

Lecture #20: Separation of Variables

I. Solution of PDEs through Separation of Variables

A. Basic Concept

1. Split a PDE of n variables into n ODEs.
2. Assume solution is a product of single variable functions, eg, $f(x, y, z) = X(x)Y(y)Z(z)$
- 3a. Substitute, and divide resulting equations into parts depending on separate variables.
- b. Set each part equal to a constant of separation.
4. Apply Boundary Conditions to solve for unknown parameters (eigenvalue) and constants in general solution.

B. Cartesian Coordinates

1. Consider solving Helmholtz eq, $\boxed{\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + k^2 \psi = 0}$
2. Assume a solution $\psi(x, y, z) = X(x)Y(y)Z(z)$ and substitute.

$$YZ \frac{d^2 X}{dx^2} + XZ \frac{d^2 Y}{dy^2} + XY \frac{d^2 Z}{dz^2} + k^2 XYZ = 0$$

↑ Note: Ordinary derivative because $X(x)$ is function of x only.

3. Divide by XYZ and collect all terms with X on one side:

$$\underbrace{\frac{1}{X} \frac{d^2 X}{dx^2}}_{\text{function of only } x} = \underbrace{-\ell^2}_{\substack{\uparrow \\ \text{Constant of} \\ \text{Separation}}} = -k^2 - \underbrace{\frac{1}{Y} \frac{d^2 Y}{dy^2} - \frac{1}{Z} \frac{d^2 Z}{dz^2}}_{\text{function of only } (y, z)}$$

a. Note: Sign of constant is arbitrary, chosen to facilitate application of BCs

$$4. \text{ Thus } \boxed{\frac{d^2 X}{dx^2} = -\ell^2 X} \text{ and } \frac{1}{Y} \frac{d^2 Y}{dy^2} = -k^2 + \ell^2 - \frac{1}{Z} \frac{d^2 Z}{dz^2} = -\underbrace{m^2}_{\text{constant!}}$$

$$5. \text{ Finally } \frac{1}{Z} \frac{d^2 Z}{dz^2} = -k^2 + \ell^2 + m^2 = -n^2$$

I. B. Continued)

6. Thus, we obtain

3 ODEs:

$$\begin{aligned} X'' &= -\ell^2 X \\ Y'' &= -m^2 Y \\ Z'' &= -n^2 Z \end{aligned}$$

where $k^2 = \ell^2 + m^2 + n^2$

Hawes (2)

7. Thus, a solution is $\psi_{\ell mn} = X_{\ell}(x) Y_m(y) Z_n(z)$

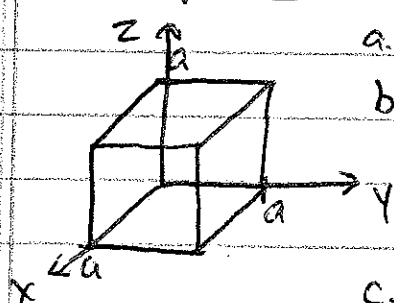
8. The most general solution is given by a linear combination

$$\Psi = \sum_{\ell, m} a_{\ell m} \psi_{\ell mn} \quad \text{where } k^2 = \ell^2 + m^2 + n^2$$

a. Application of BCs often leads to discrete values of ℓ & m , and set the value of coefficients $a_{\ell m}$.

9. NOTE: Separation can also be achieved if constant k^2 is replaced by a sum of single-variable functions, $k^2 \rightarrow f(x) + g(y) + h(z)$

10. Example: Quantum Particle in a Box



a. Particle of mass m

b. Time-independent Schrödinger Eq:

$$-\frac{1}{2} \nabla^2 \psi(x, y, z) = E \psi(x, y, z)$$

where $m = \hbar = 1$ units

Energy eigenvalue.

c. Dirichlet BCs: $\psi = 0$ at $x=0, a$; $y=0, a$; $z=0, a$.

d. Let $\psi(x, y, z) = X(x) Y(y) Z(z) \Rightarrow -\left(\frac{X''}{X} + \frac{Y''}{Y} + \frac{Z''}{Z}\right) = 2E$

e. Separate $X(x)$: $\frac{X''}{X} = -\ell^2 \Rightarrow X'' = -\ell^2 X \Rightarrow X = A \sin \ell x + B \cos \ell x$

f. Apply BCs: $X(0) = X(a) = 0$:
i. $X(0) = 0 = A \sin(0) + B \cos(0) \Rightarrow B = 0$
ii. $X(a) = 0 = A \sin(\ell a) \Rightarrow \ell a = \ell \pi$

$$\Rightarrow X(x) = A \sin\left(\frac{\ell \pi x}{a}\right) \quad \text{for } \ell = 1, 2, 3, \dots$$

I.B, 10. (Continued)

Hawes ③

g. Similar approach for $Y(y)$ and $Z(z)$ with constants $-\mu^2$ and $-\nu^2$:

$$Y_m(y) = \sin\left(\frac{m\pi y}{a}\right) \quad m=1,2,3,\dots \quad Z_n(z) = \sin\left(\frac{n\pi z}{a}\right) \quad n=1,2,3,\dots$$

h. Final condition $\lambda^2 + \mu^2 + \nu^2 = 2E \Rightarrow E_{lmn} = \frac{\pi^2}{2a^2}(\ell^2 + m^2 + n^2)$

i. Solution:

$$\psi_{lmn}(x,y,z) = A_{lmn} \sin\left(\frac{\ell\pi x}{a}\right) \sin\left(\frac{m\pi y}{a}\right) \sin\left(\frac{n\pi z}{a}\right)$$

Eigenvalues E_{lmn} positive integers

Discrete energy spectrum

C. Cylindrical Coordinates

1. Helmholtz Eq $\nabla^2 \psi + k^2 \psi = 0 \Rightarrow \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial \psi}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{\partial^2 \psi}{\partial z^2} + k^2 \psi = 0$

2. Assume $\psi(\rho, \phi, z) = P(\rho)\Phi(\phi)Z(z)$, substitute and divide by $P\Phi Z$,

$$\frac{1}{\rho P} \frac{d}{d\rho} \left(\rho \frac{dP}{d\rho} \right) + \frac{1}{\rho^2 \Phi} \frac{d^2 \Phi}{d\phi^2} + k^2 = - \frac{1}{Z} \frac{d^2 Z}{dz^2} = -\ell^2$$

separation constant

$$Z'' = \ell^2 Z$$

3. a. $\rho^2 \left[\frac{1}{\rho P} \frac{d}{d\rho} \left(\rho \frac{dP}{d\rho} \right) + \frac{1}{\rho^2 \Phi} \frac{d^2 \Phi}{d\phi^2} \right] = -\ell^2 - k^2 \equiv -n^2 \Rightarrow n^2 = \ell^2 + k^2$

b. $\frac{\rho}{P} \frac{d}{d\rho} \left(\rho \frac{dP}{d\rho} \right) + n^2 \rho^2 = \frac{m^2}{\Phi} = - \frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} \Rightarrow \Phi'' = -m^2 \Phi$

constant

4. This leaves

$$\rho \frac{d}{d\rho} \left(\rho \frac{dP}{d\rho} \right) + (n^2 \rho^2 - m^2) P = 0$$

b. Changing variables to $x = n\rho \Rightarrow (n\rho) \frac{d}{d(n\rho)} \left[(n\rho) \frac{dP}{d(n\rho)} \right] = x \frac{d}{dx} \left(x \frac{dP}{dx} \right)$

$$x^2 \frac{d^2 P}{dx^2} + x \frac{dP}{dx} + (x^2 - m^2) P = 0$$

Bessel Func Neumann Func

c. Bessel's Eq: $x^2 y'' + x y' + (x^2 - n^2) y = 0 \quad y(x) = A J_n(x) + B Y_n(x)$

I. C4 (Continued)

Hawes (4)

d. Thus, we can write solution $P_{lm}(\rho) = A J_m(l\rho) + B Y_m(l\rho)$

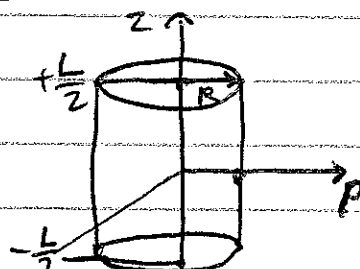
where $n^2 = l^2 + k^2$

e. ASolution: $\Psi_{lmn} = P_{lm}(\rho) \Phi_m(\phi) Z_l(z)$

f. General Solution: $\Psi(\rho, \phi, z) = \sum_{lm} a_{lm} P_{lm}(\rho) \Phi_m(\phi) Z_l(z)$

5. Ex: Cylindrical Eigenvalue Problem

a. $-\nabla^2 \Psi = \lambda \Psi$ with Dirichlet BC's $\Psi=0$ at $z=\pm L/2$ or $\rho=R$



Time-independent Schrödinger Eq (Particle in a cylindrical cavity)

b. Let's determine the ground state eigenvalue and eigenfunction.

$\Rightarrow$ Seek solution with smallest number of oscillations!

c. Assume $\Psi(\rho, \phi, z) = P(\rho) \Phi(\phi) Z(z)$. As before, with $n^2 = l^2 + \lambda$

$$Z'' = l^2 Z \Rightarrow Z = A e^{lz} + B e^{-lz}$$

$$\Phi'' = -m^2 \Phi \Rightarrow \Phi = A' \sin(m\phi) + B' \cos(m\phi)$$

d. Apply BC's to Φ : i. Periodic in ϕ with period $2\pi \Rightarrow$ any integer m

ii. Ground state $\Rightarrow$ fewest oscillations $\Rightarrow m=0 \Rightarrow \Phi(\phi) = \text{constant!}$

e. Apply BC's to Z : i. $Z(-L/2) = Z(L/2) = 0$

ii. To satisfy BC's, require $l = i\omega \Rightarrow l^2 = -\omega^2$

iii. Then, $Z'' = -\omega^2 Z \Rightarrow Z = A \sin(\omega z) + B \cos(\omega z)$

iv. Least oscillatory solution: $A=0, \frac{\omega L}{2} = \pm \frac{\pi}{2} \Rightarrow \omega = \frac{\pi}{L}$

v. $Z(z) = B \cos(\frac{\pi z}{L})$

f. P(ρ): $\rho \frac{d}{d\rho}(\rho \frac{dP}{d\rho}) + (n^2 \rho^2 - m^2) P = 0$ $P_{l0}(\rho) = A'' J_2(n\rho) + B'' Y_2(n\rho)$

I.C.S. (Continued)

Arves (5)

g. Apply BC's to P_ρ : i. Must be regular at $\rho=0$, so $B''=0$.

ii. $P_\rho(\rho=R)=0=A'' J_0(nR)$

iii. Least oscillatory solution is first zero crossing at $nR=\alpha \approx 2.4048$
 $\Rightarrow n = \frac{\alpha}{R}$

iv. Thus $P_\rho(\rho) = A'' J_0\left(\frac{\alpha \rho}{R}\right)$

h. Solution for Eigenfunction $\boxed{\psi(\rho, \phi, z) = A J_0\left(\frac{\alpha \rho}{R}\right) \cos\left(\frac{\pi z}{L}\right)}$

h. Find eigenvalue λ : i. Recall $n^2 = \ell^2 + 1$

ii. We require $\ell^2 = -\omega^2 = -\left(\frac{\pi}{L}\right)^2$ and $n^2 = \frac{\alpha^2}{R^2}$, so $\frac{\alpha^2}{R^2} = \left(\frac{\pi}{L}\right)^2 + 1$

iii. Thus $\boxed{\lambda = \frac{\pi^2}{L^2} + \frac{\alpha^2}{R^2}} \leftarrow \text{ground state energy.}$

D. Spherical Coordinates

1. Helmholtz Eq: $\nabla^2 \psi + k^2 \psi = 0 \Rightarrow \boxed{\frac{1}{r^2 \sin \theta} \left[\sin \theta \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{\sin \theta} \frac{\partial^2 \psi}{\partial \phi^2} \right] = -k^2}$

2. Assume: $\psi(r, \theta, \phi) = R(r) \Theta(\theta) \Phi(\phi)$, substitute, and divide by $R \Theta \Phi$

$$\frac{1}{R r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{1}{\Theta r^2 \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + \frac{1}{\Phi r^2 \sin^2 \theta} \frac{d^2 \Phi}{d\phi^2} = -k^2$$

3. Multiply by $r^2 \sin^2 \theta$, and rearrange

$$\frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} = -m^2 = r^2 \sin^2 \theta \left[-k^2 - \frac{1}{R r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) - \frac{1}{\Theta r^2 \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) \right]$$

$$\Rightarrow \boxed{\Phi'' = -m^2 \Phi}$$

4. Multiply RHS by $\frac{1}{\sin^2 \theta}$,

$$\frac{1}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + r^2 k^2 = \lambda = - \frac{1}{\Theta \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + \frac{m^2}{\sin^2 \theta}$$

I. D. (Continued)

$0 \leq \theta \leq \pi$ Homework 6

5. Transform $\Theta(\theta)$ using $t = \cos \theta$ ($-1 \leq t \leq 1$)

$$\boxed{(1-t^2)P''(t) - 2tP'(t) - \frac{m^2}{1-t^2}P(t) + \lambda P(t) = 0}$$
 Associated Legendre Equation

a. Solutions are Associated Legendre Functions, $\Theta(\theta) = P_l^m(\cos \theta)$

where $\lambda = l(l+1)$, l nonnegative integer and $l \geq |m|$

6. Radial Function $R(r)$: $\boxed{r^2 R'' + 2r R' + [k^2 r^2 - l(l+1)]R = 0}$

a. When $k=0 \Rightarrow$ Laplace's Equation

b. When $k \neq 0 \Rightarrow$ May transform to Bessel's Equation

7. Case $k=0$: $\boxed{r^2 R'' + 2r R' - l(l+1)R = 0}$ Laplace Equation.

a. Frobenius method trivially leads to $R(r) = Ar^l + Br^{l-1}$

b. General Solution: $\boxed{\psi(r, \theta, \phi) = \sum_{l,m} (A_{lm} r^l + B_{lm} r^{l-1}) P_l^m(\cos \theta) (A'_{lm} \sin m\phi + B'_{lm} \cos m\phi)}$

c. Apply BCs to solve for coefficients

8. Case $k \neq 0$:

a. Transform $R(r) = \frac{Z(kr)}{(kr)^{1/2}}$ to obtain

$$\boxed{x^2 Z'' + x Z' + [x^2 - (l + \frac{1}{2})^2]Z = 0}$$
 where $x = kr$

Bessel's Equation of order $l + \frac{1}{2}$.

b. Solutions are Spherical Bessel Functions

$$R(r) = A j_l(kr) + B y_l(kr) \quad \text{where } j_l(x) = \sqrt{\frac{\pi}{2x}} J_{l+\frac{1}{2}}(x)$$

$$y_l(x) = \sqrt{\frac{\pi}{2x}} Y_{l+\frac{1}{2}}(x)$$

c. General
Solution:

$$\psi(r, \theta, \phi) = \sum_{lm} [A_{lm} y_l(r) + B_{lm} y_l(r)] P_l^m(\cos \theta) [A'_{lm} \sin m\phi + B'_{lm} \cos m\phi]$$

9. NOTE: Separation also possible if $k^2 \rightarrow f(r) + \frac{g(\theta)}{r^2} + \frac{h(\phi)}{r^2 \sin^2 \theta}$

a. If $k^2 \rightarrow f(r)$ only, then $\Theta(\theta)$ and $\Phi(\phi)$ solutions remain unchanged.

b. Common Case: $k \rightarrow f(r) \Rightarrow$ Central Force Problems

c. Ex: Gravitation, electrostatics, atomic, nuclear, & particle physics.