 0 \implies n = \pm \nu.$$

Thus for $\nu \neq 0$ we have a basis of solutions $u_1(x) = x^\nu$, $u_2(x) = x^{-\nu}$. (If $\nu = 0$ there is a basis $u_1(x) = 1$, $u_2(x) = \ln x$.)

Case 1: $I_1 = (0, b)$. At b we are clearly in the limit circle case. Clearly u_1 belongs to the Hilbert space for $\nu > 0$. As for u_2 , near $x = 0$ we have

$$\int_\epsilon^1 x^{-2\nu+1} dx = \frac{1 - \epsilon^{-2\nu+2}}{2\nu+2} \implies x^{-\nu} \text{ square integrable} \iff \nu < 1.$$

For $\nu > 0$ we are in the limit circle - limit circle case provided $\nu < 1$. (In this case the spectral expansion is in terms of Fourier - Bessel series.) If $1 \leq \nu$ we are in the limit point - limit circle case. Finally, if $\nu = 0$ we are again in the limit circle - limit circle case.

Case 2: $I_2 = (0, +\infty)$. Here $+\infty$ is in the limit point case, so we have limit circle - limit point for $0 \leq \nu < 1$ and limit point - limit point for $1 \leq \nu$. The spectral expansion is in terms of the Hankel transform.

Case 3: $I_3 = (b, +\infty)$, $b > 0$. This is a limit circle - limit point case.

4.3.2 Separated boundary conditions and spectral resolutions in the limit point - limit circle case

We now consider a self-adjoint eigenvalue problem where the interval is of the form $I = [\ell, m)$, we have the (regular) limit circle case at ℓ and the limit point case at m . By introducing an appropriate change of variable we can assume $I = [0, \infty)$ with the limit point case at ∞ . Assume that the boundary condition at $\ell = 0$ is

$$B_0(u) = \sin \alpha u(0) - \cos \alpha p(0)u'(0) = 0$$

for a constant α such that $0 \leq \alpha < \pi$. To start with, we consider the regular eigenvalue problem

$$\tau u = \lambda u, \quad B_0(u) = 0, \quad B_b(u) = \cos \beta u(b) + \sin \beta p(b)u'(b) = 0$$

on the finite interval $[0, b]$, where $0 \leq \beta < \pi$. We argue as follows:

1. There exists a sequence $\{\lambda_{bn}\}$ of real eigenvalues and an ON set of corresponding eigenfunctions $\{\theta_{bn}\}$. Note that $B_0(\theta_{bn}) = B_b(\theta_{bn}) = 0$.
2. For any complex number λ let $\phi(x, \lambda), \psi(x, \lambda)$ be solutions of $\tau u = \lambda u$ such that

$$\begin{aligned} \phi(0, \lambda) &= \sin \alpha, & p(0)\phi'(0, \lambda) &= -\cos \alpha, \\ \psi(0, \lambda) &= \cos \alpha, & p(0)\psi'(0, \lambda) &= \sin \alpha. \end{aligned}$$

Then $B_0(\psi) = 0$.

3. Therefore there exist constants r_{bn} such that $\theta_{bn}(x) = r_{bn}\psi(x, \lambda_{bn})$.
4. Let $f(x)$ be a continuous function on I which vanishes outside the interval $0 \leq x \leq c$, where $0 < c < b$. Then by Parseval's equality

$$\int_0^b |f(x)|^2 k(x) dx = \sum_{n=1}^{\infty} |r_{bn}|^2 \left| \int_0^b f(x) \psi(x, \lambda_{bn}) k(x) dx \right|^2.$$

5. Let

$$g(\lambda) = \int_0^\infty f(x)\psi(x, \lambda)k(x) \, dx$$

and let $\rho_b(\lambda)$ be a monotone increasing function of λ such that

- a. ρ_b has a jump of $|r_{bn}|^2$ at each eigenvalue λ_{bn} , and is otherwise constant.
- b. $\rho_b(\lambda + 0) = \rho_b(\lambda)$.
- c. $\rho_b(0) = 0$.

Then

$$\int_0^\infty |f(x)|^2 k(x) \, dx = \int_{-\infty}^\infty |g(\lambda)|^2 \, d\rho_b(\lambda).$$

here $\rho_b(\lambda)$ is the spectral function.

Now we are ready to state our principal result. Let σ be a monotone increasing function on $(-\infty, +\infty)$. Further, let $L_c^2(\sigma)$ be the space of all complex valued functions h , measurable with respect to σ and such that

$$\int_{-\infty}^{+\infty} |h(\lambda)|^2 \, d\sigma(\lambda) < \infty.$$

We consider the eigenvalue problem $Au = \tau u$ where

$$\mathcal{D}_A = \left\{ u \in L_c^2([0, \infty), k) = \mathcal{H} : u' \text{ abs.cont.}, \tau u \in \mathcal{H}, \text{ and } B_0(u) = 0 \right\}.$$

Theorem 78 *Suppose τ is in the limit point case at $+\infty$. Then*

1. *There exists a monotone increasing function ρ on $(-\infty, +\infty)$ such that*

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

2. *If $f \in L_c^2(I, k)$ there exists $g \in L_c^2(\rho)$ such that*

$$\lim_{a \rightarrow +\infty} \int_{-\infty}^{+\infty} \left| g(\lambda) - \int_0^a f(x)\psi(x, \lambda)k(x) \, dx \right|^2 \, d\rho(\lambda) = 0,$$

i.e.,

$$g(\lambda) = \int_0^{+\infty} f(x)\psi(x, \lambda)k(x) \, dx$$

in $L_c^2(\rho)$, and

$$\int_0^{+\infty} |f(x)|^2 k(x) \, dx = \int_{-\infty}^{+\infty} |g(\lambda)|^2 \, d\rho(\lambda)$$

in $L_c^2(I, k)$.

3. Let $m_\infty(\lambda)$ be the limit point at $+\infty$. Then m_∞ is an analytic function of λ for $\text{Im } \lambda > 0$ and $\text{Im } \lambda < 0$, and

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

at points of continuity λ, μ of ρ .

4.

$$m_\infty(\ell) - m_\infty(\ell_0) = \int_{-\infty}^{+\infty} \left(\frac{1}{\lambda - \ell} - \frac{1}{\lambda - \ell_0} \right) d\rho(\lambda) + c(\ell - \ell_0)$$

where the constant $c \geq 0$ (actually we will show $c = 0$) and $\text{Im } \ell + 0 \neq 0$.

Before getting to the details of the proof of this important result, let us restate the theorem in terms of the spectral resolution of a self-adjoint differential operator. Here,

$$Au = \tau u, \quad \mathcal{D}_A = \{u \in \mathcal{D}_{A_1} : \sin \alpha u(0) - \cos \alpha p(0)u'(0) = 0\}.$$

A is a self-adjoint operator. Given any $f \in \mathcal{H} = L_c^2([0, \infty), k)$ we define the transform g of f by

$$g(\lambda) = \int_0^\infty f(x)\psi(x, \lambda)k(x) dx.$$

The expansion theorem for f takes the form

$$f(x) = \int_{-\infty}^{+\infty} g(\lambda)\psi(x, \lambda) d\rho(\lambda),$$

where $(\tau - \lambda)\psi(x, \lambda) = 0$ but in general $\psi(x, \lambda) \notin \mathcal{H}$. The spectral expansion is

$$f(x) = \int_{-\infty}^{+\infty} dE_\lambda f(x) = \int_{-\infty}^{+\infty} g(\lambda)\psi(x, \lambda) d\rho(\lambda),$$

so

$$dE_\lambda f(x) = g(\lambda)\psi(x, \lambda) d\rho(\lambda), \quad E_\lambda f(x) = \int_{-\infty}^\lambda g(\lambda)\psi(x, \lambda) d\rho(\lambda).$$

If $f \in \mathcal{D}_A$ then

$$Af(x) = \int_{-\infty}^{+\infty} \lambda g(\lambda)\psi(x, \lambda) d\rho(\lambda).$$

Corollary 31 *If $g(\lambda) \in L_c^2(\rho)$ then there exists an $f \in L_c^2(I, k)$ such that g is the transform of f .*

To finish the proof of our theorem we need two theorems that are proved in real analysis courses:

Theorem 79 (*Helly Selection Theorem*) *Let $\{h_n\}$, $n = 1, 2, \dots$ be a sequence of real monotonically increasing functions on $(-\infty, +\infty)$ and let H be a continuous nonnegative function on $(-\infty, +\infty)$. If $|h_n(\lambda)| \leq H(\lambda)$, $n = 1, 2, \dots$, $-\infty < \lambda < +\infty$, then there exists a subsequence $\{h_{n_k}\}$ and a monotonically increasing function h such that $\lim_{k \rightarrow \infty} h_{n_k}(\lambda) = h(\lambda)$ and $|h(\lambda)| \leq H(\lambda)$, $-\infty < \lambda < +\infty$.*

Theorem 80 (*Integration Theorem*) *Suppose $\{h_n\}$ is a real, uniformly bounded sequence of monotonically increasing functions on the interval $a \leq \lambda \leq c$ and suppose $\lim_{n \rightarrow \infty} h_n(\lambda) = h(\lambda)$, for $a \leq \lambda \leq c$. If f is continuous on $[a, c]$ then*

$$\lim_{n \rightarrow \infty} \int_a^c f(\lambda) dh_n(\lambda) = \int_a^c f(\lambda) dh(\lambda).$$

PROOF OF THEOREM 78: As in the lead-up to the theorem we consider the basis functions ϕ, ψ and the interval $[0, b]$ with boundary conditions B_0, B_b at the left-hand and right-hand boundary points, respectively. We have chosen ψ so that always $B_0(\psi) = 0$, so the eigenvalues and eigenvectors for this regular problem are $\{\lambda_{bn}\}$ and $\{\theta_{bn}\}$, respectively, where $\theta_{bn}(x) = r_{bn}\psi(x, \lambda_{bn})$. Now let $\text{Im } \lambda > 0$ and let $m_b(\lambda) = m(b, \beta, \lambda) \in C_b$. Set

$$\chi_b(x) = \phi(x, \lambda) + m_b(\lambda)\psi(x, \lambda), \quad [\chi_b, \chi_b](b) = 0, \quad \tau\chi_b = \lambda\chi_b.$$

Choose $m_b(\lambda)$ such that $B_b(\chi_b) = 0$. The completeness theorem for the regular problem on $[0, b]$ implies

$$\int_0^b |\chi_b(x)|^2 k(x) dx = \sum_{n=1}^{\infty} |r_{bn}|^2 \left| \int_0^b \chi_b(x) \psi(x, \lambda_{bn}) k(x) dx \right|^2.$$

Furthermore,

$$\begin{aligned} (\lambda - \lambda_{bn}) \int_0^b \chi_b(x) \psi(x, \lambda_{bn}) k(x) dx = \\ \int_0^b [\tau\chi_b(x)] \psi(x, \lambda_{bn}) k(x) dx - \int_0^b \chi_b(x) [\tau\psi(x, \lambda_{bn})] k(x) dx \end{aligned}$$

$$= [\chi_b, \psi_{bn}](b) - [\chi_b, \psi_{bn}](0) = 1,$$

because $[\chi_b, \psi_{bn}](b) = 0$ (since $B_b(\chi_b) = 0$, $B_b(\psi_{bn}) = 0$), and

$$[\chi_b, \psi_{bn}](0) = [\phi_b, \psi_{bn}](0) + \overline{m_b(\lambda)}[\psi_b, \psi_{bn}](0) = 1,$$

(since $[\phi_b, \psi_{bn}](0) = 1$ and $[\psi_b, \psi_{bn}](0) = 0$). Therefore,

$$\int_0^b \chi_b(x) \psi(x, \lambda_{bn}) k(x) \, dx = \frac{1}{\lambda - \lambda_{bn}}$$

which implies

$$\int_0^b |\chi_b(x)|^2 k(x) \, dx = \int_{-\infty}^{+\infty} \frac{d\rho_b(\mu)}{|\lambda - \mu|^2}.$$

From the Second Weyl Theorem we have

$$\int_0^b |\chi_b(x)|^2 k(x) \, dx = \frac{\operatorname{Im} m_b(\lambda)}{\operatorname{Im} \lambda}$$

so

$$\int_{-\infty}^{+\infty} \frac{d\rho_b(\mu)}{|\lambda - \mu|^2} = \frac{\operatorname{Im} m_b(\lambda)}{\operatorname{Im} \lambda}$$

We investigate this identity in the limit as $b \rightarrow +\infty$. If $\lambda = i$, then for $b > 1$, $C_1 \supset C_b$ which implies

$$\int_{-\infty}^{+\infty} \frac{d\rho_b(\mu)}{\mu^2 + 1} < \text{constant} = k$$

for all $b > 1$. Thus,

$$\int_{-a}^a d\rho_b(\mu) < k(1 + a^2)$$

for all $a > 0$. Since $\rho_b(0) = 0$, this implies

$$|\rho_b(a)| < k(1 + a^2), \quad -\infty < a < \infty.$$

It follows from the Helly Selection Theorem that there exists a limit function

$$\rho(\mu) = \lim_{b_j \rightarrow +\infty} \rho_{b_j}(\mu), \quad |\rho(\mu)| < k(1 + \mu^2).$$

This proves the first statement of Theorem 78.

Suppose $f \in \dot{C}^2([0, \infty))$. Then $f \in \mathcal{D}_A$ and

$$\int_0^\infty |\tau f(x)|^2 k(x) dx = \int_{-\infty}^\infty \left| \int_0^\infty (\tau f(x)) \psi(x, \mu) k(x) dx \right|^2 d\rho_b(\mu).$$

Since

$$g(\mu) = \int_0^\infty f(x) \psi(x, \mu) k(x) dx$$

is the transform of f we have

$$\int_0^\infty (\tau f) \psi(x, \mu) k(x) dx = \int_0^\infty f(\tau \psi) k dx = \mu g(\mu).$$

Therefore,

$$\int_0^\infty |\tau f|^2 k(x) dx = \int_0^\infty \mu^2 |g(\mu)|^2 d\rho_b(\mu).$$

Now

$$\begin{aligned} \left| \int_0^\infty |f|^2 k dx - \int_{-a}^a |g(\mu)|^2 d\rho(\mu) \right| &\leq \left| - \int_{-a}^a |g(\mu)|^2 d\rho(\mu) + \int_{-a}^a |g(\mu)|^2 d\rho_b(\mu) \right| \\ &+ \left| \int_0^\infty |f|^2 k dx - \int_{-a}^a |g(\mu)|^2 d\rho_b(\mu) \right|. \end{aligned}$$

We have

$$\begin{aligned} \left| \int_0^\infty |f|^2 k dx - \int_{-a}^a |g(\mu)|^2 d\rho_b(\mu) \right| &= \left| \left(\int_{-\infty}^{-a} + \int_a^{+\infty} \right) |g(\mu)|^2 d\rho_b(\mu) \right| \\ &= \int_\Delta |g(\mu)|^2 d\rho_b(\mu) \longrightarrow 0 \end{aligned}$$

as $a \rightarrow +\infty$. Furthermore

$$\int_\Delta |g(\mu)|^2 d\rho_b(\mu) a^2 \leq \int_\Delta \mu^2 |g(\mu)|^2 d\rho_b(\mu) \leq \int_0^\infty |\tau f|^2 k dx.$$

Therefore,

$$\left| \int_0^\infty |f|^2 k dx - \int_{-a}^a |g(\mu)|^2 d\rho(\mu) \right| \leq \frac{1}{a^2} \int_0^\infty |\tau f|^2 k dx.$$

Thus we have obtained Parseval's Theorem

$$\int_0^\infty |f|^2 k dx = \int_{-\infty}^{+\infty} |g(\mu)|^2 d\rho(\mu). \quad (4.17)$$

We could now use standard arguments to prove (4.17) for all $f \in L_c^2(I, k)$. This is the completeness proof of statement 2 in Theorem 78.

Once we have Parseval's Theorem, the proof of the expansion formula

$$f(x) = \lim_{\mu, \nu \rightarrow \infty} \int_{-\nu}^{\mu} g(\lambda) \psi(x, \lambda) d\lambda$$

becomes "standard abstract nonsense". However we give the details.

Let $f_1, f_2 \in \mathcal{H}$ with transforms $g_1, g_2 \in L_c^2(\rho)$. Then

$$\int_0^\infty f_1(x) \overline{f_2(x)} k(x) dx = \int_{-\infty}^\infty g_1(\mu) \overline{g_2(\mu)} d\rho(\mu),$$

since

$$f_1 f_2 = \frac{1}{4} \left\{ |f_1 + f_2|^2 - |f_1 - f_2|^2 + i|f_1 + if_2|^2 - i|f_1 - if_2|^2 \right\}.$$

Now let $\delta = (\lambda, \nu]$ and set

$$f_\Delta(x) = \int_\Delta g(\mu) \psi(x, \mu) d\rho(\mu)$$

where g is the transform of f . Let $F \in \mathcal{H}$ such that $F(x) \equiv 0$ for $x > a$ (say), and let G be the transform of F . Then

$$\begin{aligned} \int_0^\infty f_\Delta(x) \overline{F(x)} k(x) dx &= \int_0^a f_\Delta(x) \overline{F(x)} k(x) dx = \\ &= \int_0^a \left[\int_\Delta g(\mu) \psi(x, \mu) d\rho(\mu) \right] \overline{F(x)} k(x) dx = \int_\Delta g(\mu) \overline{G(\mu)} d\rho(\mu). \end{aligned}$$

Also,

$$\int_0^\infty f(x) \overline{F(x)} k(x) dx = \int_{-\infty}^{+\infty} g(\mu) \overline{G(\mu)} d\rho(\mu).$$

Now let $\Delta^c = (-\infty, +\infty) - \Delta$. Then

$$\int_0^\infty (f(x) - f_\Delta(x)) \overline{F(x)} k(x) dx = \int_{\Delta^c} g(\mu) \overline{G(\mu)} d\rho(\mu)$$

so

$$\begin{aligned} \left| \int_0^\infty (f - f_\Delta) \overline{F} k dx \right|^2 &\leq \int_{\Delta^c} |g(\mu)|^2 d\rho(\mu) \int_{\Delta^c} |G(\mu)|^2 d\rho(\mu) \\ &\leq \int_{\Delta^c} |g(\mu)|^2 d\rho(\mu) \int_0^\infty |F(x)|^2 k(x) dx. \end{aligned}$$

Let

$$F(x) = \begin{cases} f(x) - f_\Delta(x) & \text{if } 0 \leq x \leq a \\ = 0 & \text{if } x > a \end{cases}$$

Then

$$\int_0^a |f - f_\Delta|^2 k(x) dx \leq \int_\Delta |g(\mu)|^2 d\rho(\mu).$$

Letting $a \rightarrow +\infty$ we have

$$\int_0^\infty |f - f_\Delta|^2 k(x) dx \leq \int_\Delta |g(\mu)|^2 d\rho(\mu).$$

Thus,

$$\int_\lambda^\nu g(\mu) \psi(x, \mu) d\rho(\mu) = f_\Delta \longrightarrow f \in \mathcal{H} \text{ as } \Delta \longrightarrow (-\infty, +\infty).$$

This finishes our verification of the expansion formula.

We turn to the proofs of the fourth and third statements of the Theorem.

We know that

$$\int_{-\infty}^{+\infty} \frac{d\rho_b(\mu)}{|\lambda - \mu|^2} = \frac{\text{Im } m_b(\lambda)}{\text{Im } \lambda}, \quad \text{Im } \lambda > 0.$$

For any fixed λ with $\text{Im } \lambda > 0$ there exists a constant $c > 0$ such that

$$\int_{-\nu}^{+\nu} \frac{d\rho_b(\mu)}{|\lambda - \mu|^2} \leq c$$

for all $b > 1$ and $\mu \geq 0$. Then if we let $b \rightarrow +\infty$, it follows from the Integration Theorem that

$$\int_{-\nu}^{+\nu} \frac{d\rho(\mu)}{|\lambda - \mu|^2} \leq c.$$

Recall that

$$\int_{-\infty}^{+\infty} \frac{d\rho_b(\mu)}{\mu^2 + 1} < k$$

for all $b > 1$. This implies for all $b > 1$ that there exists a $q > 0$ such that

$$\int_\nu^{+\infty} \frac{d\rho(\mu)}{\mu^3} < \frac{q}{\nu} \quad \text{if } \nu > 1.$$

Similarly, there exists $p > 0$ such that

$$\left| \int_{-\infty}^{-\nu} \frac{d\rho_b(\mu)}{\mu^3} \right| < \frac{p}{\nu} \quad \text{if } \nu > 1$$

uniformly for all $b > 1$.

Now if $\text{Im } \lambda \neq 0$, $\text{Im } \lambda_0 \neq 0$ then

$$\int_{-\infty}^{+\infty} \left(\frac{1}{|\mu - \lambda|^2} - \frac{1}{|\mu - \lambda_0|^2} \right) d\rho_b(\mu) = \frac{\text{Im } m_b(\lambda)}{\text{Im } \lambda} - \frac{\text{Im } m_b(\lambda_0)}{\text{Im } \lambda_0}. \quad (4.18)$$

As $b \rightarrow +\infty$, $\nu \rightarrow +\infty$ the left-hand side of (4.18) behaves as

$$\begin{aligned} & \left(\int_{-\infty}^{-\nu} + \int_{-\nu}^{+\nu} + \int_{+\nu}^{+\infty} \right) \left(\frac{1}{|\mu - \lambda|^2} - \frac{1}{|\mu - \lambda_0|^2} \right) d\rho_b(\mu) \\ & \longrightarrow \int_{-\infty}^{+\infty} \left(\frac{1}{|\mu - \lambda|^2} - \frac{1}{|\mu - \lambda_0|^2} \right) d\rho(\mu), \end{aligned}$$

whereas the right-hand side of (4.18) behaves as

$$\frac{\text{Im } m_b(\lambda)}{\text{Im } \lambda} - \frac{\text{Im } m_b(\lambda_0)}{\text{Im } \lambda_0} \longrightarrow \frac{\text{Im } m_\infty(\lambda)}{\text{Im } \lambda} - \frac{\text{Im } m_\infty(\lambda_0)}{\text{Im } \lambda_0}.$$

Thus,

$$\int_{-\infty}^{+\infty} \frac{d\rho(\mu)}{|\lambda - \mu|^2} + c = \frac{\text{Im } m_\infty(\lambda)}{\text{Im } \lambda}, \quad \text{Im } \lambda > 0.$$

We can show that $c \geq 0$. Note that $\text{Im } m_\infty(\lambda)/\text{Im } \lambda > 0$. Now suppose $c < 0$. Let $\text{Re } \lambda = 0$ and choose $\text{Im } \lambda$ so large that

$$\int_{-\infty}^{+\infty} \frac{d\rho(\mu)}{|\lambda - \mu|^2} < \frac{|c|}{2}.$$

Then

$$-\frac{c}{2} + c = \frac{|c|}{2} + c > 0,$$

which is a contradiction. Thus $c \geq 0$. (Actually it can be shown that $c = 0$.)

We turn to the third statement of the Theorem. Let λ, ν be points of continuity for ρ . We have

$$\lim_{\epsilon \rightarrow +0} \int_{\nu}^{\lambda} \text{Im } m_\infty(\mu + i\epsilon) d\mu = \lim_{\epsilon \rightarrow +0} \int_{\nu}^{\lambda} d\mu \int_{-\infty}^{+\infty} \frac{\epsilon d\rho(\sigma)}{(\sigma - \mu)^2 + \epsilon^2}$$

$$\begin{aligned}
&= \lim_{\epsilon \rightarrow +0} \int_{-\infty}^{+\infty} \left[\arctan\left(\frac{\lambda - \sigma}{\epsilon}\right) - \arctan\left(\frac{\nu - \sigma}{\epsilon}\right) \right] d\rho(\sigma) \\
&= \pi \int_{\nu}^{\lambda} d\rho(\sigma) = \pi (\rho(\lambda) - \rho(\nu)),
\end{aligned}$$

because

$$\lim_{\epsilon \rightarrow 0+} \left[\arctan\left(\frac{\lambda - \sigma}{\epsilon}\right) - \arctan\left(\frac{\nu - \sigma}{\epsilon}\right) \right] = \begin{cases} \pi & \text{if } \lambda > \sigma > \nu \\ \pi/2 & \text{if } \sigma = \nu \\ -\pi/2 & \text{if } \sigma = \lambda \\ 0 & \text{otherwise.} \end{cases}$$

Therefore

$$\lim_{\epsilon \rightarrow +0} \frac{1}{\pi} \int_{\nu}^{\lambda} \operatorname{Im} m_{\infty}(\mu + i\epsilon) d\mu = \rho(\lambda) - \rho(\nu).$$

This concludes the proof of Theorem 78.

Corollary 32 *The map $f \in \mathcal{H} \longrightarrow g \in L_c^2(\rho)$ is unitary.*

REMARK: If τ is limit circle at ∞ , Theorem 78 still holds if we pick out a unique $m_{\infty}(\lambda) \in C_{\infty}$ by means of a boundary condition at ∞ :

$$B(u) = [u, v]_{\infty}, \quad v \in \mathcal{D}_+.$$

The corresponding boundary condition at b is $B_b(u) = [u, v](b)$.

We describe how to compute $m_{\infty}(\lambda)$, $\operatorname{Im} \lambda \neq 0$, in the limit point case at ∞ :

$$m_{\infty}(\lambda) = \lim_{b \rightarrow \infty} m(b, \beta, \lambda) = - \lim_{b \rightarrow \infty} \frac{\cos \phi(b, \lambda) + p(b) \phi'(b, \lambda) \sin \beta}{\cos \psi(b, \lambda) + p(b) \psi'(b, \lambda) \sin \beta}.$$

The limit is independent of β so we can set $\beta = 0$ for simplicity:

$$m_{\infty}(\lambda) = - \lim_{b \rightarrow \infty} \frac{\phi(b, \lambda)}{\psi(b, \lambda)}.$$

Example 19 *Take*

$$\tau = -\frac{d^2}{dx^2}, \quad I = [0, \infty).$$

Here the equation $\tau u = 0$ has a basis of solutions $u_1(x) = 1, u_2(x) = x$, so the problem is limit circle at 0 and limit point at ∞ . We choose the boundary

condition $B_0(u) = u'(0) = 0$. Then the basis of solutions ϕ, ψ of $\tau u = \lambda u$ such that

$$\phi(0, \lambda) = 0, \quad \phi'(0, \lambda) = -1, \quad \psi(0, \lambda) = 1, \quad \psi'(0, \lambda) = 0$$

is

$$\phi(x, \lambda) = -\frac{\sin \sqrt{\lambda} x}{\sqrt{\lambda}}, \quad \psi(x, \lambda) = \cos \sqrt{\lambda} x.$$

Thus for $\text{Im } \lambda \geq 0$ we have

$$m_\infty(\lambda) = -\lim_{b \rightarrow \infty} \frac{\phi(x, \lambda)}{\psi(x, \lambda)} = \lim_{b \rightarrow \infty} \frac{\tan \sqrt{\lambda} b}{\sqrt{\lambda}} = -\frac{1}{i\sqrt{\lambda}} = \frac{i}{\sqrt{\lambda}},$$

and, for $\epsilon > 0$,

$$\text{Im } m_\infty(\mu + i\epsilon) = \begin{cases} \frac{1}{\sqrt{\mu}} & \text{if } \mu > 0 \\ 0 & \text{if } \mu < 0 \end{cases}$$

Therefore,

$$\rho(\nu) - \rho(\lambda) = \frac{1}{\pi} \int_\lambda^\nu \frac{1}{\sqrt{\mu}} d\mu = \frac{2}{\pi} (\sqrt{\nu} - \sqrt{\lambda}),$$

and we can take

$$\rho(\mu) = \begin{cases} \frac{2}{\pi} \sqrt{\mu} & \text{if } \mu \geq 0, \\ 0 & \text{if } \mu < 0. \end{cases}$$

We conclude that the transform and expansion expressions are

$$g(\mu) = \int_0^\infty f(x) \cos \sqrt{\mu} x \, dx, \quad f(x) = \frac{1}{\pi} \int_0^\infty g(\mu) \cos \sqrt{\mu} x \, \frac{d\mu}{\sqrt{\mu}}.$$

4.3.3 Separated boundary conditions and spectral resolutions with singular behavior at each endpoint

Now we consider the case where there is singular behavior at both endpoints ℓ and m . Without loss of generality, we can assume $\ell = -\infty$ and $m = +\infty$, so $I = (-\infty, +\infty)$.

Let ϕ_1, ϕ_2 be solutions of $\tau\phi = \lambda\phi$ such that

$$\phi_1(0, \lambda) = 1, \quad p(0)\phi_1'(0, \lambda) = 0,$$

$$\phi_2(0, \lambda) = 0, \quad p(0)\phi_2'(0, \lambda) = 1,$$

for all complex λ . Let a, b be finite numbers such that $a < 0 < b$ and consider a regular eigenvalue problem on the finite interval $\delta = [a, b]$. The problem is $\tau u = \lambda u$ with boundary conditions

$$B_a(u) = \cos \alpha u(a) + \sin \alpha p(a)u'(a) = 0,$$

$$B_b(u) = \cos \beta u(b) + \sin \beta p(b)u'(b) = 0, \quad 0 \leq \alpha, \beta < \pi.$$

Then there exist a sequence of eigenvalues $\{\lambda_{\delta n}\}$ and ON eigenvectors $\{h_{\delta n}\}$ such that $\tau h_{\delta n} = \lambda_{\delta n} h_{\delta n}$, and for all f_1, f_2 square integrable on δ , we have Parseval's equality

$$\int_a^b f_1(x) \overline{f_2(x)} k(x) dx = \sum_{n=1}^{\infty} \int_a^b f_1(x) \overline{h_{\delta n}} k(x) dx \overline{\int_a^b f_2(x) \overline{h_{\delta n}} k(x) dx}. \quad (4.19)$$

Now there exist constants $\{r_{\delta n1}\}, \{r_{\delta n2}\}$ such that

$$h_{\delta n} = r_{\delta n1} \phi_1(x, \lambda_{\delta n}) + r_{\delta n2} \phi_2(x, \lambda_{\delta n})$$

for $n = 1, 2$. (We can assume that the r 's are real.) Thus for any $f \in L_c^2(I, k)$ we can write

$$\int_{\delta} |f(x)|^2 k(x) dx = \int_{-\infty}^{+\infty} \sum_{j,k=1}^n \overline{g_{\delta j}(\mu)} g_{\delta k}(\mu) d\rho_{\delta jk}(\mu),$$

where

$$g_{\delta k}(\mu) = \int_{\delta} f(x) \phi_k(x, \lambda_{\delta n}) dx$$

and $\rho_{\delta} = (\rho_{\delta jk})$ is the **spectral matrix**. The matrix elements are step functions with their only discontinuities at $\{\lambda_{\delta n}\}$. Here

$$\rho_{\delta jk}(\lambda + 0) - \rho_{\delta jk}(\lambda_{\delta n} - 0) = \sum_m r_{\delta mj} \overline{r_{\delta mk}}$$

and the sum is over all m such that $\lambda_{\delta m} = \lambda_{\delta n}$. We require that $\rho_{\delta jk}(\lambda_{\delta n} + 0) = \rho_{\delta jk}(\lambda_{\delta n})$ and $\rho_{\delta jk}(0) = 0$. Note: ρ_{δ} is a Hermitian matrix.

In the following we assume $\text{Im } \lambda \neq 0$. Let $\chi_a = \phi_1 + m_a \phi_2$ be a solution of $\tau \chi_a = \lambda \chi_a$ such that $B_a(\chi_a) = 0$. Thus $m_a \in C_a$ and $[\chi_a, \chi_a](a) = 0$. Further, let $\chi_b = \phi_1 + m_b \phi_2$ be a solution of $\tau \chi_b = \lambda \chi_b$ such that $B_b(\chi_b) = 0$, which implies $m_b \in C_b$ and $[\chi_b, \chi_b](b) = 0$. Note that χ_a, χ_b are linearly independent and

$$W(\chi_a, \chi_b) = [\chi_a, \overline{\chi_b}](x) \equiv [\chi_a, \overline{\chi_b}](0) = m_b(\lambda) - m_a(\lambda).$$

Now we apply the Parseval equality (4.19) to

$$f_1(x) = \begin{cases} \chi_a(x, \lambda) & a \leq x \leq 0 \\ 0 & 0 < x \leq b, \end{cases} \quad f_2(x) = \begin{cases} 0 & a \leq x < 0 \\ \chi_b(x, \lambda) & 0 \leq x \leq b, \end{cases}$$

We consider three cases.

1.

$$\int_{\delta} |f_1(x)|^2 k(x) dx = \int_a^0 |\chi_a|^2 k dx = \sum_{n=1}^{\infty} \left| \int_a^0 \chi_a \overline{h_{\delta n}} k dx \right|^2.$$

To evaluate the left-hand side of this equation we observe that

$$\begin{aligned} 2i \operatorname{Im} \lambda \int_a^0 |\chi_a|^2 k dx &= \int_a^0 (\tau \chi_a) \overline{\chi_a} k dx - \int_a^0 \chi_a (\overline{\tau \chi_a}) k dx \\ &= [\chi_a, \chi_a](0) - [\chi_a, \chi_a](a) = [\chi_a, \chi_a](0) = -2i \operatorname{Im} m_a(\lambda). \end{aligned}$$

To evaluate the right-hand side of the equation we note that

$$\begin{aligned} (\lambda - \lambda_{\delta n}) \int_a^0 \chi_a \overline{h_{\delta n}} k dx &= [\chi_a, h_{\delta n}](0) - [\chi_a, h_{\delta n}](a) = [\chi_a, h_{\delta n}](0) \\ &= [\phi_1 + m_a(\lambda)\phi_2, r_{\delta n 1}\phi_1 + r_{\delta n 2}\phi_2](0) = \overline{r_{\delta n 2}} - \overline{r_{\delta n 1}} m_a(\lambda), \end{aligned}$$

because

$$[\phi_1, \phi_1] = [\phi_2, \phi_2] = 0, \quad [\phi_1, \phi_2] = 1.$$

Thus the identity becomes

$$-\frac{\operatorname{Im} m_a(\lambda)}{\operatorname{Im} \lambda} = \sum_n \frac{|r_{\delta n 2}|^2 + |r_{\delta n 1}|^2 |m_a(\lambda)|^2 - \overline{r_{\delta n 2}} r_{\delta n 1} \overline{m_a(\lambda)} - r_{\delta n 2} \overline{r_{\delta n 1}} m_a(\lambda)}{|\lambda - \lambda_{\delta n}|^2}.$$

2.

$$\int_{\delta} |f_2(x)|^2 k(x) dx = \int_0^b |\chi_b|^2 k dx = \sum_{n=1}^{\infty} \left| \int_0^b \chi_b \overline{h_{\delta n}} k dx \right|^2.$$

To evaluate the left-hand side of this equation we observe that

$$2i \operatorname{Im} \lambda \int_0^b |\chi_b|^2 k dx = [\chi_b, \chi_b](b) - [\chi_b, \chi_b](0) = -[\chi_b, \chi_b](0) = 2i \operatorname{Im} m_b(\lambda).$$

To evaluate the right-hand side of the equation we note that

$$(\lambda - \lambda_{\delta n}) \int_0^b \chi_b \overline{h_{\delta n}} k dx = [\chi_b, h_{\delta n}](b) - [\chi_b, h_{\delta n}](0) = -[\chi_b, h_{\delta n}](0)$$

$$= -[\phi_1 + m_b(\lambda)\phi_2, r_{\delta n1}\phi_1 + r_{\delta n2}\phi_2](0) = -\overline{r_{\delta n2}} + \overline{r_{\delta n1}}m_b(\lambda),$$

Thus the identity becomes

$$\frac{\operatorname{Im} m_b(\lambda)}{\operatorname{Im} \lambda} = \sum_n \frac{|r_{\delta n2}|^2 + |r_{\delta n1}|^2 |m_b(\lambda)|^2 - \overline{r_{\delta n2}} r_{\delta n1} \overline{m_b(\lambda)} - r_{\delta n2} \overline{r_{\delta n1}} m_b(\lambda)}{|\lambda - \lambda_{\delta n}|^2}.$$

3.

$$\int_{\delta} f_1(x) \overline{f_2(x)} k(x) dx = 0 = \sum_{n=1}^{\infty} \int_a^0 \chi_a \overline{h_{\delta n}} k dx \int_0^b \chi_b \overline{h_{\delta n}} k dx.$$

From the computations above we thus find

$$0 = \sum_n \frac{(\overline{r_{\delta n2}} - \overline{r_{\delta n1}} m_a(\lambda))(-r_{\delta n2} + r_{\delta n1} \overline{m_b(\lambda)})}{|\lambda - \lambda_{\delta n}|^2} =$$

$$\sum_n \frac{-|r_{\delta n2}|^2 + r_{\delta n2} \overline{r_{\delta n1}} m_a(\lambda) + r_{\delta n1} \overline{r_{\delta n2}} \overline{m_b(\lambda)} - |r_{\delta n1}|^2 m_a(\lambda) \overline{m_b(\lambda)}}{|\lambda - \lambda_{\delta n}|^2}.$$

We can express these three identities in terms of the spectral matrix $\rho_{\delta} = (\rho_{\delta jk})$. Indeed, noting that $\rho_{\delta 12} = \rho_{\delta 21}$, we can write the identities as

1.

$$-\frac{\operatorname{Im} m_a(\lambda)}{\operatorname{Im} \lambda} = \int_{-\infty}^{+\infty} \frac{d\rho_{\delta 22}(\mu) + d\rho_{\delta 11}(\mu) |m_a(\lambda)|^2 - d\rho_{\delta 12}(\mu)(m_a(\lambda) + \overline{m_a(\lambda)})}{|\lambda - \mu|^2},$$

2.

$$\frac{\operatorname{Im} m_b(\lambda)}{\operatorname{Im} \lambda} = \int_{-\infty}^{+\infty} \frac{d\rho_{\delta 22}(\mu) + d\rho_{\delta 11}(\mu) |m_b(\lambda)|^2 - d\rho_{\delta 12}(\mu)(m_b(\lambda) + \overline{m_b(\lambda)})}{|\lambda - \mu|^2},$$

3.

$$0 = \int_{-\infty}^{+\infty} \frac{-d\rho_{\delta 22}(\mu) - d\rho_{\delta 11}(\mu) m_a(\lambda) \overline{m_b(\lambda)} + d\rho_{\delta 12}(\mu)(m_a(\lambda) + \overline{m_b(\lambda)})}{|\lambda - \mu|^2}.$$

Note that we have three linear equations for the three measures $d\rho_{\delta 11}, d\rho_{\delta 12}, d\rho_{\delta 22}$. Straightforward elimination yields the results

$$\int_{-\infty}^{+\infty} \frac{d\rho_{\delta 11}(\mu)}{|\lambda - \mu|^2} = \frac{\operatorname{Im} M_{\delta 11}(\lambda)}{\operatorname{Im} \lambda}, \quad M_{\delta 11}(\lambda) = \frac{1}{m_a(\lambda) - m_b(\lambda)}, \quad (4.20)$$

$$\int_{-\infty}^{+\infty} \frac{d\rho_{\delta 22}(\mu)}{|\lambda - \mu|^2} = \frac{\operatorname{Im} M_{\delta 22}(\lambda)}{\operatorname{Im} \lambda}, \quad M_{\delta 22}(\lambda) = \frac{m_a(\lambda)m_b(\lambda)}{m_a(\lambda) - m_b(\lambda)}, \quad (4.21)$$

$$\int_{-\infty}^{+\infty} \frac{d\rho_{\delta 12}(\mu)}{|\lambda - \mu|^2} = \int_{-\infty}^{+\infty} \frac{d\rho_{\delta 21}(\mu)}{|\lambda - \mu|^2} = \frac{\operatorname{Im} M_{\delta 12}(\lambda)}{\operatorname{Im} \lambda}, \quad M_{\delta 12}(\lambda) = \frac{1}{2} \frac{m_a(\lambda) + m_b(\lambda)}{m_a(\lambda) - m_b(\lambda)}. \quad (4.22)$$

Note that a consequence of (4.20) is the inequality

$$\frac{\operatorname{Im} (m_b - m_a)}{\operatorname{Im} \lambda} = \int_{-\infty}^{+\infty} \frac{|m_a - m_b|^2 d\rho(\mu)}{|\lambda - \mu|^2} \geq 0.$$

This implies that $m_a(\lambda)$ and $m_b(\lambda)$ are in opposite half planes for $\operatorname{Im} \lambda \neq 0$.

Just as in the limit circle - limit point case we can let $\delta = [a, b] \rightarrow (-\infty, +\infty)$ and use the Helly selection Theorem to show that there exists a sequence of intervals $\delta_n = [a_n, b_n] \rightarrow (-\infty, +\infty)$, and corresponding boundary conditions B_{a_n}, B_{b_n} such that $\rho_{\delta_n jk}(\mu) \rightarrow \rho_{jk}(\mu)$ for $j, k = 1, 2$. Further we can show that the matrix function $\rho(\mu) = (\rho_{jk}(\mu))$ is

- a. Hermitian (Indeed we can assume that it is real and symmetric.)
- b. The symmetric spectral matrix satisfies $\rho(\lambda) - \rho(\mu) \geq 0$ if $\lambda > \mu$.
- c. Each ρ_{jk} is of finite total variation on any finite μ - interval.

In the limit point case at $-\infty$ and $+\infty$, ρ is unique, since $C_{a_n} \rightarrow \text{pt.}$ and $C_{b_n} \rightarrow \text{pt.}$ as $n \rightarrow \infty$. If there is a limit circle endpoint (say $+\infty$) then to define a unique extension we need a boundary condition $B_\infty(u) = [u, v]_\infty$, $v \in \mathcal{D}_+$. Now take $B_{b_n}(u) = [u, v](b_n)$ and define $m_{b_n}(\lambda) \in C_b(\lambda)$ by $B_{b_n}(\chi_{b_n}) = 0$, $\chi_{b_n} = \phi_1 + m_{b_n}\phi_2$.

We conclude that in all cases we obtain a limit spectral matrix $\rho(\mu)$ such that

$$\rho_{jk}(\nu) - \rho_{jk}(\lambda) = \lim_{\epsilon \rightarrow 0+} \int_{\lambda}^{\nu} \operatorname{Im} M_{jk}(\mu + i\epsilon) d\mu \quad (4.23)$$

where

$$M_{11}(\lambda) = \frac{1}{m_{-\infty}(\lambda) - m_\infty(\lambda)}, \quad M_{22}(\lambda) = \frac{m_{-\infty}(\lambda)m_\infty(\lambda)}{m_{-\infty}(\lambda) - m_\infty(\lambda)}, \quad (4.24)$$

$$M_{12}(\lambda) = M_{21}(\lambda) = \frac{1}{2} \frac{m_{-\infty}(\lambda) + m_{\infty}(\lambda)}{m_{-\infty}(\lambda) - m_{\infty}(\lambda)}. \quad (4.25)$$

Note: In the limit point - limit point case we have

$$m_{-\infty}(\lambda) = - \lim_{a \rightarrow -\infty} \frac{\phi_1(a, \lambda)}{\phi_2(a, \lambda)}, \quad m_{+\infty}(\lambda) = - \lim_{b \rightarrow +\infty} \frac{\phi_1(b, \lambda)}{\phi_2(b, \lambda)}.$$

The derivation and proof of the expansion theorem follows by analogy with the limit circle - limit point case, and we just present the results. Let $L_c^2(\rho)$ be the Hilbert space of all vectors $g(\mu) = \{g_1(\mu), g_2(\mu)\}$ such that

$$\|g\|^2 = \int_{-\infty}^{\infty} \sum_{j,k=1}^2 g_j(\mu) \overline{g_k(\mu)} d\rho_{jk}(\mu) < \infty,$$

where

$$(g, h) = \int_{-\infty}^{\infty} \sum_{j,k=1}^2 g_j(\mu) \overline{h_k(\mu)} d\rho_{jk}(\mu).$$

Note that $\|g\| \geq 0$. Now let $f \in \mathcal{H} = L_c^2(I, k)$. We define the transforms $g = \{g_1, g_2\}$ of f by

$$g_j(\mu) = \lim_{a \rightarrow -\infty, b \rightarrow +\infty} \int_a^b f(x) \phi_j(x, \mu) k(x) dx$$

where the convergence is in the Hilbert space norm. The limit exists and $g \in L_c^2(\rho)$. Furthermore, for $f^{(1)}, f^{(2)} \in L_c^2(I, k)$, we have the Parseval equality

$$\int_{-\infty}^{\infty} f^{(1)}(x) \overline{f^{(2)}(x)} k(x) dx = \int_{-\infty}^{\infty} \sum_{j,k=1}^2 g_j^{(1)}(\mu) \overline{g_k^{(2)}(\mu)} d\rho_{jk}(\mu),$$

i.e., the map $f \in \mathcal{H} \longrightarrow g = \{g_1, g_2\} \in L_c^2(\rho)$ is unitary. The expansion theorem is

$$f(x) = \int_{-\infty}^{\infty} \sum_{j,k=1}^2 \phi_j(x, \mu) g_k(\mu) d\rho_{jk}(\mu),$$

where the convergence is in \mathcal{H} .

Example 20 Consider the eigenvalue problem $\tau u = \lambda u$ where

$$\tau u = -u'' + \frac{\nu^2 - \frac{1}{4}}{x^2} u, \quad I = (0, +\infty), \quad 0 < \nu.$$

If we set $u = \sqrt{x}v(x)$ then the equation $\tau u = \lambda u$ becomes

$$-v'' - \frac{v'}{x} + \frac{\nu^2}{x^2}v = \lambda v$$

or

$$-\frac{1}{x}(xv')' + \frac{\nu^2}{x^2}v = \lambda v,$$

which is Bessel's equation.

Set $\lambda = 0$ and look for solutions of $\tau u = 0$ of the form $u = x^\alpha$. Such solutions exist provided $\alpha = 1/2 \pm \nu$. From this result we conclude that our problem is limit circle at 0 if $0 < \nu < 1$ and limit point at 0 if $\nu \geq 1$. It is limit point at $+\infty$ for all $\nu > 0$.

Now we compute a basis of solutions of $\tau u = \lambda u$ near $x = 0$. We use the trial solutions

$$u(x) = \sum_{n=0}^{\infty} a_n x^{n+\alpha}, \quad \alpha = 1/2 + \nu, 1/2 - \nu.$$

From this we find the two solutions

$$u_1(x) = \sqrt{x}J_\nu(\sqrt{\lambda}x), \quad u_2(x) = \sqrt{x}J_{-\nu}(\sqrt{\lambda}x),$$

where

$$J_\nu(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{\Gamma(\nu + n + 1)} \left(\frac{x}{2}\right)^{2n-\nu}$$

and the series converges for $0 < |x| < \infty$.

Note: The Gamma function is defined by

$$\Gamma(\beta) = \int_0^{\infty} e^{-t} t^{\beta-1} dt, \quad \text{Re } \beta > 0,$$

and extended by analytic continuation for all complex $\nu \neq 0, -1, -2, \dots$. It obeys the identities

$$\Gamma(\beta + 1) = \beta\Gamma(\beta), \quad \Gamma(\beta)\Gamma(1 - \beta) = \frac{\pi}{\sin \pi\beta}.$$

In the special case $\beta = n + 1$ where $n = 0, 1, 2, \dots$ the first identity becomes $\Gamma(n + 1) = n!$. Clearly, $u - 1, u - 2$ are linearly independent unless ν is an integer. Then $J_{-n}(x) = (-1)^n J_n(x)$.

We need to find solutions that form a basis for all ν . Note that

$$J_\nu(x) = \frac{(x/2)^\nu}{\Gamma(\nu+1)} \left(1 + O(x^2)\right), \quad J'_\nu(x) = \frac{(x/2)^{\nu-1}}{2\Gamma(\nu)} \left(1 + O(x^2)\right).$$

Thus the Wronskian is given by $xW(J_\nu(x), J_{-\nu}(x)) \equiv C$ or

$$W(J_\nu, J_{-\nu})(x) = -\frac{2 \sin \nu \pi}{\pi x} + O(x) = \frac{C}{x},$$

or $W(J_\nu, J_{-\nu})(x) = -\frac{2 \sin \nu \pi}{\pi x}$. We define the Neumann function by

$$Y_\nu(x) = \frac{J_\nu(x) \cos \nu \pi - J_{-\nu}(x)}{\sin \nu \pi}.$$

Using the L'Hôpital theorem we can verify that the $Y_n(x) = \lim_{\nu \rightarrow n} Y_\nu(x)$ exists and defines a solution of Bessel's equation for $\nu = n$. Further, we have Lommel's formula

$$W(J_\nu(x), Y_\nu(x)) = \frac{\cos \nu \pi}{\sin \nu \pi} W(J_\nu, J_\nu) - \frac{1}{\sin \nu \pi} W(J_\nu, J_{-\nu}) = -\frac{1}{\sin \nu \pi} W(J_\nu, J_{-\nu}) = \frac{2}{\pi x},$$

so $\{J_\nu, Y_\nu\}$ is a basis of solutions of Bessel's equation for all $\nu \neq 0, -1, \dots$. A second important basis is $\{H_\nu^{(1)}, H_\nu^{(2)}\}$ where the Hankel functions are defined by

$$H_\nu^{(1)}(x) = J_\nu(x) + iY_\nu(x) = \frac{J_{-\nu}(x) - e^{-\nu\pi i} J_\nu(x)}{i \sin \nu \pi},$$

$$H_\nu^{(2)}(x) = J_\nu(x) - iY_\nu(x) = \frac{J_{-\nu}(x) - e^{+\nu\pi i} J_\nu(x)}{-i \sin \nu \pi}.$$

Now fix a finite number c , $0 < c$ and construct the associated basis of solutions of $\tau u = \lambda u$ at c :

$$\phi_2(x, \lambda) = -\frac{\pi}{2} \sqrt{xc} \left(J_\nu(\sqrt{\lambda}x) Y_\nu(\sqrt{\lambda}c) - Y_\nu(\sqrt{\lambda}x) J_\nu(\sqrt{\lambda}c) \right),$$

$$\phi_1(x, \lambda) = \frac{\pi}{2} \sqrt{xc\lambda} \left(J_\nu(\sqrt{\lambda}x) Y'_\nu(\sqrt{\lambda}c) - Y_\nu(\sqrt{\lambda}x) J'_\nu(\sqrt{\lambda}c) \right) - \frac{1}{2c} \phi_2(x, \lambda).$$

Then a straightforward calculation making use of the Wronskian formulas yields

$$\phi_2(c, \lambda) = 0, \quad \phi'_2(c, \lambda) = 1, \quad \phi_1(c, \lambda) = 1, \quad \phi'_1(c, \lambda) = 0.$$

Now assume $\nu \geq 1$, i.e., 0 is limit point. Then

$$\int_0^c |\sqrt{x} J_{-\nu}(\sqrt{\lambda}x)|^2 dx = \infty, \quad \int_0^c |\sqrt{x} J_{\nu}(\sqrt{\lambda}x)|^2 dx < \infty.$$

We find

$$m_0(\lambda) = \lim_{c \rightarrow 0} -\frac{\phi_1(x, \lambda)}{\phi_2(x, \lambda)} = \frac{\sqrt{\lambda} J'_{\nu}(\sqrt{\lambda}c)}{J_{\nu}(\sqrt{\lambda}c)} + \frac{1}{2c},$$

and, also,

$$\phi_1(x, \lambda) + m_0(\lambda)\phi_2(x, \lambda) = \sqrt{\frac{x}{c}} \frac{J_{\nu}(\sqrt{\lambda}x)}{J_{\nu}(\sqrt{\lambda}c)}.$$

One can show that

$$H_{\nu}^{(1)}(x) \sim \left(\frac{2}{\pi x}\right)^{1/2} \frac{e^{i(x-\nu\pi/2-\pi/4)}}{\Gamma(\nu+1/2)}, \quad x \longrightarrow +\infty.$$

Therefore

$$\int_c^{\infty} |\sqrt{x} H_{\nu}^{(1)}(\sqrt{\lambda}x)|^2 dx < \infty$$

if $\text{Im } \lambda > 0$, and $\sqrt{x} H_{\nu}^{(1)}(\sqrt{\lambda}x)$ is the only solution that is square integrable at $+\infty$. Thus

$$\phi_1(x, \lambda) + m_{\infty}(\lambda)\phi_2(x, \lambda) = K\sqrt{x} H_{\nu}^{(1)}(\sqrt{\lambda}x). \quad (4.26)$$

To evaluate the constant K we set $x = c$ and find $1 = K\sqrt{c} H_{\nu}^{(1)}(\sqrt{\lambda}c)$. Then differentiating (4.26) with respect to x and setting $x = c$ we obtain

$$m_{\infty}(\lambda) = \frac{\sqrt{\lambda} H_{\nu}^{(1)'}(\sqrt{\lambda}c)}{H_{\nu}^{(1)}(\sqrt{\lambda}c)} + \frac{1}{2c}.$$

Now we can compute the spectral measures for this limit point - limit point case. We have

$$M_{11}(\lambda) = \frac{1}{m_0(\lambda) - m_{\infty}(\lambda)} = \frac{J_{\nu}(\sqrt{\lambda}c) H_{\nu}^{(1)}(\sqrt{\lambda}c)}{\sqrt{\lambda} W(H_{\nu}^{(1)}(\sqrt{\lambda}x), J_{\nu}(\sqrt{\lambda}x))} = \frac{i\pi c}{2} J_{\nu}(\sqrt{\lambda}c) H_{\nu}^{(1)}(\sqrt{\lambda}c),$$

since

$$H_{\nu}^{(1)}(x) = \frac{J_{-\nu}(x) - e^{-\nu\pi i} J_{\nu}(x)}{i \sin \nu\pi} \longrightarrow W(H_{\nu}^{(1)}, J_{\nu}) = \frac{2}{i\pi c \sqrt{\lambda}}.$$

Now we let λ in the upper halfplane become real and positive μ :

$$\pi d\rho_{11}(\mu) = \lim_{\epsilon \rightarrow 0+} M_{11}(\mu + i\epsilon) = \frac{\pi c}{2} J_\nu^2(\sqrt{\mu}c).$$

If λ in the upper halfplane become real and positive μ , then we find $d\rho_{11}(\mu) = 0$. We obtain similar results for the other spectral measures. There is no spectrum for $\mu < 0$, but for $\mu > 0$ we find

$$\pi d\rho_{22}(\mu) = \lim_{\epsilon \rightarrow 0+} M_{22}(\mu + i\epsilon) = m_0^2(\mu) \operatorname{Im} M_{11}(\mu),$$

$$\pi d\rho_{12}(\mu) = \pi d\rho_{21}(\mu) = \lim_{\epsilon \rightarrow 0+} M_{12}(\mu + i\epsilon) = m_0(\mu) \operatorname{Im} M_{11}(\mu).$$

These (apparently c -dependent) results will simplify greatly once we work out the expansion theorem. In particular the dependence on c will drop out, as it must. Let $f, h \in \mathcal{H}$. then

$$\begin{aligned} \int_0^\infty f(x) \overline{h(x)} dx &= (f, h) = \int_{-\infty}^\infty \sum_{j,k=1}^2 \int_0^\infty f(x) \phi_j(x, \mu) dx \overline{\int_0^\infty h(t) \phi_k(t, \mu) dt d\rho_{jk}(\mu)} \\ &= \int_{-\infty}^\infty \int_0^\infty f(x) [\phi_1(x, \mu) + m_0(\mu) \phi_2(x, \mu)] dx \overline{\int_0^\infty h(t) [\phi_1(t, \mu) + m_0(\mu) \phi_2(t, \mu)] dt d\rho_{11}(\mu)} \\ &= \int_0^\infty \int_0^\infty f(x) \sqrt{x} J_\nu(\sqrt{\mu}x) dx \overline{\int_0^\infty h(t) \sqrt{t} J_\nu(\sqrt{\mu}t) dt d\mu}. \end{aligned}$$

At this point we recognise the Hankel transform: Let $f \in \mathcal{H}$ and define the Hankel transform of f as

$$g(\mu) = \int_0^\infty f(x) \sqrt{x} J_\nu(\sqrt{\mu}x) dx.$$

The expansion formula is

$$\begin{aligned} f(x) &= \int_0^\infty \sum_{j,k=1}^2 \int_0^\infty f(t) \phi_j(t, \mu) dt \phi_k(x, \mu) d\rho_{jk}(\mu) \\ &= \int_0^\infty \left[\int_0^\infty f(t) (\phi_1(t, \mu) + m_0(\mu) \phi_2(t, \mu)) dt \right] [\phi_1(x, \mu) + m_0(\mu) \phi_2(x, \mu)] d\rho_{11}(\mu) \\ &= \frac{1}{2} \int_0^\infty g(\mu) \sqrt{x} J_\nu(\sqrt{\mu}x) d\mu. \end{aligned}$$

Example 21 *Hermite functions.* We will go into enough detail in this example to indicate how the spectrum is calculated, but not write down the full expansion theorem. Consider the operator

$$\tau u = -u'' + x^2 u, \quad I = (-\infty, +\infty).$$

We are interested in the eigenvalue problem $\tau u = \lambda u$. If we set $\lambda = 0$ then the equation is $-u'' + x^2 u = 0$. This is clearly the limit point - limit point case. Indeed, consider the solution $u(x)$ of this equation such that $u(1) = u'(1) = 1$. Since $u''(x) = x^2 u(x)$ we see that the second derivative is positive, so that the first derivative is increasing. Thus this solution grows monotonically as $x \rightarrow +\infty$ and is not square integrable. A similar argument works for negative $x \rightarrow -\infty$: choose the solution such that $u(-1) = 1, u'(-1) = -1$.

We choose ϕ_1, ϕ_2 such that $\tau \phi_j = \lambda \phi_j$, $j = 1, 2$ and such that

$$\phi_1(0, \lambda) = 1, \quad \phi_1'(0, \lambda) = 0, \quad \phi_2(0, \lambda) = 0, \quad \phi_2'(0, \lambda) = 1.$$

Note: If $u(x)$ is a solution of $\tau u = \lambda u$ then so is $u(-x)$. Therefore $\phi_1(-x, \lambda)$ is a solution such that $\phi_1(0, \lambda) = 1, \phi_1'(0, \lambda) = 0$ so $\phi_1(-x, \lambda) \equiv \phi_1(x, \lambda)$. Similarly, $\phi_2(-x, \lambda)$ is a solution such that $\phi_2(0, \lambda) = 0, \left. \frac{d}{dx} \phi_2(-x, \lambda) \right|_{x=0} = -1$, so $\phi_2(-x, \lambda) \equiv -\phi_2(x, \lambda)$. Therefore, since

$$m_\infty(\lambda) = \lim_{b \rightarrow \infty} -\frac{\phi_1(x, \lambda)}{\phi_2(x, \lambda)},$$

and the numerator is even whereas the denominator is odd, we have

$$m_{-\infty}(\lambda) = \lim_{a \rightarrow -\infty} -\frac{\phi_1(x, \lambda)}{\phi_2(x, \lambda)} = -m_\infty(\lambda).$$

Now we construct a square integrable solution of our differential equation, using a contour integral. Set

$$u(x, \lambda) = e^{-x^2/2} \int_{\infty}^{(0+)} e^{-xz - z^2/4} z^{-(\lambda+1)/2} dz$$

where the contour in the complex z -plane goes along the line $z = x + i\epsilon_1$ just above the positive real axis from $x + \infty$ until it reaches the circle $z = \epsilon e^{i\theta}$ of radius ϵ . Then it moves counterclockwise around the circle and goes back

along the line $z = x - i\epsilon_1$ just below the positive real axis to $+\infty - i\epsilon$. We interpret the many-valued function $z^{-(\lambda+1)/2}$ in the integrand as

$$z^{-(\lambda+1)/2} = \exp\left[-\frac{1}{2}(\lambda+1)\ln z\right]$$

where $\ln z$ is the branch of the complex logarithm that is real for positive z . Now differentiating under the integral sign, which is permitted due to the rapid decay of the integrand along the contour, we find

$$\begin{aligned} (\tau - \lambda)u(x, \lambda) &= e^{-x^2/2} \int_{\infty}^{(0+)} (-x^2 + 1 - 2xz - z^2 - \lambda + x^2) e^{-xz - z^2/4} z^{-(\lambda+1)/2} dz \\ &= 2e^{-x^2/2} \int_{\infty}^{(0+)} \frac{d}{dz} (e^{-xz - z^2/4} z^{-\lambda+1/2}) dz = 0. \end{aligned}$$

The $u(x, \lambda)$ is a solution of the differential equation. Furthermore, for fixed λ it is straightforward analysis to get the bound

$$|u(x, \lambda)| \leq Ce^{-x^2/2+x}$$

as $x \rightarrow \infty$. It follows that

$$\int_0^{\infty} |u(x, \lambda)|^2 dx < \infty.$$

Since we are limit point at $+\infty$ it follows that, to within a constant multiple, $u(x, \lambda)$ is the only solution square integrable at $+\infty$. We conclude that there is a nonzero constant K such that

$$u(x, \lambda) = K (\phi_1(x, \lambda) + m_{\infty}(\lambda)\phi_2(x, \lambda)).$$

Now, $u(0, \lambda) = K$ and $u'(0, \lambda) = Km_{\infty}(\lambda)$. Therefore,

$$m_{\infty}(\lambda) = \frac{u'(0, \lambda)}{u(0, \lambda)} = -\frac{\int_{\infty}^{(0+)} e^{-xz - z^2/4} z^{-\lambda+1/2} dz}{\int_{\infty}^{(0+)} e^{-xz - z^2/4} z^{-\lambda-1/2} dz}.$$

Proceeding in this way it is straightforward, but tedious, to compute the complete spectral resolution and expansion theorem.

Example 22 In order to show that our spectral machinery yields correct results in familiar cases, and to improve understanding of the method, we

conclude with a regular self-adjoint boundary value problem where we already know the spectral expansion. Consider the problem

$$\tau u = -u'', \quad I = [0, \pi], \quad B_0(u) = u(0) = 0, \quad B_\pi(u) = u(\pi) = 0.$$

This is clearly the limit circle - limit circle case. Here we take a basis of solutions for the differential equation as

$$\phi_1(x, \lambda) = \phi(x, \lambda) = \cos(\sqrt{\lambda}x), \quad \phi_2(x, \lambda) = \psi(x, \lambda) = \frac{\sin(\sqrt{\lambda}x)}{\sqrt{\lambda}}.$$

We will adopt the method of the proof of Theorem 78 to restudy this problem. Let $\chi_b(x, \lambda)$ be the solution $\chi_b(x, \lambda) = \phi_1(x, \lambda) + m_b(\lambda)\phi_2(x, \lambda)$, such that $B_b(\chi_b) = 0$. Then

$$B_b(\chi_b) = 0 = \phi_1(b, \lambda) + m_b(\lambda)\phi_2(b, \lambda)$$

so

$$m_b(\lambda) = -\frac{\phi_1(b, \lambda)}{\phi_2(b, \lambda)} = -\frac{\sqrt{\lambda} \cos(\sqrt{\lambda}b)}{\sin(\sqrt{\lambda}b)}.$$

Therefore,

$$m_\pi(\lambda) = \lim_{b \rightarrow \pi} -\frac{\phi_1(b, \lambda)}{\phi_2(b, \lambda)} = -\frac{\sqrt{\lambda} \cos(\sqrt{\lambda}\pi)}{\sin(\sqrt{\lambda}\pi)}.$$

It follows that the spectral measure is given by

$$\rho(\nu) - \rho(\gamma) = \lim_{\epsilon \rightarrow 0+} \frac{1}{\pi} \int_\gamma^\nu \operatorname{Im} m_\pi(\mu + i\epsilon) d\mu = -\frac{1}{\pi} \int_\gamma^\nu \operatorname{Im} \left(\frac{\sqrt{\mu + i\epsilon} \cos(\sqrt{\mu + i\epsilon}\pi)}{\sin(\sqrt{\mu + i\epsilon}\pi)} \right) d\mu.$$

Note that $m_\pi(\mu)$ is real and that

$$m_\pi(\lambda) = -\frac{\sqrt{\lambda} \cos(\sqrt{\lambda}\pi)}{\sin(\sqrt{\lambda}\pi)}$$

is analytic in the λ -complex plane, except for simple poles at the points $\lambda = 1, 2^2, 3^2, \dots, n^2, \dots$ with residue $-2n^2/\pi$. This follows from the fact that

$$\frac{d}{d\lambda} \left(\frac{\sin \sqrt{\lambda}\pi}{\sqrt{\lambda}} \right) \Big|_{\lambda=n^2} = \left(\frac{\pi \cos \sqrt{\lambda}\pi}{2\lambda} - \frac{1}{2} \frac{\sin \sqrt{\lambda}\pi}{\lambda^{3/2}} \right) \Big|_{\lambda=n^2} = \frac{(-1)^n \pi}{2n^2}.$$

From this we can see that $\rho(\mu)$ has a jump $+2n^2/\pi$ at the points $\mu = n^2$, $n = 1, 2, \dots$, and is otherwise constant. Thus from the proof of Theorem

78 we get the following expansion result. Given any $f \in \mathcal{H}$ we define the transform of f by

$$g(\mu) = \int_0^\pi f(x) \psi(x, \mu) \, dx = \int_0^\pi f(x) \frac{\sin(\sqrt{\lambda}x)}{\sqrt{\lambda}} \, dx.$$

Then the expansion theorem says

$$f(x) = \int_0^\infty g(\mu) \frac{\sin(\sqrt{\lambda}x)}{\sqrt{\lambda}} \, d\rho(\mu) = \sum_{n=1}^\infty g(n^2) \frac{2n^2}{\pi} \frac{\sin(nx)}{n} = \frac{2}{\pi} \sum_{n=1}^\infty h(n) \sin(nx),$$

where

$$h(n) = \int_0^\pi f(x) \sin(nx) \, dx.$$

This is just the Fourier sine series for f .