Lecture 12  Sturm-Liouville problem

1. Definition and examples

2. Self-adjointness

3. Orthogonality, reality, uniqueness

4. Phase formalism

Sturm-Liouville (S-L) problem

1. **Definition**
   
   **Given:**
   
   (1) **Differential operator**
   
   \[
   \hat{L}u = \left[ \frac{d}{dx} p(x) \frac{d}{dx} + q(x) \right] u(x)
   \]
   
   where \( p(x) > 0 \), \( p'(x) \), \( q(x) \) are real continuous functions on an interval \( a < x < b \)
   
   (2) **Boundary conditions**
   
   \( \lambda_0 u(a) + \lambda_1 u'(a) = 0 \), \( \lambda_2 u(b) + \beta_1 u'(b) = 0 \)
   
   (mixed Dirichlet-Neumann b.c.)
   
   \( \lambda_i's \), \( \beta_i's \) are real
   
   **Solve:** the eigenvalue equation
   
   \[
   \hat{L}u(x) + \lambda W(x) u(x) = 0 \]
   
   where \( W(x) \geq 0 \), \( a < x < b \).
1. Harmonic vibrations of a non-uniform elastic spring

\[ \frac{d}{dx} \left[ k(x) \frac{d}{dx} u(x) \right] + p(x) \omega^2 u(x) = 0 \]

\[ \begin{align*}
    k(x) > 0 &= \text{elastic modulus} \\
p(x) &= \text{mass density} \\
\omega &= \text{vibration frequency}
\end{align*} \]

2. One-dimensional heat flow / diffusion

\[ c_v(x) \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left[ k(x) \frac{\partial T}{\partial x} \right] \]

\[ \begin{align*}
    c_v &= \text{specific heat} \\
k &= \text{thermal conductivity}
\end{align*} \]

Look for decaying-in-time solutions \( T(x,t) = u(x) e^{-\lambda t} \)

\[ \frac{d}{dx} k(x) \frac{du}{dx} + \lambda c_v(x) u(x) = 0. \]

3. E & M Problems: \( \nabla^2 V = 0, \quad (\nabla^2 + k^2) V = 0 \)

lead to the S-L problems upon separation of variables

(a) Spherical coordinates: \( V = R(r) U(\theta) \cos m \phi \)

Substitution \( x = r \cos \theta \) yields associated Legendre equation

\[ \left( 1-x^2 \right) u'' - 2x u' + \left[ n(n+1) - \frac{n^2}{1-x^2} \right] u(x) = 0 \]

\[ \frac{d}{dx} \left( 1-x^2 \right) \frac{d}{dx} u, \quad \lambda = q(x) \quad [\text{Arfken}] \quad (8.64) \]

\[ (12.71) \]

so \( p = 1-x^2. \)
(b) cylindrical coordinates: separation of variables yields Bessel equation

\[ x^2 u'' + xu' + (x^2 - v^2) u = 0 \]

[to be precise, \( v \) = integer in the E&M problem, while \( x = \text{const} \times (\text{radial distance}) \)].

As written, the Bessel eq. is not in the S-L form yet. But if we divide by \( x \), we get

\[ xu'' + u' + (x - \frac{v^2}{x}) u = 0 \]

Now rescale the indep. variable \( x = \sqrt{\lambda} \ t \), then

\[ \frac{1}{\sqrt{\lambda}} t \frac{d^2 u}{dt^2} + \frac{1}{\sqrt{\lambda}} \frac{du}{dt} + \left( \sqrt{\lambda} t - \frac{1}{\sqrt{\lambda}} \frac{v^2}{t} \right) u(t) = 0 \]

\[ \frac{d}{dt} \left( t \frac{du}{dt} \right) + \left( \lambda t - \frac{v^2}{t} \right) u = 0 \]

**Question:** Consider ODE \( p_0(x) u'' + p_1(x) u'(x) + p_2(x) u = 0 \). Can we bring it to the S-L form \( \hat{L} u(x) + \lambda w(x) u(x) = 0 \)?

**A:** Yes, by multiplying the general eigenvalue equation \( \hat{L} u + \lambda p(x) u(x) = 0 \) by \( \left[ \frac{p(x)}{p_0(x)} \right] \), \( p(x) \equiv \exp \int \frac{p_1(t)}{p_0(t)} \ dt \).

[Arfken, Eq. (9.7)]
Furthermore, as long as \( p(x), w(x) > 0 \), we can reduce the S-L to a Schrodinger eq. by Liouville substitution

\[
\begin{align*}
\xi &= \xi(x) = \int_a^x \sqrt{\frac{w(t)}{p(t)}} \, dt \quad \text{(new indep. variable)} \\
\psi(\xi) &= u(x) \left[ p(x) w(x) \right]^{1/4} \quad \text{(new dependent var.)}
\end{align*}
\]

\[
\frac{d^2}{d\xi^2} \psi(\xi) + \left[ E - V(\xi) \right] \psi(\xi) = 0,
\]

where

\[
V(\xi) = \frac{9}{w} + (pw)^{-1/4} \frac{d^2}{d\xi^2} (pw)^{1/4}; \quad E = \lambda.
\]


4. The Schrödinger eq. is, of course, in the S-L form.

Conclusion: the S-L is general and ubiquitous in mathematical physics.

Our objective: understand the properties of \( \{ u(x), \lambda \} \).
Quick detour: Scalar product, matrix element

- Scalar product of two functions:

\[
\langle u | v \rangle = \int_a^b u^*(x) v(x) \, dx
\]

Properties:

\[
\langle u | v_1 + v_2 \rangle = \langle u | v_1 \rangle + \langle u | v_2 \rangle
\]

\[
\langle u | \lambda v \rangle = \lambda \langle u | v \rangle
\]

\[
\langle v | u \rangle = \langle u | v \rangle^*
\]

- Matrix element:

\[
\langle u | \hat{L} | v \rangle \equiv \langle u | \hat{L} \hat{v} \rangle = \int_a^b dx \, u^*(x) \hat{L}(x) \hat{v}(x)
\]

Self-adjoint operators:

\[
\langle u | \hat{L} | v \rangle = \langle v | \hat{L} | u \rangle^*
\]

Consider \( \hat{L} = \frac{d}{dx} p(x) \frac{d}{dx} + q(x) \)

\[
\langle u | \hat{L} | u \rangle = \int_a^b dx \, u^*(x) \left[ (pu')' + qu(x) \right]
\]

by parts

\[
= p(x) u^*(x) u'(x) \bigg|_a^b + \int_a^b dx \left\{ -pu' \frac{d}{dx} u^* + q u^* u \right\}
\]

again

\[
= p(x) [u^* u' - (u^*)' u] \bigg|_a^b + \int_a^b dx \, u \left[ (pu')' + q u^* \right]
\]

\[
= p(x) [u^* u' - (u^*)' u] \bigg|_a^b + \langle u | \hat{L} | u \rangle^*
\]

Example: \( u, v = 0 \) at \( x=0, b \) (Dirichlet) \( \Rightarrow \) \( \langle u | \hat{L} | v \rangle = \langle u | \hat{L} | v \rangle^* \).
Basic properties of self-adjoint (Hermitian) operators:

1) Eigenvalues are real:
\[ \hat{L}|u\rangle = \lambda |u\rangle, \quad \lambda \in \mathbb{R} \]

2) Eigenfunctions that belong to \( \lambda_1 \neq \lambda_2 \) are orthogonal
\[ \hat{L}|u_1\rangle = \lambda_1 |u_1\rangle, \quad \hat{L}|u_2\rangle = \lambda_2 |u_2\rangle \Rightarrow \langle u_1|u_2\rangle = 0. \]
(2) **Self-adjointness property**

We want to establish more carefully when
\[
\langle u | \hat{L} | u \rangle = \langle u | \hat{L} | u \rangle^* \quad \text{holds.}
\]

This highlights the role of boundary conditions (b.c.)

On the previous page we found:
\[
\langle u | \hat{L} | u \rangle - \langle u | \hat{L} | u \rangle^* = p(x)(u^* u' - u^*' u') \big|_a^b.
\]

Now, \( u^* u' - u^*' u = \det \begin{bmatrix} u^* & u^* \\ u & u' \end{bmatrix} \),

The boundary conditions give
\[
M(x) \begin{bmatrix} \phi_0 \\ \phi_1 \end{bmatrix} = \begin{bmatrix} d_0 u^*(a) + d_1 u^{'*(a)} \\ d_0 u(a) + d_1 u(a) \end{bmatrix} = \begin{bmatrix} (d_0 u + d_1 u')^* \\ d_0 u + d_1 u \end{bmatrix} = [0],
\]

Unless \( d_0 = d_1 = 0 \), we must have \( \det M(x) = 0 \).

Therefore, the boundary term at \( x = a \) vanishes for all allowed \( u, v \) if and only if

(a) \( d_1^2 + d_2^2 > 0 \), \( p(a) \) arbitrary \quad \text{regular S-L problem}

(b) \( d_1 = d_2 = p(a) = 0 \) \quad \text{(singular S-L p.)}

The similar statement holds for \( x = b \) if \( a \to b, \lambda \to \beta \).

Q: Why call \( p(a) = 0 \) case singular?
A: \[
u'' + \frac{p'(x)}{p(x)} u' + \frac{q(x) + \lambda w(x)}{p(x)} u = 0.\]
Orthogonality, uniqueness, reality

We saw that \( \hat{L}u + \lambda w(x)u(x) = 0 \) is equivalent to

\[
\left[ \frac{d^2}{dx^2} - V(\xi) \right] \psi(\xi) + \lambda \psi(\xi) = 0
\]

This is Hermitian.

Thus, all \( \lambda \) are real, and for \( \lambda_1 \neq \lambda_2 \)

\[
0 = \langle \psi_1 | \psi_2 \rangle = \int \frac{\psi_1^*(\xi) \psi_2(\xi)}{\sqrt{S(\xi)}} d\xi
\]

\[
= \int_a^b u_1^*(p(x)\frac{1}{4}u_2(p(x)\frac{1}{4}(\frac{w(x)}{p(x)})^{1/2}) dx
\]

\[
= \int_a^b u_1^*u_2(x) w(x) dx = \langle u_1 | u_2 \rangle_w
\]

[Orthogonality with the weight \( w(x) \)].

\( \lambda \)'s are non-degenerate if the SL problem is regular

\((w > 0, p > 0, q \) are well-behaved\)

Proof: since \( \lambda \) is real, Re & Im parts of any
eigenfunction is again an eigenfunction \( \Rightarrow \) can assume they
are always real. For two such functions \( u_1, u_2 \)

\[
\det M(x) = \det \left| \begin{array}{cc} u_1 & u_2 \\ u_1' & u_2' \end{array} \right| = w(x) \quad (\text{Wronskian})
\]

We saw that \( W(\xi) = 0 \).

Abel formula \( W(x) = \frac{\text{Const}}{p(x)} \Rightarrow W(x) = 0 \Rightarrow u_1, u_2 \) are
linearly dependent.
Note: there are also other formulations of the S-L problem, such as those with periodic boundary conditions, e.g.,

\[ u(a) = u(b) \]

In such a problem, the degeneracy may and does occur:

\[ \frac{d^2 y}{dx^2} + \lambda y = 0 \]

has periodic solutions

\[ y(0) = y(2\pi) \] of two kinds,

\[ y = \cos mx \quad \text{and} \quad y = \sin mx \]

\( (\lambda = m^2) \).
Phase formalism - a convenient approach to analyze
the behavior of \( u(x) \).
We have: \( \frac{d}{dx} p(x) \frac{du}{dx} + Q(x) u = 0 \), \( Q(x) = q(x) + 2 \omega x \).
Consider the Poincaré phase portrait in the phase plane

\[
\begin{align*}
\begin{cases}
    u(x) &= r(x) \sin \Theta(x) \quad \text{"coordinate"} \\
p(x)u'(x) &= r(x) \cos \Theta(x) \quad \text{"momentum"}
\end{cases}
\end{align*}
\]

\[
\begin{align*}
r^2 &= u^2 + p^2 (u')^2 \\
\theta &= \arctan \left[ \frac{u}{pu'} \right]
\end{align*}
\]

The transformation to the \((r, \Theta)\) - variables is non-singular
because \( r \neq 0 \) at all \( x \) (otherwise \( u = u' = 0 \Rightarrow u = 0 \)).
The "equations of motion" for \( \Theta \) and \( r \) are:

\[
\begin{align*}
\begin{cases}
\frac{d\Theta}{dx} &= Q(x) \sin^2 \Theta + \frac{1}{p(x)} \cos^2 \Theta \\
\frac{dr}{dx} &= \frac{1}{2} \left[ \frac{1}{p(x)} - Q(x) \right] r(x) \sin 2\Theta(x)
\end{cases}
\end{align*}
\]

From (2), \( r(x) = r(a) \exp \left\{ \frac{1}{2} \int_{a}^{x} \left( \frac{1}{p} - Q \right) \sin 2\Theta \, dx \right\} \)
Simple check: if \( p(x) = \frac{1}{Q(x)} = \text{const} \),

\[
\frac{d\theta}{dx} = Q \quad \Rightarrow \quad \theta = \theta_0 + Q \cdot (x-a) \quad r = \text{const}
\]

\[
\Rightarrow \quad u = r \sin \left[ Q \cdot (x-a) + \theta_0 \right]
\]

which indeed satisfies

\[
\frac{1}{Q} \frac{d^2 u}{dx^2} + Q \cdot x = 0. \quad \text{(harmonic osc. eq.)}
\]

In general, we expect the phase portrait shown above: the solution oscillates and has zeros, \( u(x) = 0 \), whenever \( \theta = \pi \cdot n \).

Boundary conditions:

\[
\left. \lambda_0 \cdot u + \lambda_1 \cdot u' \right|_a = 0 \quad \Rightarrow \quad \theta(a) = \arctan \left[ -\frac{\lambda_1}{\lambda_0} \frac{1}{p(a)} \right], \quad \lambda_0 < 0
\]

\[
\tan \left[ \theta(b) \right] = -\frac{\beta_k}{\beta_0} \frac{1}{p(b)} \quad \Rightarrow \quad \theta(b) = \arctan \left[ -\frac{\beta_k}{\beta_0} \frac{1}{p(b)} \right] + \pi \cdot n.
\]

\[
\frac{\partial}{\partial \lambda} \left( \frac{d\theta}{dx} \right) = \frac{\partial}{\partial \lambda} Q(x) \cdot \sin^2 \theta = W(x) \sin^2 \theta \geq 0.
\]

**Larger \( \lambda \) \Rightarrow steeper growth of \( \theta(x) \).**

It can be shown that for large enough \( \lambda \) the solution should exist, in fact, there is \( \infty \)-number of discrete eigenvalues (for \( b-a < \infty \)):

\[
\lambda_0 < \lambda_1 < \lambda_2 < \ldots
\]
Large $\lambda$ behavior

\[ \frac{d\theta}{dx} = \frac{Q(x) \sin^2 \theta}{p(x)} + \frac{1}{p(x)} \cos \theta \]

Expect very rapid growth of $\theta(x) \Rightarrow$ rapid crossings of $\theta = \pi n$ lines, i.e., rapid oscillations. It can be shown that

\[ \tan \theta \sim \frac{1}{\sqrt{pQ}} \tan \left[ \int_{a}^{x} \sqrt{\frac{Q(t)}{p(t)}} + y \right] , \quad \lambda \to +\infty \]

This is done most conveniently in the Schrödinger representation

\[ \left[ \frac{d^2}{dx^2} + \lambda - V(x) \right] \psi(x) = 0. \]

At large $\lambda$, $V$ can be neglected $\Rightarrow$

\[ \psi(x) \sim C \sin \left( \sqrt{\lambda} x + y \right) , \]

\[ U(x) \sim \frac{C}{[p(x)w(x)]^{1/4}} \sin \left( \sqrt{\lambda} \int_{a}^{x} \sqrt{\frac{w(t)}{p(t)}} dt + y \right) . \]

This leads to the Bohr-Sommerfeld quantization condition

\[ \sqrt{\lambda} \int_{a}^{b} \sqrt{\frac{w(x)}{p(x)}} dx = 2\pi n + 2(\theta - \theta_0) . \]

If $J < \infty$, then $\lambda$'s are discrete and $\lambda_n \sim \left( \frac{2\pi}{J} \right)^2 n^2$.\[ \lambda_n \to \infty \text{ as } n \to \infty \]
Sturm comparison theorem

Let's return to the dependence of phase \( \theta \) on \( x \) and \( \lambda \).

Let \( x_j, x_{j+1} \) be two consecutive zeros of \( u_i(x) \) (at \( \lambda = \lambda_i \)).

Clearly, this means that \( \theta(x_{j+1}) - \theta(x_j) = \pi \).

For any \( \lambda \geq \lambda_1 \) we then have \( \theta \left| \frac{x_{j+1}^{(i)}}{x_j^{(i)}} \right| > \pi \implies \)

\( u_2(x) \) must cross one of the \( \theta = \pi n \) lines \( \Rightarrow \)

there is a zero of \( u_2(x) \) on the interval \((x_j^{(i)}, x_{j+1}^{(i)})\).

(see Figure).
Variational principle for the eigenvalues

We already proved that the eigenvalues of the S-L problem form the sequence $\lambda_0 < \lambda_1 < \ldots < \lambda_n < \ldots$

$\lambda_n = O(n^2) \Rightarrow \infty, \ n \to \infty.$

There is a general fact that the smallest eigenvalue $\lambda_0$ of any Hermitean operator $\hat{A}$ can be found from the variational principle:

$$\lambda_0 = \min \langle u | \hat{A} | u \rangle \text{ subject to the constraint}$$

$$\langle uu \rangle = 1$$

Indeed, for a finite-dim. Hilbert space there is an orthonormal basis of eigenvectors $\{u_0, u_1, u_2, \ldots, u_{n-1}\}$ so that $|u> = \sum_{i=0}^{n-1} c_i |u_i>$$

$$\langle uu \rangle = \sum_i |c_i|^2 = 1,$$

$$\langle uu | \hat{A} | uu \rangle = \sum_i \lambda_i |c_i|^2 > \sum_i \lambda_0 |c_i|^2 = \lambda_0$$

and, of course, $\langle u_0 | \hat{A} | u_0 \rangle = \lambda_0.$
For the S-L problem, \( \frac{d}{dx} p \frac{du}{dx} + q(x) u(x) + \lambda w(x) u = 0 \) (\( \omega \)-dimensional Hilbert space) the variational principle also exists provided \( p(x), w(x) \geq 0 \):

\[
\lambda_0 = \min \langle u | \hat{L} | u \rangle ; \quad \langle uu \rangle_w = \int_a^b u^2(x) w(x) = 1
\]

Note that
\[
\langle u | \hat{L} | u \rangle = \int_a^b u \left[ - \left( p u' \right)' - q u \right] dx .
\]

Integrating by parts,
\[
= \int_a^b \left[ p(u')^2 - q u^2 \right] dx
\]

**Derivation:** To handle the constraint, use Lagrange multipliers method; \( \min F \), where \( F \) is the functional

\[
F[u] = \int_a^b \left\{ p(x) \left( \frac{du}{dx} \right)^2 - q(x) u^2(x) - \lambda w(x) u^2 \right\} dx .
\]

According to the variational principle, the extremal function satisfies the Euler-Lagrange equation

\[
\frac{d}{dx} \frac{\delta L}{\delta u'} - \frac{\delta L}{\delta u} = 0 ,
\]

which is the same as our S-L problem. Next, we have

\[
\min \langle u | \hat{L} | u \rangle = - \min \langle u | \hat{L} | u \rangle = \min \langle u | \lambda w u \rangle
\]

\[
= \min \lambda = \lambda_0 .
\]
Variational method for other eigenvalues

(a) In a finite-dimensional Hilbert space

\[ \lambda_1 = \min \langle u | \hat{A} | u \rangle \quad \text{under constraints} \]
\[
\begin{align*}
\langle u | u \rangle &= 1 \\
\langle u | u_0 \rangle &= 0 \quad (\text{i.e., } |u\rangle \text{ is orthogonal to } |u_0\rangle) 
\end{align*}
\]

Indeed, in this case \[ |u\rangle = \sum_{i=0}^{n-1} c_i |u_i\rangle \] and \[ c_0 = 0 \]

so that \[ \langle u | \hat{H} | u \rangle = \sum_{i=1}^{n-1} \lambda_i |c_i|^2 \geq \lambda_1 \sum_{i=1}^{n-1} |c_i|^2 = \lambda_1 \]

Similarly, for eigenvalue \( \lambda_m \), \( m > 0 \), we must impose constraints

\[ \langle u | u_i \rangle = 0 \quad \text{for } i = 0, 1, \ldots, m-1. \]

(b) For the S-L problem it is, by analogy,

\[ \lambda_n = \min \langle u | -\hat{L} | u \rangle \]

under constraints

\[ \langle u | u \rangle = 1, \quad \langle u | u_i \rangle = 0, \quad i = 0, 1, \ldots, n-1. \]
Equivalent formulation

\[ \lambda_n = \min \frac{\langle u_1 - \hat{\lambda_1} u \rangle}{\langle uu \rangle_w} \quad \text{for} \quad u \neq 0 \quad \text{and} \]

the constraints \( \langle u_i u \rangle = 0 \), \( i = 0, 1, \ldots, n-1 \)

This variational principle enables us to prove completeness of the eigenfunction basis:

for any \( u(x) \) that satisfies the boundary conditions, there exist eigenfunction expansion \( u(x) = \sum_{n=0}^{\infty} c_i u_i(x) \), where

\[ c_i = \langle u_i \mid u \rangle_w \]

that converges in the \( W \)-norm:

\[ \langle \delta_n \mid \delta_n \rangle_w \to 0, \quad n \to \infty \]

Here \( \delta_n = u(x) - \sum_{m=0}^{n-1} c_i u_i(x) \) \( (n\text{-th residual}) \).

Proof: \( |\delta_n\rangle \) is orthogonal to all \( |u_i\rangle \), \( i=0, \ldots, n-1 \), and so

\[ \frac{\langle \delta_n \mid \hat{\lambda}_1 \mid \delta_n \rangle}{\langle \delta_n \mid \delta_n \rangle_w} = \lambda_n, \quad \text{i.e.}, \quad \langle \delta_n \mid \delta_n \rangle_w < \frac{\langle \delta_n \mid \hat{\lambda}_1 \mid \delta_n \rangle}{\lambda_n} \]

Since \( \lambda_n \to \infty \), \( n \to \infty \) we just need to show that

the numerator is bounded.
This follows from the equality

\[ \langle \delta_n \mid \hat{\mathbf{L}} \mid \delta_n \rangle = \sum\limits_{i=0}^{n-1} \lambda_i \mathbf{c}_i^2 \]

and the fact that at sufficiently large \( m \), \( \lambda_n > 0 \).

(proof left for homework)