Chapter 8 Sturm-Liouville Theory

Eigenvalue problems of the form

$$\mathcal{L}\,\psi(x) = \lambda\,\psi(x) \quad \text{with} \quad \mathcal{L}(x) = p_0(x)\frac{d^2}{dx^2} + p_1(x)\frac{d}{dx} + p_2(x)$$

where λ is a parameter (eigenvalue) determined by the boundary conditions

$\mathcal{L}(x)$ is <u>self-adjoint</u> if $p_0'(x) = p_1(x)$ which allows to write $\mathcal{L}(x)$ as $\mathcal{L}(x) = \frac{d}{dx}\left[p_0(x)\frac{d}{dx}\right] + p_2(x)$ such that

$$\mathcal{L}u = (p_0 u')' + p_2 u$$

Consider the integral $\int_a^b v^*(x)\,\mathcal{L}u(x)\,dx$

Integrate by parts:

$$\int_a^b v^*(x)\,\mathcal{L}u(x)\,dx = \int_a^b \{v^*(p_0u')' + v^*p_2u\}\,dx = \left[v^*p_0u'\right]_a^b +$$

$$+ \int_a^b \{-(v^*)'p_0u' + v^*p_2u\}\,dx = \left[v^*p_0u' - (v^*)'p_0u\right]_a^b + \int_a^b \{[p_0(v^*)']'u + v^*p_2u\}\,dx$$

$$= \left[v^*p_0u' - (v^*)'p_0u\right]_a^b + \int_a^b (\mathcal{L}v)^*u\,dx \quad \text{where it is assumed } p_0 \text{ real.}$$

If $\int_a^b v^*(x)\mathcal{L}u(x)\,dx = \langle v|\mathcal{L}u\rangle$ has properties of scalar product (must satisfy $\langle v|v\rangle \geq 0$, be linear and $\langle v|\mathcal{L}u\rangle^* = \langle \mathcal{L}u|v\rangle$)

and the boundary terms $\left[v^*p_0u' - (v^*)'p_0u\right]_a^b = 0$ then the <u>operator is self-adjoint</u>, i.e. $\langle v|\mathcal{L}u\rangle = \langle \mathcal{L}v|u\rangle$

(The <u>equation</u> is self-adjoint if $\mathcal{L}u = (p_0u')' + p_2u$)

The boundary terms vanish for Dirichlet boundary conditions i.e. $u(x), v(x)$ vanish at the boundary. Also for Neumann boundary conditions, i.e. $u'(x), v'(x)$ vanish at the boundary. Typically also for periodic systems where

$v^*p_0u'\big|_a = v^*p_0u'\big|_b$ for all u and v on the space

Assume $\mathcal{L}u = \lambda_u u$ and $\mathcal{L}v = \lambda_v v$ and $\lambda_u \neq \lambda_v$, both real.

we have $\int_a^b v^* \mathcal{L}u\,dx = \int_a^b v^* \lambda_u u\,dx = \lambda_u \int_a^b v^* u\,dx$ and

$\int_a^b (\mathcal{L}v)^* u\,dx = \int_a^b (\lambda_v v)^* u\,dx = \lambda_v \int_a^b v^* u\,dx$ so that

$$(\lambda_u - \lambda_v) \int_a^b v^* u\,dx = \left[p_0 (v^* u' - (v^*)' u)\right]_a^b$$

If the boundary conditions are such that the right hand side vanishes, then $\int_a^b v^* u\,dx \equiv \langle v|u\rangle = 0$ and the functions v and u (corresponding to different eigenvalues) are orthogonal over $[a,b]$ with scalar product $\int_a^b w(x) v^*(x) u(x)\,dx$ where $w(x)$ is a weight function (here $w(x) \equiv 1$).

If the operator is self-adjoint, i.e. $\langle v|\mathcal{L}u\rangle = \langle \mathcal{L}v|u\rangle$ then the eigenvalues are real:

$$\lambda_u \langle u|u\rangle = \langle u|\mathcal{L}u\rangle = \langle \mathcal{L}u|u\rangle = \lambda_u^* \langle u|u\rangle$$

Hermitian (self-adjoint) operators have

- real eigenvalues
- orthogonal eigenfunctions that form a complete set (basis for) the Hilbert space defined by the boundary conditions
- Hilbert space is a (complex) linear vector space with scalar product
- $\mathcal{L}^+ = \mathcal{L}$

Hermiticity for operators $\langle v|\mathcal{L}u\rangle = \langle \mathcal{L}v|u\rangle$ is a stronger condition than self-adjointness for ODE's

$$\langle v|\mathcal{L}u\rangle = \left[v^* p_0 u' - (v^*)' p_0 u\right]_a^b + \langle \mathcal{L}v|u\rangle$$

A general second-order ODE which is not on self-adjoint form can be made self-adjoint by multiplying with

$$w(x) = \frac{1}{P_0(x)} \exp\left\{ \int^x \frac{P_1(s)}{P_0(s)} ds \right\} \quad \text{so that}$$

[compare integrating factor]

$$w(x)\mathcal{L}(x)\psi(x) = w(x)\lambda\psi(x)$$

With $\mathcal{L}(x) = P_0(x)\frac{d^2}{dx^2} + P_1(x)\frac{d}{dx} + P_2(x)$ we find

$$w(x)\mathcal{L}(x)\psi(x) = \exp\left\{\int^x \frac{P_1(s)}{P_0(s)} ds\right\}\frac{d^2\psi}{dx^2} + \frac{P_1(x)}{P_0(x)}\exp\left\{\int^x \frac{P_1(s)}{P_0(s)} ds\right\}\frac{d\psi}{dx} + \frac{P_2(x)}{P_0(x)}\exp\left\{\int^x \frac{P_1(s)}{P_0(s)} ds\right\}\psi(x)$$

Here $\frac{d}{dx}\exp\left\{\int^x \frac{P_1(s)}{P_0(s)} ds\right\} = \frac{P_1(x)}{P_0(x)}\exp\left\{\int^x \frac{P_1(s)}{P_0(s)} ds\right\}$ so that

$$w(x)\mathcal{L}(x)\psi(x) = \frac{d}{dx}\left\{w(x)\frac{d\psi}{dx}\right\} + w(x)P_2(x)\psi(x) \quad \text{self-adjoint}$$

Doing the partial integrations we obtain

$$\int_a^b v^* w \mathcal{L} u \, dx = \left[v^* \bar{P}_0 u' - (v^*)'\bar{P}_0 u\right]_a^b + \int_a^b w(\mathcal{L}v)^* u \, dx$$

If the boundary terms vanish we have $\langle v|\mathcal{L}u\rangle = \langle \mathcal{L}v|u\rangle$ when the scalar product is defined including the weight function as $\langle v|u\rangle = \int_a^b v^*(x)u(x)w(x)\,dx$

Orthogonality: $(\lambda_u - \lambda_v)\int_a^b v^* u w \, dx = \left[w P_0 (v^* u' - (v^*)' u)\right]_a^b$

if the right hand side vanishes then u and v are orthogonal on $[a,b]$ with weight factor $w(x)$ when $\lambda_u \neq \lambda_v$

Example: Laguerre functions (solutions to the H-atom radial Schrödinger equation): $\mathcal{L}\psi = \lambda\psi$ with

$$\mathcal{L} = x\frac{d^2}{dx^2} + (1-x)\frac{d}{dx}$$

and (a) ψ non-singular on $0 \le x < \infty$

and (b) $\lim_{x\to\infty}\psi(x) = 0$

With $p_0(x) = x$ and $p_1(x) = 1-x$ the operator is not self-adjoint. Becomes self-adjoint through the weight factor

$$w(x) = \frac{1}{x} \exp\left\{ \int^x \frac{1-s}{s}\,ds \right\} = \frac{1}{x} e^{\ln x - x} = e^{-x}$$

Is the operator $e^{-x}\mathcal{L}(x)$ self-adjoint (Hermitian) on this function space?

$$\Big[\underbrace{x e^{-x}}_{p_0 w(x)} (v^* u' - (v^*)' u)\Big]_0^\infty$$

for $x = 0$ the value is $= 0$ (multiplication by x)

for $x \to \infty$ —— " —— since $u, v \xrightarrow[x\to\infty]{} 0$

Thus, the operator is self-adjoint and the eigenfunctions (Laguerre polynomials) are orthogonal on $[0, \infty)$ with scalar product $\langle v|u\rangle = \int_0^\infty v^*(x)\, u(x)\, e^{-x} dx$ (different eigenvalues)

Legendre equation $\mathcal{L}y(x) = -(1-x^2)y'' + 2xy'(x) = \lambda y(x)$

Equation for ϑ-dependence when ∇^2 is separated in spherical polar coordinates with $x = \cos\vartheta$ so that $-1 \leq x \leq 1$. We require nonsingular solutions over the range of $-1 \leq x \leq 1$.

At $x = \pm 1$ we have a regular singularity since

$\mathcal{L}y(x) = y'' - \frac{2x}{1-x^2} y'$ gives divergence at $x = \pm 1$

but $\frac{(x+1)2x}{(1+x)(1-x)} = \frac{2x}{1-x}$ is regular for $x \to -1$

and $\frac{(x-1)2x}{(1+x)(1-x)} = -\frac{2x}{1+x}$ is regular for $x \to +1$

Attempt a series solution $y(x) = \sum_{j=0}^\infty a_j x^{s+j}$

$$y' = \sum_{j=0}^{\infty} a_j (s+j)\, x^{s+j-1} \quad ; \quad y'' = \sum_{j=0}^{\infty} a_j (s+j)(s+j-1)\, x^{s+j-2}$$

We get

$$-(1-x^2)\sum_{j=0}^{\infty} a_j (s+j)(s+j-1) x^{s+j-2} + 2x \sum_{j=0}^{\infty} a_j (s+j) x^{s+j-1} - \lambda \sum_{j=0}^{\infty} a_j x^{s+j} =$$

$$= -a_0 s(s-1) x^{s-2} - a_1 s(s+1) x^{s-1} + \sum_{j=0}^{\infty} \Big[a_j \{ (s+j)(s+j-1) + 2(s+j) - \lambda \} -$$

$$- a_{j+2} (s+j+2)(s+j+1) \Big] x^{s+j} = 0$$

Indicial equation $s(s-1) = 0$

For $s=0$ a_1 is indeterminate but $\mathcal{L}$ preserves parity and we can set $a_1 = 0$ making all odd terms vanish (2-step relation)

$$s=0: \quad a_{j+2} = \frac{j(j-1) + 2j - \lambda}{(j+2)(j+1)} a_j = \frac{j(j+1) - \lambda}{(j+2)(j+1)} a_j$$

Does the series converge for $|x| = 1$?

Ratio test inconclusive : $\dfrac{a_{j+2} x^{j+2}}{a_j x^{j}} \xrightarrow[\substack{j\to\infty \\ |x|=1}]{} \dfrac{j(j+1)}{(j+1)(j+2)} \to 1$

Gauss' test: if for large n $\quad \dfrac{u_n}{u_{n+1}} = 1 + \dfrac{h}{n} + \dfrac{B(n)}{n^2}$ where

$B(n)$ is bounded for n sufficiently large then

$\sum_n u_n$ converges for $h > 1$ and diverges for $h \le 1$

We have $\dfrac{a_{2j}}{a_{2j+2}} = \dfrac{(2j+1)(2j+2)}{2j(2j+1) - \lambda} = \dfrac{(2j+1)(2j+2)}{2j(2j+1)\left(1 - \frac{\lambda}{2j(2j+1)}\right)} \approx$

(only even terms)

$$\approx \frac{(2j+1)(2j+2)}{2j(2j+1)} \left\{ 1 + \frac{\lambda}{2j(2j+1)} \right\} = \frac{2j+2}{2j} + \frac{2j+2}{2j} \cdot \frac{\lambda}{2j(2j+1)} =$$

$$= 1 + \frac{1}{j} + \frac{\lambda}{2j(2j+1)} + \frac{\lambda}{2j^2(2j+1)} \longrightarrow 1 + \frac{1}{j} + \frac{B(j)}{j^2} \quad \lambda/4$$

$h = 1 \to$ divergence

By choosing the eigenvalue $\lambda = l(l+1)$ with l even makes the series terminate and we have a polynomial which is non singular for $|x| \leq 1$

The root $s=1$ requires $a_1 = 0$ and we have

$$a_{j+2} = \frac{(j+1)(j+2)-\lambda}{(j+2)(j+3)} a_j$$ which also diverges at $|x|=1$

Terminates for $\lambda = (l+1)(l+2)$ with l even giving polynomials of degree $l+1$, i.e. odd so we have $\lambda = l(l+1)$ with l odd and all functions are obtained by combining the solutions.

Hermite equation $\mathcal{L}y = -y'' + 2xy' = \lambda y \qquad -\infty < x < \infty$

$\mathcal{L}$ becomes Hermitian with scalar product

$$\langle f|g\rangle = \int_{-\infty}^{\infty} f^*(x) g(x) e^{-x^2} dx$$ We want our solutions to have finite norm, i.e. $\langle y_n | y_n \rangle < \infty$

Series solution gives $- \sum_{j=0}^{\infty} a_j (s+j)(s+j-1) x^{s+j-2} + 2 \sum_{j=0}^{\infty} a_j (s+j) x^{s+j} -$

$$- \lambda \sum_{j=0}^{\infty} a_j x^{s+j} = 0$$

Indicial equation: $s(s-1) = 0$ and recurrence relation

$$a_{j+2} = \frac{2(s+j) - \lambda}{(s+j+2)(s+j+1)} a_j$$

For $s=0$ set $a_1 = 0$ and develop even solution as

$$a_{j+2} = \frac{2j - \lambda}{(j+2)(j+1)} a_j$$ with $\frac{a_{j+2}}{a_j} \xrightarrow[j\to\infty]{} \frac{2}{j}$

Power series for $e^{x^2} = 1 + x^2 + \frac{1}{2!} x^4 + \dots = \sum_{k=0}^{\infty} \frac{1}{k!} x^{2k}$ (convergent for all x)

Compare coefficients for powers x^{j+2} and x^{j}

$$\frac{x^{j+2}}{x^j} : \frac{j!}{(j+1)!} = \frac{1}{j+1} = \frac{2}{2j+2} = \frac{2}{k+2} \to \frac{2}{k}$$ (only even powers)

Thus the power series behaves as e^{x^2} and cannot be normalized over $(-\infty, \infty)$ unless it terminates, i.e. $\lambda = 2j$ for some j giving a polynomial (Hermite polynomial)

Odd solutions obtained from root $s = 1$.

Another view of weight factor.

The Schrödinger equation for the harmonic oscillator (atomic units $\hbar = e = m_e = 1$) self-adjoint

$$-\frac{1}{2}\frac{d^2\psi}{dx^2} + \frac{1}{2}x^2\psi = E\psi \qquad \text{with } \langle\psi|\psi\rangle \text{ finite} \Rightarrow \psi(x) \underset{x\to\pm\infty}{\longrightarrow} 0$$

Asymptotically $\frac{d^2\psi}{dx^2} \sim x^2\psi \rightarrow \psi(x) \sim e^{-\frac{1}{2}x^2}$

$$\frac{d\psi}{dx} = \frac{d}{dx}e^{-\frac{1}{2}x^2} = -x e^{-\frac{1}{2}x^2}$$

$$\frac{d^2\psi}{dx^2} = -(1-x^2)e^{-\frac{1}{2}x^2} \qquad x \text{ large} \longrightarrow \frac{d^2\psi}{dx^2} \approx +x^2 e^{-\frac{1}{2}x^2}$$

Ansatz: $\psi(x) = P(x)e^{-\frac{1}{2}x^2}$

$$\psi' = P'e^{-\frac{1}{2}x^2} - xPe^{-\frac{1}{2}x^2}$$

$$\psi'' = \left[P'' - 2xP' + (x^2-1)P\right]e^{-\frac{1}{2}x^2}$$

The equation: $\psi'' + (2E - x^2)\psi = 0$

Gives $P'' - 2xP' + (2E-1)P = 0$ Hermite equation

The orthogonality is from the Schrödinger equation

$$\langle\psi_n|\psi_m\rangle = \int_{-\infty}^{\infty}\psi_n^*\psi_m\,dx = \int_{-\infty}^{\infty}H_n^*(x)e^{-\frac{1}{2}x^2}\cdot H_m(x)e^{-\frac{1}{2}x^2}dx =$$

$$= \int_{-\infty}^{\infty}H_n^*(x)\,H_m(x)\,\underbrace{e^{-x^2}}_{w(x)}dx$$

Ex. Deuteron

Variational principle: $\langle\psi_n|\psi_m\rangle = \delta_{nm}$. $H\psi_n = E_n\psi_n$

$\{\psi_n\}$ complete basis $\rightarrow f(x) = \sum_n a_n\psi_n$ and

$\langle H\rangle = \sum_n |a_n|^2 E_n \geqslant E_0$; E_0 (lowest eigenvalue is lower bound