Lecture 32 Variational Functional

\[ \omega^2 [\rho] = \frac{\int_a^b \left[ c_1 \rho'^2 + V \rho^2 \right]dx}{\int_a^b \rho^2 dx} \]

Just like \( \langle E \rangle = \frac{\int_a^b \hat{\Psi}^* \mathcal{H} \hat{\Psi} dx}{\int_a^b \hat{\Psi}^* \hat{\Psi} dx} \)

adjust \( \rho \) to minimize \( \langle E \rangle \)

\( \rho \) which minimizes \( \omega^2 [\rho] \) satisfies

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

Example: Uniform string \( \rho, \Omega = \text{const} \)

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

\[ \rho' = l-2x \]

\[ \omega^2 = \frac{1}{2} \int_0^l (l-2x)^2 dx \]

\[ \omega^2 = \frac{1}{6} \left[ \int_0^l (l^2 - 4lx + 4x^2) dx \right] \]

\[ = \frac{1}{6} \left[ \frac{l^3}{3} - \frac{2l}{4} + 1/5 \right] = \frac{10 l^2}{6 l^2} \]
Exact: \( p_1 = \sin \left( \frac{\pi x}{L} \right) \)
\[
\omega^2 [p_1] = \left( \frac{\pi}{L} \right)^2 \int_0^L \sigma \cdot S \cdot \sin^2 \left( \frac{\pi x}{L} \right) dx
\]
\[
\omega_1^2 = \pi^2 \frac{c^2}{6L^2} = 9.8696 \frac{c}{6L^2}
\]
\[
10 \frac{c}{6L^2} \text{ is } 1.3 \% \text{ above exact } \omega_1^2
\]

**EigenFunctions**

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

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

\[-\frac{d}{dx} \left( \frac{c}{L} \frac{d \rho_n}{dx} \right) + V \rho_n = \omega_n^2 \sigma \rho_n \]

\[n = 1, 2, \ldots \infty\]

Assumptions:

1. \( \omega_n^2 \rightarrow \infty \) as \( n \rightarrow \infty \).
   
   Large \( n \) has large # of nodes and thus large \( \frac{\omega}{c} \) contribution to variational functional.

2. \( \omega_n \geq 0 \) for all \( n \).
   Equivalent to a stability criteria for the string.
Prove Orthogonality of Eigenfunctions

Consider two eigenfunctions

\[ \frac{d}{dx} (2PP') - VP_p = -\omega_p^2 \sigma P_p \quad (A) \]

\[ \frac{d}{dx} (2P_q') - VP_q = -\omega_q^2 \sigma P_q \quad (B) \]

Multiply (A) by \( P_q \) and subtract \( P_p \) from \( \int_b^a \). Integrate:

\[ \int_a^b \frac{d}{dx} \left[ P_q^\dagger P_p - P_p^\dagger P_q^\dagger \right] dx = \left[ (\omega_q^2) - \omega_p^2 \right] \int_a^b \sigma P_q \sigma P_p \]

Note \( \int_a^b \sigma P_q \sigma P_p \) term cancels

\[ = \left( P_q^\dagger P_p^\dagger - P_p^\dagger P_q^\dagger \right) \bigg|_a^b = 0 \]

This vanishes for any b.c. Example

periodic upper limit = lower.

\[ \left[ (\omega_q^2) - \omega_p^2 \right] \int_a^b \sigma P_q \sigma P_p \ dx = 0 \]

If \( q = p \) \( \Rightarrow \) \( (\omega_p^2) - \omega_p^2 = 0 \) \( \Rightarrow \) \( \omega_p^2 \) is real.

If \( \omega_q^2 \neq \omega_p^2 \)

\[ \int_a^b \sigma P_q \sigma P_p \ dx = 0 \quad q \neq p \]

Eigenfunctions are orthogonal. Important general result.
Choose normalization $F_0$, $p=q$. Also choose eigenfunctions real.

\[ \int_a^b p_0 p_p p_q \, dm = \int_a^b p_p q \, dm \]

\[ dm = \delta(x) \, dx \]

**Completeness of eigenfunctions**

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

\[ f(x) = \sum_{n=1}^{\infty} a_n \, p_n(x) \]

If expansion is valid, project cut coeff. $a_n = \int_a^b p_n(x) \, f(x) \, dm$.

Consider error in a finite expansion.

\[ S_N = \int_a^b \left[ f(x) - \sum_{n=1}^{N} a_n \, p_n(x) \right] \, dm \geq 0 \]

Eigenfunctions are complete if

\[ \lim_{N \to \infty} S_N = 0 \]

**Proof:** Consider

\[ g_N(x) = \delta^{1/2} \sum_{n=1}^{N} a_n \, p_n(x) \]

\[ g_N \] is orthogonal to the first $N$ eigenfunctions.

\[ \int_a^b g_N(x) \, p_n(x) \, dm = 0 \quad n = 1, \ldots, N \]

because $a_n$ is the projection of $f$ on $p_n$.
② $g_N$ is normalized

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

This is just def. of $g_N$

Note for any function $g$

$$w^2 [g] \geq w^2_1$$

lowest eigenvalue

IF $g$ is orthogonal to $p_1$ \implies

$$w^2 [g] \geq w^2_2$$

2nd lowest eigenvalue

e tc ...

$$w^2 [g_N] \geq w^2_{N+1}$$

because $g_N$ is orthogonal to first $N$ eigenfunctions.

Explicitly calculate

$$w^2 [g_N] = \int_a^b \left[ 2 g_N^2 \, + \, V g_N^2 \right] \, dx$$

$$\underbrace{\int_a^b g_N^2 \, dm}_{S_b^a g_N^2 \, dm}$$

See text.

$$w^2 [g_N] = \frac{1}{S_N^b} \left( \sum_{n=1}^{\infty} \frac{w_n^2}{a_n^2} \right) S_b^a f^2 \, dm - \sum_{n=1}^{\infty} \frac{w_n^2}{a_n^2}$$

$$\geq w^2_{N+1}$$

Quantity in brackets is positive so
\[
\int_0^a 2f^2 \, \sigma_b \, \frac{f^2}{d\mu} \, d\mu \geq \frac{W^2_{N+1}}{W^2_N}
\]

\[
\sigma_N \leq \frac{\int_0^a 2f^2 \, \sigma_b \, \frac{f^2}{d\mu} \, d\mu}{W^2_{N+1}}
\]

Numerator is independent of N. As \( N \to \infty \), \( W^2_{N+1} \to \infty \) by assumption.

\[
\Rightarrow \quad \lim_{N \to \infty} \sigma_N = 0
\]

This proves completeness.

Thus very general results:

(A) Eigenfunctions are orthonormal:

\[
\int_a^b \psi_p \, \psi_q \, d\mu = \delta_{pq}
\]

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

\[
F(x) = \sum_{n=1}^{\infty} a_n f_n(x)
\]