Sturm-Lioville Theory

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→ If $\mathcal{L} = \mathcal{L}^{+}$, then the linear differential operator $\mathcal{L}$ is said to be self-adjoint.

→ If $\mathcal{L} = \mathcal{L}^{+}$ AND the boundary terms are zero, then $\mathcal{L}$ is said to be Hermitian.

Note: for matrices (finite dimensional space) self-adjoint is the same as Hermitian. Arfken textbook does not bother to distinguish the two.

Example: Show that $\mathcal{L} = \frac{d^2}{dx^2}$ is self-adjoint and find the conditions for $\mathcal{L}$ to be Hermitian in $x \in [a,b]$.

$$\int_a^b dx\, f^*(x)\, \mathcal{L}\, g(x) = \int_a^b dx\, f^*(x) \frac{d^2 g}{dx^2}$$

$$= \int_a^b \cancel{dx}\, f^*(x) \frac{d}{\cancel{dx}}\left(\frac{dg}{dx}\right) \quad \leftarrow \int u\, dv, \quad u = f^*(x),\ dv \to \frac{dg}{dx}$$

$$= f^*(x) \frac{dg}{dx}\Big|_a^b - \int_a^b d[f^*(x)] \frac{dg}{dx}$$

$$= f^*(x) \frac{dg}{dx}\Big|_a^b - \int_a^b dx \frac{df^*}{dx}\frac{dg}{dx}$$

$$= f^*(x) \frac{dg}{dx}\Big|_a^b - \int_a^b \cancel{dx} \frac{df^*}{dx}\frac{dg}{\cancel{dx}} \quad \leftarrow \int u\, dv, \quad u = \frac{df^*}{dx},\ dv \leftarrow g(x)$$

$$= f^*(x) \frac{dg}{dx}\Big|_a^b - \left[\frac{df^*}{dx} g(x)\Big|_a^b - \int_a^b d\left(\frac{df^*}{dx}\right) g(x)\right]$$

boundary terms →

$$= f^*(x) \frac{dg}{dx}\Big|_a^b - \frac{df^*}{dx} g(x)\Big|_a^b + \int_a^b dx \frac{d^2 f^*}{dx^2} g(x)$$

$$= \int_a^b dx\, [\mathcal{L} f(x)]^* g(x) + \underline{f^*(x) \frac{dg}{dx}\Big|_a^b - \frac{df^*}{dx} g(x)\Big|_a^b}$$

(self-adjoint)

To make it Hermitian, we must set

$$\left[f^*(x) \frac{dg}{dx} - \frac{df^*}{dx} g(x)\right]_a^b = 0$$

1 → We can set $f(a) = g(a) = f(b) = g(b) = 0$ (Dirichlet boundary conditions)

2 → We can set $f'(a) = g'(a) = f'(b) = g'(b) = 0$ (Neumann boundary conditions)

Q3. For what values of α will $\mathcal{L} = \alpha \frac{d}{dx}$ becomes self-adjoint? Under what condition will $\mathcal{L}$ become Hermitian?

⇒ treat α as a complex number

Recall from 111 that Hermitian matrices have real eigenvalues & their eigenvectors are orthogonal. The same is true for Hermitian linear differential operators.

real eigenvalues → important in Q.M

* things that we measure are expected to be real-valued

energy operator $-\hbar \frac{\vec{\nabla}^2}{2m}$

position operator $\vec{r}$

momentum operator $\frac{\hbar}{i}\vec{\nabla}$ > $\underline{\vec{\nabla} = \hat{i}\frac{\partial}{\partial x} + \hat{j}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z}}$

Observables (physical quantities) ⟷ Hermitian linear operators

possible outcome of measurement ⟷ eigenvalues of Hermitian operators

Consider the two eigenfunctions of $\mathcal{L}$, that is $\phi_n(x)$ and $\phi_m(x)$

$$\mathcal{L}\,\phi_n(x) = \lambda_n \phi_n(x)$$

$$\mathcal{L}\,\phi_m(x) = \lambda_m \phi_m(x)$$

Take the m^{th} eigenvalue-eigenfunction relation & multiply it with $\phi_n^*(x)$ and then integrate:

$$\int_a^b dx\, \phi_n^*(x) \left[\mathcal{L}\,\phi_m(x) = \lambda_m \phi_m(x)\right]$$

$$\int_a^b dx\, \phi_n^*(x)\, \mathcal{L}\,\phi_m(x) = \lambda_m \int_a^b dx\, \phi_n^*(x)\, \phi_m(x) \quad ❤$$

Do the same for the n^{th} relation

$$\int_a^b dx\, \phi_m^*(x)\, \mathcal{L}\,\phi_n(x) = \lambda_n \int_a^b dx\, \phi_m^*(x)\, \phi_n(x)$$

Take complex conjugate

$$\int_a^b dx\, \phi_m(x) [\mathcal{L}\,\phi_n(x)]^* = \lambda_n^* \int_a^b dx\, \phi_m(x)\, \phi_n^*(x) \quad ■$$

We want $\mathcal{L}$ to be Hermitian, which means

$$\int_a^b dx\, [\mathcal{L}\,\phi_n(x)]^* \phi_m(x) = \int_a^b dx\, [\mathcal{L}^{+} \phi_n(x)]^* \phi_m(x) \quad \Leftarrow \text{definition of Hermitian operator}$$

$$= \int_a^b dx\, \phi_n^*(x)\, \mathcal{L}\,\phi_m(x) \quad \Leftarrow \text{reverse IBP}$$

Thus, because $\mathcal{L}$ is Hermitian, the left hand side ■ is equal to the the LHS of ❤

Subtracting ■ with ❤, we get

$$0 = \lambda_m \int_a^b dx\, \phi_n^* \phi_m(x) - \lambda_n^* \int_a^b dx\, \phi_m(x)\, \phi_n^*(x)$$

$$0 = \underline{(\lambda_m - \lambda_n^*)} \int_a^b dx\, \phi_n^*(x)\, \phi_m(x) \quad ✓$$

$m \neq n$, we expect $\lambda_m \neq \lambda_n^*$ (hindi si $(\lambda_m - \lambda_n^*)$ ang magpapa zero kay RHS)

$$\int_a^b dx\, \phi_n^*(x)\, \phi_m(x) = 0 \quad \text{for } m \neq n$$

but what is this?

$$\langle \phi_n | \phi_m \rangle = 0 \quad \text{for } m \neq n$$

⇒ statement of orthogonality

⇒ you can also show that the eigenvalues are real for $m = n$

We concentrate on a specific form of differential operator

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

where $p_0(x)$, $p_1(x)$, and $p_2(x)$ are known real functions $p_0(x) \neq 0$ in the chosen function space.

If $p_1(x) = \frac{dp_0}{dx}$, then $\mathcal{L}_x$ becomes self-adjoint ($\mathcal{L}_x = \mathcal{L}_x^{+}$)

We can write $\mathcal{L}_x = p_0(x)\frac{d^2}{dx^2} + \frac{dp_0}{dx}\frac{d}{dx} + p_2(x)$

$$\mathcal{L}_x = \frac{d}{dx}\left[p_0(x)\frac{d}{dx}\right] + p_2(x)$$

Example: Consider an equation involving Laplacian $\vec{\nabla}^2$ in spherical form

$$\vec{\nabla}^2 \psi(\vec{r}) = k^2 \psi(\vec{r}) \ ; \quad k \text{ is a scalar function}, \ \psi(\vec{r}) \text{ unknown scalar function}$$

$$\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial}{\partial\phi}\right]\psi(\vec{r}) = k^2 \psi(\vec{r})$$

Notice that the differential operators in r & θ take the self-adjoint form of $\mathcal{L}_x$

Proof that $\mathcal{L}_x = \frac{d}{dx}\left[p_0(x)\frac{d}{dx}\right] + p_2(x)$ is self-adjoint

$$\int_a^b f^*(x)\, \mathcal{L}_x\, g(x)\, dx = \int_a^b f^* \left[\frac{d}{dx}\left(p_0 \frac{dg}{dx}\right) + p_2 g\right] dx$$

$$= \int_a^b f^* \frac{d}{dx}\left(p_0 \frac{dg}{dx}\right) dx + \int_a^b f^* p_2 g\, dx$$

$$= f^* p_0 \frac{dg}{dx}\Big|_a^b - \int_a^b p_0 \frac{dg}{dx}\frac{df^*}{dx} dx + \int_a^b f^* p_2 g\, dx$$

$$= f^* p_0 \frac{dg}{dx}\Big|_a^b - \int_a^b \frac{dg}{dx} p_0 \frac{df^*}{dx} dx + \int_a^b f^* p_2 g\, dx$$

$$= f^* p_0 \frac{dg}{dx}\Big|_a^b - \left[g\, p_0 \frac{df^*}{dx} - \int_a^b g\, d\left(p_0 \frac{df^*}{dx}\right)\right] + \int_a^b f^* p_2 g\, dx$$

$$= f^* p_0 \frac{dg}{dx}\Big|_a^b - g(x)\, p_0(x) \frac{df^*}{dx}\Big|_a^b + \underbrace{\int_a^b \frac{d}{dx}\left(p_0 \frac{df^*}{dx}\right) g(x)\, dx + \int_a^b p_2(x) f^*(x)\, g(x)\, dx}_{\int_a^b dx \left[\frac{d}{dx}\left(p_0 \frac{df}{dx}\right) + p_2\right]^* g(x)}$$

$$= \left(p_0(x) f^*(x) \frac{dg}{dx} - p_0(x)\, g(x) \frac{df^*}{dx}\right)\Big|_a^b + \int_a^b \mathcal{L}_x f^*(x)\, g(x)\, dx$$

$$= \text{boundary terms} + \int_a^b (\mathcal{L}_x f(x))^* g(x)\, dx$$

↳ will vanish if we choose either the Diriclet or the Neumann boundary conditions

Suppose $p_1(x) \neq \frac{dp_0}{dx}$, that is $\mathcal{L}_x$ is not self-adjoint. We can make $\mathcal{L}_x$ self-adjoint by multiplying it by some weight function

$$\rho(x) = \frac{1}{p_0(x)} \exp\left(\int^x \frac{p_1(x')}{p_0(x')} dx'\right)$$

Exercise: show that if $p_1(x) = \frac{dp_0}{dx}$, the weight function is 1.

$$\mathcal{L} = \rho(x)\, \mathcal{L}_x$$

$$= \frac{1}{p_0(x)} \exp\left(\int^x \frac{p_1(x')}{p_0(x')} dx'\right)\left[p_0(x)\frac{d^2}{dx^2} + p_1(x)\frac{d}{dx} + p_2(x)\right]$$

$$= \underbrace{\exp\left(\int^x \frac{p_1(x')}{p_0(x')} dx'\right)}_{\bar{p}_0(x)}\frac{d^2}{dx^2} + \underbrace{\frac{p_1(x)}{p_0(x)} \exp\left(\int^x \frac{p_1(x')}{p_0(x')} dx'\right)}_{\bar{p}_1(x)}\frac{d}{dx} + \underbrace{\frac{p_2(x)}{p_0(x)} \exp\left(\int^x \frac{p_1(x')}{p_0(x')} dx'\right)}_{\bar{p}_2(x)}$$

Thus,

$$\mathcal{L} = \frac{d}{dx}\left(\bar{p}_0(x)\frac{d}{dx}\right) + \bar{p}_2(x) \quad \text{[Sturm-Liouville form]}$$