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,
   e.g., $f(x,y,z) = X(x)\,Y(y)\,Z(z)$
3. a. Substitute, and divide resulting equations into parts depending on separate variables.
   b. Set each parts equal to a <u>constant of separation</u>.
4. Apply Boundary Conditions to solve for unknown parameter (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.

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

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

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

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

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

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

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

I. B. (Continued)

6. Thus, we obtain 3 ODEs: $\boxed{\begin{aligned} X'' &= -\ell^2 X \\ Y'' &= -m^2 Y \\ Z'' &= -n^2 Z \end{aligned}}$ where $\boxed{k^2 \equiv \ell^2 + m^2 + n^2}$

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

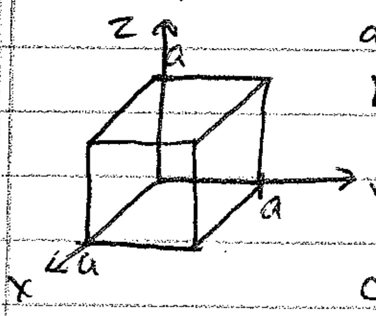
8. The most general solution is given by a linear combination

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

a. Application of BCs often leads to discrete values of ℓ ℓm, 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, $k^2 \to f(x) + g(y) + h(z)$

10. Example: Quantum Particle in a Box



a. Particle of mass m

b. Time-independent Schrödinger Eq: $-\frac{1}{2}\nabla^2 \psi(x,y,z) = E\,\psi(x,y,z)$ ← Energy eigenvalue.
where $m = \hbar = 1$ units

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

f. Apply BCs: $X(0) = X(a) = 0$:
i. $X(0) = 0 = A\cancel{\sin(0)}^{0} + B\cos(0)^{1} \Rightarrow B = 0$
ii. $X(a) = 0 = A\sin(\lambda a) \to \lambda a = \ell\pi$

$\Rightarrow X_\ell(x) = A\sin\left(\frac{\ell\pi x}{a}\right)$ for $\ell = 1, 2, 3, \ldots$

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

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

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

Eigenvalues ℓ, m, n positive integers

$\Downarrow$

~~Discrete energy~~ spectrum

i. Solution:

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

C. Cylindrical Coordinates

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

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

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

separation constant

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

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

4.
a. This leaves $$\rho\frac{d}{d\rho}\left(\rho\frac{dP}{d\rho}\right) + \left(n^2\rho^2 - m^2\right)P = 0$$

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

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

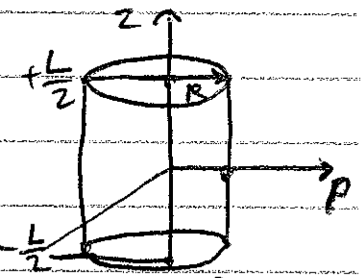
c. Bessel's Eq: $\boxed{x^2y'' + xy' + \left(x^2 - n^2\right)y = 0}$ $\quad y(x) = A\underset{\text{Bessel Func}}{J_n(x)} + B\underset{\text{Neumann Func}}{Y_n(x)}$

I. C.4 (Continued)

d. Thus, we can write solution $P_{\ell m}(\rho) = A J_m(n\rho) + B_m Y(n\rho)$ where $n^2 = \ell^2 + k^2$

e. A Solution: $\psi_{\ell m n} = P_{\ell m}(\rho)\Phi_m(\phi) Z_\ell(z)$

f. General Solution: $\boxed{\Psi(\rho,\phi,z) = \sum_{\ell m} a_{\ell m} P_{\ell m}(\rho)\Phi_m(\phi) Z_\ell(z)}$



5. Ex: Cylindrical Eigenvalue Problem

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

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 $\boxed{n^2 = \ell^2 + \lambda}$

$$Z'' = \ell^2 Z \Rightarrow Z = Ae^{\ell z} + Be^{-\ell z}$$

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

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) = $ constant!

e. Apply BC's to Z: i. $Z(-\frac{L}{2}) = Z(+\frac{L}{2}) = 0$

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

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. $P(\rho)$: $\rho\frac{d}{d\rho}(\rho\frac{dP}{d\rho}) + (n^2\rho^2 - \cancel{m^2})P = 0$ $\quad P_{\ell 0}(\rho) = A''J_0(n\rho) + B''Y_0(n\rho)$

I. C. 5. (Continued)

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

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

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

iv. Thus $P_{\ell 0}(\rho)=A'' J_0\left(\frac{\alpha\rho}{R}\right)$

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 $n^2=\ell^2+\lambda$

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

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

D. Spherical Coordinates

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

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

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

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

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

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

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

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

I. D. (Continued) $0 \le \theta \le \pi$

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

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

a. Solutions are Associated Legendre Functions, $\Theta(\theta) = P_\ell^m(\cos\theta)$
where $\lambda = \ell(\ell+1)$, ℓ nonnegative integer and $\ell \ge |m|$

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

a. When $k=0 \Rightarrow$ Laplace's Equation
b. When $k \ne 0 \Rightarrow$ May transform to Bessel's Equation

7. <u>Case $k=0$:</u> $$\boxed{r^2R'' + 2rR' - \ell(\ell+1)R = 0}$$ <u>Laplace Equation.</u>

a. Frobenius method trivially leads to $R(r) = Ar^\ell + Br^{-\ell-1}$
b. <u>General Solution:</u> $$\boxed{\psi(r,\theta,\phi) = \sum_{\ell,m}(A_{\ell m}r^\ell + B_{\ell m}r^{-\ell-1})P_\ell^m(\cos\theta)(A'_{\ell m}\sin m\phi + B'_{\ell m}\cos m\phi)}$$
c. Apply BCs to solve for coefficients

8. <u>Case $k \ne 0$:</u>
a. Transform $R(r) = \frac{Z(kr)}{(kr)^{\frac{1}{2}}}$ to obtain

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

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

b. Solutions are <u>spherical Bessel functions</u>

$R(r) = A\,j_\ell(kr) + B\,y_\ell(kr)$ where $j_\ell(x) = \sqrt{\frac{\pi}{2x}}\,J_{\ell+\frac{1}{2}}(x)$

$y_\ell(x) = \sqrt{\frac{\pi}{2x}}\,Y_{\ell+\frac{1}{2}}(x)$

c. General Solution: $\boxed{\psi(r,\theta,\phi) = \sum_{\ell m} \left[A_{\ell m} j_\ell(kr) + B_{\ell m} y_\ell(kr)\right] P_\ell^m(\cos\theta) \left[A'_{\ell m} \sin m\phi + B'_{\ell m} \cos m\phi\right]}$

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

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

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

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