11/8/00

Lecture 32 Variational Functional

$$\omega^2[\rho] = \frac{\int_a^b [\tau \rho'^2 + V\rho^2]\,dx}{\int_a^b \sigma \rho^2\,dx}$$

Just like

$$\langle E \rangle = \int \psi^* \hat{H} \psi \,d\tau \Big/ \int \psi^* \psi \,d\tau$$

adjust ψ to minimize $\langle E \rangle$

ρ which minimizes $\omega^2[\rho]$ satisfies Sturm-Liouville eq.

$$-\frac{d}{dx}\left[\tau(x)\frac{d\rho}{dx}\right] + V(x)\rho = \omega^2 \sigma(x)\rho$$

<u>Example</u>: Uniform string $\sigma, \tau = \text{const.}$ $V = 0$

Fixed ends. $\rho(0) = \rho(l) = 0$

Guess a smooth trial function that satisfies b.c.

$$\rho(x) = x(l-x)$$

Note normalization does not matter

$$\rho' = l - 2x$$

$$\omega^2 = \frac{\tau \int_0^l (l-2x)^2\,dx}{\sigma \int_0^l [x(l-x)]^2\,dx}$$

$$\omega^2 = \frac{\tau}{\sigma}\,\frac{\int_0^l [l^2 - 4xl + 4x^2]\,dx}{\int_0^l x^2 dx\,(l^2 - 2lx + x^2)}$$

$$= \frac{\tau}{\sigma l^2}\,\frac{[1 - 4/2 + 4/3]}{[\frac{1}{3} - 2/4 + 1/5]} = \boxed{10\,\frac{\tau}{\sigma l^2}}$$

Exact $\rho_1 = \sin(\pi x/\ell)$

$$\omega^2[\rho_1] = \left(\frac{\pi}{\ell}\right)^2 \tau \frac{\int_0^\ell \cos^2\left(\frac{\pi x}{\ell}\right) dx}{\sigma \int_0^\ell \sin^2\left(\frac{\pi x}{\ell}\right) dx}$$

$$\omega_1^2 = \pi^2 \frac{\tau}{\sigma \ell^2} = 9.8696 \frac{\tau}{\sigma \ell^2}$$

$10 \frac{\tau}{\sigma \ell^2}$ is 1.3% above exact ω_1^2

<u>Eigenfunctions</u>

$$-\frac{d}{dx}\left[\tau \frac{d\rho}{dx}\right] + V\rho = \omega^2 \sigma \rho$$

The B.C. (be they fixed, natural, mixed or periodic) can only be satisfied for certian eigenvalues

$$-\frac{d}{dx}\left(\tau \frac{d}{dx}\rho_n\right) + V \rho_n = \omega_n^2 \sigma \rho_n$$

$$n = 1, 2, \ldots \infty$$

Assumptions (1) $\omega_n^2 \to \infty$ as $n \to \infty$. [Large n has large # of nodes and thus large $\tau \rho'^2$ contribution to variational functional.]

(2) $\omega_n^2 \geq 0$ for all n Equivalent to a stability criteria for the string

Prove <u>Orthogonality of Eigenfunctions</u>

Consider two eigenfunctions

$$\frac{d}{dx}(\tau \rho_p')' - V\rho_p = -\omega_p^2 \sigma \rho_p \qquad (A)$$

$$\frac{d}{dx}(\tau \rho_q') - V\rho_q = -\omega_q^2 \rho_q \qquad (B)$$

Multiply (A) by ρ_q^* and subtract ρ_p times complex conj of (B). Integrate from $\int_a^b dx$.

$$\int_a^b \frac{d}{dx}\left[\rho_q^* \tau \rho_p' - \rho_p \tau \rho_q'^*\right] dx = \left[(\omega_q^2)^* - \omega_p^2\right] \int_a^b dx\, \rho_q^* \sigma \rho_p$$

Note $\rho_q^* V \rho_p$ term cancels

$$= \left(\rho_q^* \tau \rho_p' - \rho_p \tau \rho_q'^*\right)\Big|_a^b = 0$$

This vanishes for any b.c. Example periodic upper limit = lower.

$$\left[(\omega_q^2)^* - \omega_p^2\right] \int_a^b \rho_q^* \sigma \rho_p \, dx = 0$$

If $q = p \Rightarrow (\omega_p^2)^* - \omega_p^2 = 0 \Rightarrow \boxed{\omega_p^2 \text{ is real}}$

If $\omega_q^2 \neq \omega_p^2$

$$\boxed{\int_a^b \rho_q^* \sigma \rho_p \, dx = 0} \qquad q \neq p$$

Eigenfunctions are orthogonal. Important general result.

Can chose normalization for $p=q$. Also can chose eigenfunctions real

$$\boxed{\int_a^b \rho_p \rho_q \, dm = \delta_{pq}}$$

$$dm \equiv \sigma(x)\, dx$$

<u>Completeness of eigenfunctions</u>

Expand any function $f(x)$ that satisfies b.c. in eigenfunctions

$$f(x) = \sum_{n=1}^{\infty} a_n \rho_n(x)$$

If expansion is valid project out coef.

$$a_n = \int_a^b \rho_n(x) f(x) \, dm$$

Consider error in a finite expansion

$$\delta_N \equiv \int_a^b \left[f(x) - \sum_{n=1}^{N} a_n \rho_n(x) \right]^2 dm \geq 0$$

Eigenfunctions are complete if

$$\lim_{N \to \infty} \delta_N = 0$$

<u>Proof</u>: Consider $g_N(x) \equiv \delta_N^{-1/2} \left[f - \sum_{n=1}^{N} a_n \rho_n \right]$

① g_N is orthogonal to the first N eigenfunctions

$$\int_a^b g_N(x) \rho_n(x) \, dm = 0 \qquad n = 1, \dots, N$$

because a_n is the projection of f on ρ_n

(2) g_N is normalized

$$\int_a^b g_N^2 \, dm = 1$$

This is just def. of δ_N

Note for any function g

$$\omega^2[g] \geq \omega_1^2 \qquad \text{lowest eigenvalue}$$

If g is orthogonal to $\rho_1 \Rightarrow$

$$\omega^2[g] \geq \omega_2^2 \qquad \text{2nd lowest eigenvalue}$$

etc. so

$$\omega^2[g_N] \geq \omega_{N+1}^2$$

because g_N is orthogonal to first N eigenfunctions.

Explicitly calculate

$$\omega^2[g_N] = \frac{\int_a^b [\tau g_N'^2 + V g_N^2] \, dx}{\int_a^b g_N^2 \, dm}$$

See text.

$$\omega^2[g_N] = \frac{1}{\delta_N} \left\{ \omega^2[f] \int_a^b f^2 dm - \sum_{n=1}^{N} \omega_n^2 a_n^2 \right\}$$

$$\geq \omega_{N+1}^2$$

Quantity in brackets is positive so

$$\frac{1}{\delta_N} \, \omega^2[f] \int_0^b f^2 \, dm \geq \omega_{N+1}^2$$

or $$\delta_N \leq \frac{\omega^2[f] \int_a^b f^2 \, dm}{\omega_{N+1}^2}$$

Numerator is independent of N. As $N \to \infty$
$\omega_{N+1}^2 \to \infty$ by assumption

$$\Rightarrow \boxed{\lim_{N \to \infty} \delta_N = 0}$$

This proves completeness.

Thus very general results

(A) Eigenfunctions are orthonormal

$$\int_a^b \rho_p \rho_q \, dm = \delta_{pq}$$

(B) Eigenfunctions are complete $\Rightarrow$ can expand any function (satisfying b.c.)

$$f(x) = \sum_{n=1}^{\infty} a_n \rho_n(x)$$