11/9/11

834 Lecture 14

Lecture Plan
- Loose ends on Fourier transforms
- Numerov method for numerically solving S-eqn 68-70
- First pass at Sturm-Liouville theory

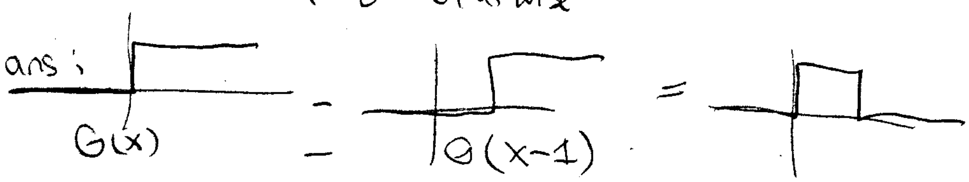
Before class:
- Start up 834 page + Mathematica
  - but don't put screen down

On board:
Warm-ups:

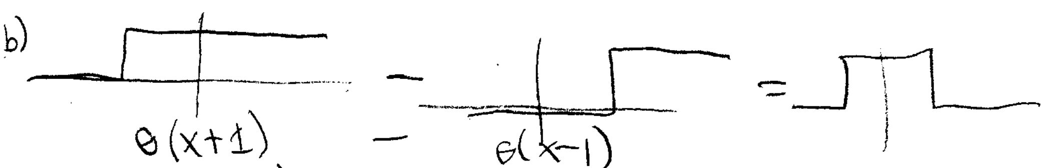
1 a) Write $f(x) = \begin{cases} x & \text{if } 0 \le x \le 1 \\ 0 & \text{otherwise} \end{cases}$ in terms of Θ functions

b) Write $f(x) = \begin{cases} e^x & \text{if } -1 \le x \le 1 \\ 0 & \text{otherwise} \end{cases}$ in terms of Θ functions

a) ans:



b)

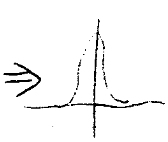


2 What is $\int_{-\infty}^{\infty} e^{ik(x-x_0)}\, dk$? ans: $2\pi\,\delta(x-x_0)$

cf. discussion $\delta^3(\vec r) = \frac{1}{4\pi r^2}\delta(r)$ $\Downarrow$ $\int_0^\infty \delta(r)\,dr = 1$

$\int_{-\infty}^{\infty} e^{-ik(x-x_0)}\, dk$? ans: $2\pi\,\delta(x-x_0)$

symmetric so only half included

relevant for PS#7 prob. 4c $\Rightarrow$ $\int_0^\infty \cos kx\, dk$? ans: $\pi\,\delta(k)$ (not $2\pi\,\delta(k)$) $\Rightarrow$  $\int_0^\infty \delta(k)\, dk = \frac{1}{2}$ here

11/9/11

Recap on Sine and Cosine Transforms (on board at beginning)

a) $F_c[f] = F_c(k) = \sqrt{\frac{2}{\pi}} \int_0^\infty f(x) \cos kx \, dx$

b) $F_s[f] = F_s(k) = \sqrt{\frac{2}{\pi}} \int_0^\infty f(x) \sin kx \, dx$

c) $F_c\left[\frac{df}{dx}\right] = -\sqrt{\frac{2}{\pi}} f(0) + k F_s(k)$

d) $F_s\left[\frac{df}{dx}\right] = -k F_c(k)$

e) $F_c\left[\frac{d^2f}{dx^2}\right] = -\sqrt{\frac{2}{\pi}} \left.\frac{df}{dx}\right|_{x=0} - k^2 F_c(k)$

f) $F_s\left[\frac{d^2f}{dx^2}\right] = k\sqrt{\frac{2}{\pi}} f(0) - k^2 F_s(k)$

- $f(x)$ for $x>0$ only (or $f(x)$ known to be even or odd)
- In diffusion problem: use a) + e) since 2nd order and $\left.\frac{\partial \rho(y,t)}{\partial y}\right|_{y=0}$ given
- Note: rate $r = \int_0^\infty dy \left.\frac{\partial \rho}{\partial t}\right|_{t=0}$ checks $m \cdot \frac{\text{atoms}/m^3}{s} = \text{atoms}/m^2 s$ ✓

proportional to $\delta(y)$

Any questions?

- Do (124), cases i) and ii) simultaneously

Consider $\int_{-\infty}^\infty e^{ikx} \, dk = 2\pi\delta(x)$

$\int_{-\infty}^\infty e^{-ikx} \, dk = 2\pi\delta(x)$

but this $\delta(x)$ means that $\int_0^\infty \delta(x)dx = \frac{1}{2}\int_{-\infty}^\infty \delta(x)\,dx = \frac{1}{2}$

sum $\int_{-\infty}^\infty (e^{ikx} + e^{-ikx}) dk = 2\int_{-\infty}^\infty \cos kx \, dk = 4\pi\delta(x)$

since even

$\Rightarrow \int_{-\infty}^\infty \cos kx \, dk = 2\pi\delta(x)$ or $\int_0^\infty \cos kx \, dk = \pi\delta(x)$

11/9/11

Initial conditions and Causality in Fourier Transform Theory

Based on Lea, example 7.4

Key take-away point: causality (response only happens after a driving term starts) is reflected in location of poles of Fourier transform. (cf. homework PS#7 problem 3)

Electron at rest initially, then $\vec{E}(t) = \Theta(t)\vec{E}_0 e^{-\alpha t}$ acts (so $t>0$ only)

- Damping force $\vec{F}_d = -\gamma\vec{v}$, $\gamma > 0$
- Find motion of electron. Causality $\vec{v}(t) = 0$ for $t<0$!

$\vec{F} = m\vec{a}$: $\quad m\frac{d\vec{v}}{dt} = -\gamma\vec{v} - e\vec{E}(\vec{x}, t)$

- looks 3-Dimensional but motion is only in one-dimension $\Rightarrow$ from $\vec{E}_0$

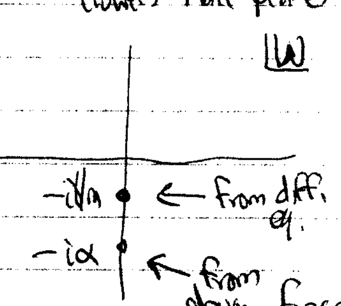
Take FT with $F(\omega) = \int_{-\infty}^{\infty} f(t) e^{i\omega t} dt$ ← note choice of signs for time FT $\Rightarrow$ only pay attention to t dependence

$$\Rightarrow \tilde{\vec{E}}(\omega) = \frac{\vec{E}_0}{\sqrt{2\pi}}\int_0^\infty e^{-\alpha t} e^{i\omega t} dt = \frac{\vec{E}_0}{\sqrt{2\pi}}\frac{1}{i\omega - \alpha} e^{-\alpha t} e^{i\omega t}\Big|_0^\infty = \frac{\vec{E}_0}{\sqrt{2\pi}}\frac{1}{\alpha - i\omega} = \frac{\vec{E}_0}{\sqrt{2\pi}}\frac{i}{\omega + i\alpha}$$

key ↗ 0 $\qquad$ pole in definite (lower) half plane

$$\mathcal{F}[\text{equation}] \Rightarrow -i\omega m\tilde{\vec{v}}(\omega) + \gamma\tilde{\vec{v}}(\omega) = -e\tilde{\vec{E}}(\omega)$$

$$\Rightarrow \tilde{\vec{v}}(\omega) = \frac{1}{-i\omega m + \gamma}\frac{-e\vec{E}_0}{\sqrt{2\pi}}\frac{i}{\omega + i\alpha} = \frac{e}{m}\frac{\vec{E}_0}{\sqrt{2\pi}}\frac{1}{\omega + i\gamma/m}\frac{1}{\omega + i\alpha}$$



* Causality requires transform have no poles in the upper half plane.

$$\vec{v}(t) = \frac{1}{2\pi}\frac{e}{m}\vec{E}_0\int_{-\infty}^{\infty}\frac{1}{\omega + i\gamma/m}\frac{1}{\omega + i\alpha} e^{-i\omega t} d\omega$$

If $t<0$, close in upper half plane $\Rightarrow \vec{v}(t<0) = 0$!

BC's: $\vec{v} = 0$ at $t=0$, $\vec{v} \to 0$ as $t \to \infty$

$$\Rightarrow \vec{v}(t) = \Theta(t)\frac{1}{2\pi}\frac{e}{m}\vec{E}_0(-2\pi i)\left(\frac{e^{-i(-i\alpha)t}}{(-i\alpha + i\gamma/m)} + \frac{e^{-i(-i\gamma/m)t}}{(-i\gamma/m + i\alpha)}\right) = \boxed{\frac{e\vec{E}_0}{\cancel{\alpha m} - \gamma}\left(e^{-\alpha t} - e^{-\frac{\gamma t}{m}}\right)}$$

11/9/11

Removable singularities in contour integrals

Compare

a) $\displaystyle\int_{-\infty}^{\infty} \frac{\sin kx}{x}\,dx = \pi\left[\theta(k) - \theta(-k)\right]$

b) $\displaystyle P\int_{-\infty}^{\infty} \frac{\sin kx}{x}\,dx = \pi\left[\theta(k) - \theta(-k)\right]$

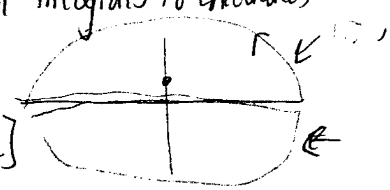
$\varepsilon \to 0^{+}$ implied

c) $\displaystyle\int_{-\infty}^{\infty} \frac{\sin kx}{x - i\varepsilon}\,dx = \pi\left[\theta(k) - \theta(-k)\right]$

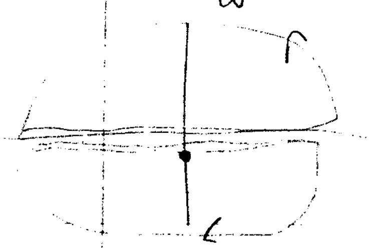
d) $\displaystyle\int_{-\infty}^{\infty} \frac{\sin kx}{x + i\varepsilon}\,dx = \pi\left[\theta(k) - \theta(-k)\right]$

Analysis: Apparent pole at $x=0$, but $\lim_{x\to 0} \frac{\sin kx}{x} \to \frac{kx}{x} = k$
so not a real pole ⇒ "removable"
This means that a) = b) = c) = d) because $\varepsilon \to 0$ limits are all the same (nothing funny happens at $x=0$!)
⇒ use whichever is most convenient (e.g. fewest integrals to calculate)

c) $$\frac{1}{2i}\int_{-\infty}^{\infty} \frac{\overset{i)}{e^{ikx}} - \overset{ii)}{e^{-ikx}}}{x - i\varepsilon} = \frac{1}{2i}\Big[\theta(k)\big[\overset{i)}{(2\pi i)}\cdot 1 - \overset{ii)}{(-2\pi i)}\cdot 0\big] + \theta(-k)\big[\overset{i)}{(-2\pi i)}\cdot 0 - \overset{ii)}{(+2\pi i)}\cdot 1\big]\Big]$$
$$= \pi\left[\theta(k) - \theta(-k)\right]$$



d) $$\frac{1}{2i}\int_{-\infty}^{\infty} \frac{e^{ikx} - e^{-ikx}}{x + i\varepsilon} = \frac{1}{2i}\Big[\theta(k)\big[(2\pi i)\cdot 0 - (-2\pi i)\cdot 1\big] + \theta(-k)\big[(-2\pi i)\cdot 1 - (2\pi i)\cdot 0\big]\Big]$$



$$= \pi\left[\theta(k) - \theta(-k)\right] \quad ✓$$

11/9/11

- Undetermined coefficients for diff. eqs. and integrals

Suppose $\frac{df(x)}{dx} + af(x) = b_0 + b_1 x + b_2 x^2$. What is $f(x)$?

First solve $\frac{df_1}{dx} + af_1 = 0 \Rightarrow f_1(x) = Ce^{-ax}$ C = constant

Now take $f(x) = f_1(x) + d_0 + d_1 x + d_2 x^2$ d_i are "undetermined coefficients"

substitute $\Rightarrow \frac{df}{dx} + af = \cancel{\left(\frac{df_1}{dx} + af_1\right)}^{\,0} + d_1 + 2d_2 x + a(d_0 + d_1 x + d_2 x^2)$

$$= b_0 + b_1 x + b_2 x^2$$

equate coefficients of each x^n:
$$b_0 = d_1 + ad_0$$
$$b_1 = 2d_2 + ad_1$$
$$b_2 = ad_2$$

Solve: $d_2 = \frac{b_2}{a}$; $d_1 = (b_1 - 2d_2)/a = \frac{b_1}{a} - \frac{2b_2}{a}$;
$d_0 = (b_0 - d_1)/a = b_0/a - b_1/a^2 + 2b_2/a^2$

Diffusion case: $b_1 = b_2 = 0 \Rightarrow f(x) = Ce^{-ax} + b_0/a$ ✓
$f(0) = C + b_0/a$ so $C \neq f(0)$ here!

- Same idea used by Mathematica for many integrals,

special case of Risch algorithm

  - Basic principle: The form of many indefinite integrals can be known with undetermined coefficients (rational functions of polynomials, trig, exp.)
    - derivatives are easy to program $\Rightarrow$ work backwards

example $I = \int x^2 e^x \, dx = ax^2 e^x + bxe^x + ce^x$ Find a, b, c

$x^2 e^x = \frac{d}{dx}(ax^2 e^x + bxe^x + ce^x) = 2axe^x + ax^2 e^x + be^x + bxe^x + ce^x$

$x^2 e^x$, xe^x , e^x

$\Rightarrow 1 = a$, $0 = 2a + b$, $0 = b + c$ $\Rightarrow a = 1, b = -2, c = 2$

$\Rightarrow I = x^2 e^x - 2xe^x + 2e^x$ ✓

11/9/11

Fourier Transform: convolution

Suppose $F(k) = \mathcal{F}[f(x)]$ and $G(k) = \mathcal{F}[g(x)]$

Then $H(k) = F(k)\,G(k) \xrightarrow[\text{transform}]{\text{inverse}} h(x)$

Is $h(x) = f(x)\,g(x)$? No! What is it?

$$h(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} H(k)\, e^{ikx}\, dk$$

note different x variables

substitute
$$= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x_1)\, e^{-ikx_1}\, dx_1\right]\left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(x_2)\, e^{-ikx_2}\, dx_2\right] e^{ikx}\, dk$$

Where is k dependence? All in exponents: $e^{-ik(x_1+x_2-x)}$

$\Rightarrow$ do k integral first $\int_{-\infty}^{\infty} e^{-ik(x_1+x_2-x)}\, dk = 2\pi\,\delta(x_1+x_2-x)$

$$\Rightarrow h(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2\, f(x_1)\, g(x_2)\, \delta(x_1+x_2-x) \quad \Rightarrow x_2 = x - x_1$$

$$= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx_1\, f(x_1)\, g(x-x_1)$$

convolution!

11/9/11

Sturm-Liouville Introduction

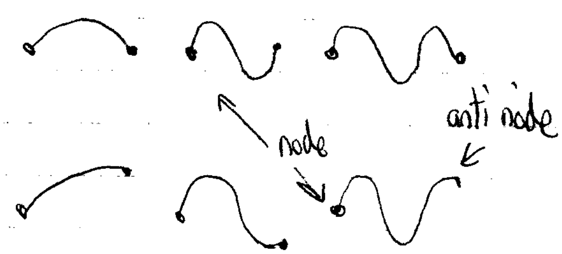
What are Sturm-Liouville problems?

Start with probably the simplest example, the familiar Helmholtz equation on $x \in [0, L]$ (ie $0 \le x \le L$):

$$\frac{d^2y}{dx^2} + k^2 y = 0$$

· Physical situation dictates boundary conditions:

i) vibrating string fixed at ends
$y(0) = 0, \quad y(L) = 0$



ii) pressure (sound) wave in pipe closed at one end
$y(0) = 0, \quad y'(L) = 0$

[Aside: which is the open end?]

more general: a mix of conditions on y and y': $(\alpha y + \beta y')\Big|_{x=L} = 0$

Features:

(that is, $y(x)$ satisfies equation and boundary condition)

- only certain values of k work $\Rightarrow$ eigenvalue problem
- corresponding eigenfunctions
  eg. i) $\Rightarrow y_n(x) = A_n \sin k_n x \Rightarrow k_n L = n\pi \Rightarrow k_n = \frac{n\pi}{L}$
- we can choose A_n so normalized. They are also orthogonal

$$\Rightarrow \int_0^L y_n(x)\, y_m(x) = \delta_{nm} \quad \text{(if normalized)}$$

- From Fourier sine series, we know that $\{y_n(x)\}$ are a complete set on $[0, L]$ $\Rightarrow$ any $f(x) = \sum_{n=1}^{\infty} a_n y_n(x)$ with $f(x)$ same B.C.'s

11/9/11

Another set of applications come from Laplace's equation $\nabla^2\Phi = 0$ (or generalizations).

- We'll particularly consider how it plays out with different coordinate systems. Just as a warm-up, consider cylindrical coordinates.

- The Jackson covers tell us that in cylindrical coordinates

$$\nabla^2\psi = \frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\psi}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\phi^2} + \frac{\partial^2\psi}{\partial z^2}$$

- Look for separation of variables solution to $\nabla^2\Phi$: $\Phi = R(\rho)W(\phi)Z(z)$

$$\Rightarrow \frac{1}{\rho}\frac{d}{d\rho}\left(\rho\frac{dR}{d\rho}\right)WZ + \frac{1}{\rho^2}RZ\frac{d^2W}{d\phi^2} + RW\frac{d^2Z}{dz^2} = 0$$

Collect all R, W, Z's in separate terms by dividing by RWZ:

$$\underbrace{\frac{1}{R\rho}\frac{d}{d\rho}\left(\rho\frac{dR}{d\rho}\right) + \frac{1}{\rho^2}\frac{1}{W}\frac{d^2W}{d\phi^2}}_{\text{no } Z\text{'s}} + \underbrace{\frac{1}{Z}\frac{\partial^2 Z}{dz^2}}_{\text{only } Z\text{'s}} = 0 \Rightarrow \frac{1}{Z}\frac{d^2Z}{dz^2} = \text{constant} = k^2$$

later: when $k^2, -k^2$?

so $Z(z) \propto e^{\pm kz}$

Now isolate W term by multiplying by ρ^2

$$\Rightarrow \rho\frac{1}{R}\frac{d}{d\rho}\left(\rho\frac{dR}{d\rho}\right) + \underbrace{\frac{1}{W}\frac{d^2W}{d\phi^2}}_{\text{only } \phi\text{'s}} + k^2\rho^2 = 0$$

only ϕ's $\Rightarrow \frac{1}{W}\frac{d^2W}{d\phi^2} = -m^2$

$$*\frac{R}{\rho} \Rightarrow \boxed{\frac{d}{d\rho}\left(\rho\frac{dR}{d\rho}\right) - m^2\frac{R}{\rho} + k^2\rho R = 0}$$ Bessel's equation!

Generalize: $f(\rho)$, $g(\rho)$, eigenvalue λ, $w(\rho)$ "weight"

$\Rightarrow$ Sturm-Liouville in general form

(cf. similar exercise with ∇^2 in spherical, eg. $\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) + \ldots$)

11/9/11

General Sturm-Liouville form for $y(x)$ equation:

$$\frac{d}{dx}\left(f(x)\frac{dy}{dx}\right) - g(x)\,y + \lambda\, w(x)\, y = 0$$

where $w(x) \geq 0$ on $a \leq x \leq b$ $\left(x \in [a,b]\right)$

and boundary conditions:

$$\left.\left(\alpha_1 y + \beta_1 \frac{dy}{dx}\right)\right|_{x=a} = 0 \qquad \left.\left(\alpha_2 y + \beta_2 \frac{dy}{dx}\right)\right|_{x=b} = 0 \qquad \text{B.C.'s}$$

[Vocabulary: $\alpha = 0 \Rightarrow \frac{dy}{dx} = 0$ $\Rightarrow$ Neumann conditions;
$\beta = 0 \Rightarrow y = 0 \Rightarrow$ Dirichlet conditions;]

Problem: Find λ's for which there are non-trivial (that is, $y(x)$ is not identically zero) solutions. $\Rightarrow$ eigenvalues and eigenfunctions, λ_n, $y_n(x)$

(Here: take $y_n(x)$'s to be real but generally complex)

General solution: linear combination of orthogonal eigenfunctions

① orthogonal is with respect to weight $w(x)$: $\int_a^b w(x)\, y_m(x)\, y_n(x)\, dx = \delta_{mn}$ (if normalized). $w(x) \neq 1$ in general!

[general: $\int_a^b w(x)\, y_n^* y_m\, dx = \delta_{nm}$

② completeness on $x \in [a,b]$

$$f(x) = \sum_{n=0}^{\infty} a_n y_n(x) \Rightarrow a_m = \frac{\int_a^b f(x)\, y_m(x)\, w(x)\, dx}{\int_a^b [y_m(x)]^2 w(x)\, dx}$$

$\leftarrow = 1$ if normalized

$\equiv I_n$

[$|y_m(x)|^2$ if complex]

substitute for y_n $\Rightarrow$ sifting!

$$\Rightarrow \sum_n \frac{y_n(x)\, y_n(x')\, w(x')}{I_n} = \delta(x-x')$$

cf. $1 = \sum_n |y_n\rangle\langle y_n|$

③ eigenvalues λ_n are real

④ self-adjoint: if $\mathcal{L}y \equiv \frac{d}{dx}\left(f(x)\frac{dy}{dx}\right) - g(x)\, y$

$$\Rightarrow \int_a^b y_n \mathcal{L} y_m\, dx = \int_a^b y_m \mathcal{L} y_n\, dx$$

because surface terms vanish from BC's

11/9/11

Proof of orthogonality: cf. $\langle \psi_n | H | \psi_m \rangle = (E_n - E_m)\langle \psi_n | \psi_m \rangle$

$\Rightarrow$ nondegenerate $\Rightarrow \langle \psi_n | \psi_m \rangle = \delta_{nm}$

$$y_n * \left[\frac{d}{dx}\left(f(x)\frac{dy_m}{dx}\right) - g(x)\, y_m + \lambda_m w(x)\, y_m = 0 \right]$$

$$y_m * \left[\frac{d}{dx}\left(f(x)\frac{dy_n}{dx}\right) - g(x)\, y_n + \lambda_n w(x)\, y_n = 0 \right]$$

subtract and integrate $\int_a^b dx$

note weight!

$$\int_a^b dx \left[y_n \frac{d}{dx}\left(f(x)\frac{dy_m}{dx}\right) - y_m \frac{d}{dx}\left(f(x)\frac{dy_n}{dx}\right)\right] = (\lambda_n - \lambda_m)\int_a^b w(x)\, y_m y_n \, dx$$

like with Hamiltonian: partially integrate both terms:

$$-\frac{dy_n}{dx} f(x) \frac{dy_m}{dx} - (-)\frac{dy_m}{dx} f(x) \frac{dy_n}{dx} = 0$$

Surface terms? $\left[y_n f(x) \frac{dy_m}{dx} - y_m f(x) \frac{dy_n}{dx} \right]\Big|_a^b$

vanish if: a) $f(b) = f(a) = 0$

b) $\alpha_1 y + \beta_1 \frac{dy}{dx} = 0$ at each end

If either $y = 0$, or $\frac{dy}{dx} = 0$, then done.

Otherwise $\frac{dy}{dx} = -\frac{\alpha_1}{\beta_1} y \Rightarrow \frac{\alpha_1}{\beta_1} f(x)\left[y_n y_m - y_m y_n \right]\Big|_a^b = 0$

Degeneracies? $\lambda_n = \lambda_m$ for $y_n \neq y_m$? Come back to this!