8: STURM-LIOUVILLE THEORY

Characterization of the general features of eigen-problems arising from second-order *ordinary differential equations* (ODE) is known as **Sturm-Liouville theory**.

The matters of interest here, and the subject matter of the current chapter, include:

1. The conditions under which a second order ODE can be written as an eigenvalue equation with a self-adjoint (Hermitian) operator,
2. Methods for the solution of ODEs subject to boundary conditions, and
3. The properties of the solutions to ODE eigenvalue equations.

The Sturm-Liouville theory therefore deals with eigenvalue problems of the form

$$\mathcal{L}\, u(x) = \lambda\, u(x) \qquad (8.7)$$

where $\mathcal{L}$ is a linear second-order differential operator, of the general form

$$\mathcal{L}(x) = p_0(x)\frac{d^2}{dx^2} + p_1(x)\frac{d}{dx} + p_2(x). \qquad (8.8)$$

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The key matter at issue here is to identify the conditions under which $\mathcal{L}$ is a Self-Adjoint ODE or a Hermitian operator

$\mathcal{L}$ is known in differential equation theory as **self-adjoint** if

$$\boldsymbol{p_1(x) = p_o'(x)} \qquad \textbf{(8.9)}$$

Using (8.9) in (8.8) and through (8.7) we obtain

$$p_o(x)\,\frac{d^2u}{dx^2} + p_o'(x)\,\frac{du}{dx} + p_2(x)\,u = \lambda\,u \qquad (8.10a)$$

Or $\qquad p_o u'' + p_o'\,u' + p_2\,u = \lambda\,u$

Or $\qquad (p_o u')' + p_2\,u = \lambda\,u \qquad (8.10b)$

Or $\qquad \mathcal{L}\,u(x) = \lambda\,u(x) \qquad$ [see Eq. (8.7)]

where $\mathcal{L}\,u(x)$ can now be written as

$$(p_o u')' + p_2\,u \qquad (8.11)$$

Consider the expectation value equation ➔ $\int_a^b v^*(x)\mathcal{L}\,u(x)dx$

Inserting $(p_o u')' + p_2\,u$ [Eq.(8.11)] in place of $\mathcal{L}\,u(x)$ in above integral

$\int_a^b v^*(x)\,[(p_o u')' + p_2\,u]\,dx$ Or $\int_a^b [\,v^*(x)\,(p_o u')' + v^*(x)\,p_2\,u\,]\,dx$

Now integrating by parts with second term $(p_o u')'$ (assuming that p_o is real)

$$\int_a^b v^*(x)\mathcal{L}u(x)\,dx = \int_a^b \left[v^*\left(p_0 u'\right)' + v^* p_2 u\right]dx = \left[v^* p_0 u'\right]_a^b + \int_a^b \left[-(v^*)' p_0 u' + v^* p_2 u\right]dx.$$

Another integration by parts with first term as $(v^*)'p_o$ leads to

$$\int_a^b v^*(x)\mathcal{L}u(x)\,dx = \left[v^* p_0 u' - (v^*)' p_0 u\right]_a^b + \int_a^b \left[\left[p_0 (v^*)'\right]' u + v^* p_2 u\right]dx$$

$$= \left[v^* p_0 u' - (v^*)' p_0 u \right]_a^b + \int_a^b (\mathcal{L}v)^* u \, dx. \qquad (8.12)$$

Equation (8.12) shows that, if the boundary terms $[\cdots]_a^b$ vanish and the scalar product is an unweighted integral from *a* to *b*, then the operator $\mathcal{L}$ is self-adjoint, as that term was defined for operators. In passing, we observe that the notion of self-adjointness in differential equation theory is weaker than the corresponding concept for operators in our Hilbert spaces, due to the lack of a requirement on the boundary terms. We again stress that the Hilbert-space definition of self-adjoint depends not only on the form of $\mathcal{L}$ but also on the definition of the scalar product and the boundary conditions.

Looking further at the boundary terms, we see that they are surely zero if *u* and v both vanish at the endpoints *x* = *a* and *x* = *b* (a case of what are termed *Dirichlet* boundary conditions). The boundary terms are also zero if both *u'* and v' vanish at *a* and *b* (*Neumann* boundary conditions). Even if neither Dirichlet nor Neumann boundary conditions apply, it may happen (particularly in a periodic system, such as a crystal lattice) that the boundary terms vanish because $v^* p_0 u' \big|_a = v^* p_0 u' \big|_b$ for all *u* and v.

Specializing Eq. (8.12) to the case that *u* and v are eigenfunctions of $\mathcal{L}$ with respective real eigenvalues λ_u and λ_v, that equation reduces to

$$(\lambda_u - \lambda_v) \int_a^b v^* u \, dx = \left[p_0 (v^* u' - (v^*)' u) \right]_a^b. \qquad (8.13)$$

It is thus apparent that if the boundary terms vanish and $\lambda_u \neq \lambda_v$, then *u* and v must be orthogonal on the interval (*a* , *b*). This is a specific illustration of the orthogonality requirement for eigenfunctions of a Hermitian operator in a Hilbert space.

MAKING AN ODE SELF-ADJOINT

Some of the differential equations that are important in physics involve operators $\mathcal{L}$ that are self-adjoint in the differential-equation sense, meaning that they satisfy Eq. (8.9); others are not. However, if an operator does not satisfy Eq. (8.9), it is known how to multiply it by a quantity that converts it into self-adjoint form. Letting such a quantity be designated w(x) , the Sturm-Liouville eigenvalue problem of Eq. (8.7) becomes

$$w(x)\mathcal{L}(x)\psi(x) = w(x)\lambda\psi(x), \qquad (8.14)$$

an equation that has the same eigenvalues λ and eigen-functions $\psi(x)$ as the original problem in Eq. (8.7). If now w(x) is chosen to be

$$w(x) = p_0^{-1} \exp\left(\int \frac{p_1(x)}{p_0(x)} dx \right), \qquad (8.15)$$

where p_0 and p_1 are the quantities in $\mathcal{L}$ as given in Eq. (8.8), we can by direct evaluation find that

$$w(x)\mathcal{L}(x) = \overline{p}_0 \frac{d^2}{dx^2} + \overline{p}_1 \frac{d}{dx} + w(x)p_2(x), \tag{8.16}$$

$$\overline{p}_0 = \exp\left(\int \frac{p_1(x)}{p_0(x)}dx\right), \quad \overline{p}_1 = \frac{p_1}{p_0}\exp\left(\int \frac{p_1(x)}{p_0(x)}dx\right). \tag{8.17}$$

It is then straightforward to show that $\overline{p}_0' = \overline{p}_1$, so $w\mathcal{L}$ satisfies the self-adjoint condition.

If we now apply the process represented by Eq. (8.12) to $w\mathcal{L}$, we get

$$\int_a^b v^*(x)w(x)\mathcal{L}u(x)\,dx = \left[v^*\overline{p}_0 u' - (v^*)'\,\overline{p}_0 u\right]_a^b + \int_a^b w(x)\,(\mathcal{L}v)^*\,u\,dx. \tag{8.18}$$

{ (*Assignment*: Prove the above relation Eq.(8.18) }

If the boundary terms vanish, Eq. (8.18) is equivalent to $\langle v|\mathcal{L}|u\rangle = \langle \mathcal{L}v|u\rangle$ when the scalar product is defined to be

$$\langle v|u\rangle = \int_a^b v^*(x)u(x)w(x)\,dx. \tag{8.19}$$

Again considering the case that u and v are eigenfunctions of $\mathcal{L}$, with respective eigenvalues λ_u and λ_v, Eq. (8.18) reduces to

$$(\lambda_u - \lambda_v)\int_a^b v^*u\,w\,dx = \Big[w p_0\left(v^*u' - (v^*)'u\right)\Big]_a^b, \tag{8.20}$$

where p_0 is the coefficient of y'' in the original ODE. We thus see that if the right-hand side of Eq. (8.20) vanishes, then u and v are orthogonal on (a, b) with weight factor w when $\lambda_u \neq \lambda_v$. In other words, our choice of scalar product definition and boundary conditions have made $\mathcal{L}$ a self-adjoint operator in our Hilbert space, thereby producing an eigenfunction orthogonality condition.

Summarizing, we have the useful and important result:

> *If a second-order differential operator $\mathcal{L}$ has coefficients $p_0(x)$ and $p_1(x)$ that satisfy the self-adjoint condition, Eq. (8.9), then it is Hermitian, given (a) a scalar product of uniform weight and (b) boundary conditions that remove the endpoint terms of Eq. (8.12).*
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> *If Eq. (8.9) is not satisfied, then $\mathcal{L}$ is Hermitian if (a) the scalar product is defined to include the weight factor given in Eq. (8.15), and (b) boundary conditions cause removal of the endpoint terms in Eq. (8.18).*

Note that once the problem has been defined such that $\mathcal{L}$ is Hermitian, then the general properties proved for Hermitian problems apply: the eigenvalues are real; the eigenfunctions are (or if degenerate can be made) orthogonal, **using the relevant scalar product definition**.

Problems:

- Check if the following polynomial can be written in the form of eigenvalue equation.
- Also check if they are Hermitian, Determine the weight function w(x) to convert them into a Hermitian operation wherever possible.

Simple harmonic oscillator

$y'' + \omega^2 y = 0$,

Legendre[a]

$(1 - x^2)y'' - 2xy' + l(l+1)y = 0$,

Hermite

$y'' - 2xy' + 2\alpha y = 0$

Bessel

$x^2 y'' + xy' + (x^2 - n^2)y = 0$

Chebyshev

$(1 - x^2)y'' - xy' + n^2 y = 0$

Confluent hypergeometric

$xy'' + (c - x)y' - ay = 0$,

Hypergeometric

$x(x-1)y'' + [(1 + a + b)x + c]y' + aby = 0$

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