Lecture #11: Spherical Bessel Functions and Legendre Functions

I. Spherical Bessel Functions

A. Spherical Symmetry

1. When performing a separation of variables for the Helmholtz Equation in spherical coordinates,

$$\nabla^2\psi + k^2\psi = 0 \qquad \text{where } \psi(r,\theta,\phi) = R(r)\,\Theta(\theta)\,\Phi(\phi)$$

we obtain a radial equation

$$\boxed{r^2\frac{d^2R}{dr^2} + 2r\frac{dR}{dr} + \left[k^2r^2 - \ell(\ell+1)\right]R = 0}$$

where ℓ is an integer to satisfy BCs of angular equations.

2. Substitute $R(kr) = \dfrac{Z(kr)}{(kr)^{\frac{1}{2}}}$ to obtain

$$\boxed{r^2\frac{d^2Z}{dr^2} + r\frac{dZ}{dr} + \left[k^2r^2 - \left(\ell+\tfrac{1}{2}\right)^2\right]Z = 0}$$

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

Solutions: $J_{\ell+\frac{1}{2}}(kr)$ & $Y_{\ell+\frac{1}{2}}(kr)$

3. Def: Spherical Bessel Functions (integer n)

$$\boxed{\begin{aligned}
j_n(x) &= \sqrt{\frac{\pi}{2x}}\,J_{n+\frac{1}{2}}(x)\\
y_n(x) &= \sqrt{\frac{\pi}{2x}}\,Y_{n+\frac{1}{2}}(x)\\
h_n^{(1)}(x) &= \sqrt{\frac{\pi}{2x}}\,H^{(1)}_{n+\frac{1}{2}}(x) = j_n(x) + i y_n(x)\\
h_n^{(2)}(x) &= \sqrt{\frac{\pi}{2x}}\,H^{(2)}_{n+\frac{1}{2}}(x) = j_n(x) - i y_n(x)
\end{aligned}}$$

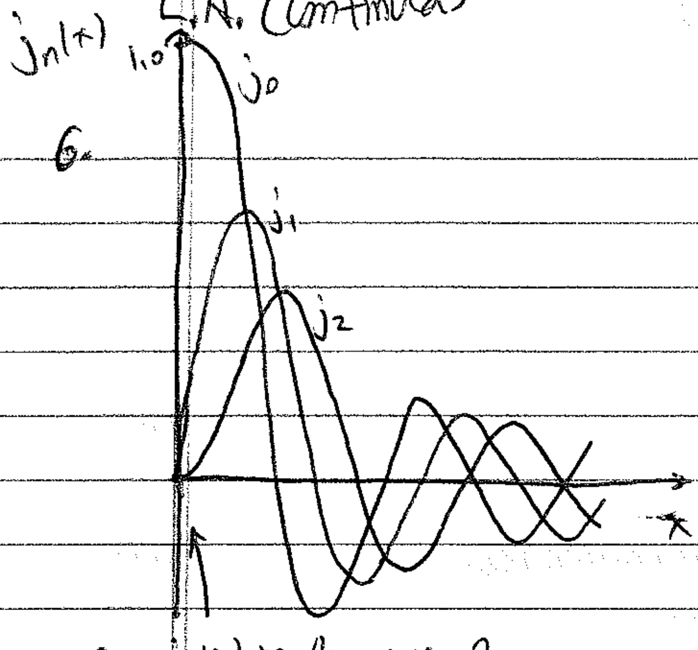
4. Definition of $Y_{n+\frac{1}{2}}(x)$ yields $\boxed{y_n(x) = (-1)^{n+1} j_{-n-1}(x)}$

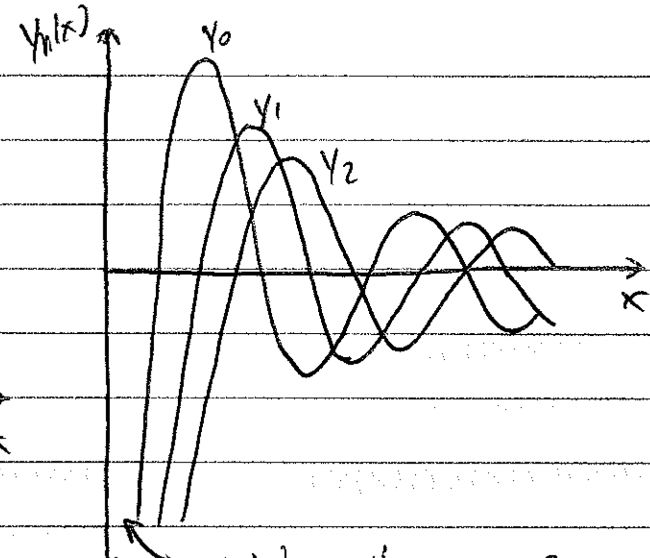
5. Series Form: $\boxed{j_n(x) = \sqrt{\dfrac{\pi}{2x}}\displaystyle\sum_{s=0}^{\infty}\frac{(-1)^s}{s!\,\Gamma(s+n+\frac{3}{2})}\left(\frac{x}{2}\right)^{2s+n+\frac{1}{2}}}$

or $j_n(x) = \dfrac{x^n}{(2n+1)!!}\displaystyle\sum_{s=0}^{\infty}\frac{(-1)^s}{s!\,(n+\frac{3}{2})_s}\left(\frac{x}{2}\right)^{2s}$ where Pochhammer symbol $(n+\frac{3}{2})_s$

I. A. (Continued)

6.





a. $j_n(x)$ regular at $x=0$

$$\lim_{x\to 0} j_n(x) \propto x^{n}$$

b. $y_n(x)$ irregular at $x=0$.

$$\lim_{x\to 0} y_n(x) \propto x^{-n-1}$$

7. Closed Form:

$$j_0(x) = \frac{\sin x}{x} \qquad y_0(x) = -\frac{\cos x}{x}$$

$$h_0^{(1)}(x) = \frac{-i}{x} e^{ix} \qquad h_0^{(2)}(x) = \frac{i}{x} e^{-ix}$$

B. Constructing Spherical Hankel Functions

1. a. The asymptotic expansion of $H_{n+\frac{1}{2}}(x)$ terminates for half-integral order,

$$H_{n+\frac{1}{2}}(x) = \sqrt{\frac{2}{\pi x}}\, e^{\pm i[x+(n+1)\frac{\pi}{2}]}\left[P_{n+\frac{1}{2}}(x) \pm i\, Q_{n+\frac{1}{2}}(x)\right]$$

b. Thus, we can write

$$h_n^{(1)}(x) = (-i)^{n+1} \frac{e^{ix}}{x} \sum_{n=0}^{\infty} \frac{i^s}{s!\,(2x)^s} \frac{(n+s)!}{(n-s)!}$$

2. Taking Re and Im parts, you may construct $h_n^{(2)}$, j_n, y_n, for example

$$h_1^{(1)}(x) = e^{ix}\left(-\frac{1}{x} - \frac{i}{x^2}\right)$$

$$h_2^{(1)}(x) = e^{ix}\left(\frac{i}{x} - \frac{3}{x^2} - \frac{3i}{x^3}\right) \qquad \text{etc.}$$

I. (Continued)

C. Recurrence Relations

1. Using recurrence relations for $J_\nu(x)$, $Y_\nu(x)$, $H_\nu(x)$, we can generate recurrence relations for spherical Bessel functions:

$$f_{n-1}(x) + f_{n+1}(x) = \frac{2n+1}{x} f_n(x)$$

$$n f_{n-1}(x) + (n+1) f_{n+1}(x) = (2n+1) f_n'(x)$$

where $f_n \rightarrow j_n, y_n$, or h_n

2. Also, useful derivative relations, $\frac{d}{dx}\left[x^{n+1} f_n(x)\right] = x^{n+1} f_{n-1}(x)$

$$\frac{d}{dx}\left[x^{-n} f_n(x)\right] = -x^{-n} f_{n+1}(x)$$

3. Rayleigh Formulas (analogous to Rodrigues Formulas)

$$j_n(x) = (-1)^n x^n \left(\frac{1}{x}\frac{d}{dx}\right)^n \left(\frac{\sin x}{x}\right) \quad \text{, etc.}$$

D. Small Argument ($x \ll 1$) and Asymptotic ($x \gg 1$) Limits

1. For $x \ll 1$, $\quad j_n(x) \simeq \dfrac{x^n}{(2n+1)!!}$ $\quad$ where $(2n-1)!! = \dfrac{(2n)!}{2^n n!}$

$$y_n(x) \simeq \frac{(2n-1)!!}{x^{n+1}}$$

2. Asymptotic Values: Using asymptotic values of J_ν, Y_ν, H_ν, ...

a. $\quad j_n(x) \sim \frac{1}{x}\sin\left(x - \frac{n\pi}{2}\right) \qquad y_n(x) \sim -\frac{1}{x}\cos\left(x - \frac{n\pi}{2}\right)$

$$h_n^{(1)} \sim (-i)^{n+1} \frac{e^{ix}}{x} \qquad h_n^{(2)} \sim i^{n+1} \frac{e^{-ix}}{x}$$

requiring $x \gg n(n+1)/2$.

b. Standing (j_n & y_n) and traveling ($h_n^{(1)}$ & $h_n^{(2)}$) spherical waves.

I. (Continued)

E. Orthogonality and Zeros

1. Using the orthogonality condition of $J_n(x)$, we can derive

$$\boxed{\int_0^a j_n\left(\alpha_{np}\frac{r}{a}\right) j_n\left(\alpha_{nq}\frac{r}{a}\right) r^2 dr = \frac{a^3}{2}\left[j_{n+1}(\alpha_{np})\right]^2 \delta_{pq}}$$

where α_{np} is the p-th zero of j_n.

a. NOTE: Weight factor r^2 (not r as with J_n).
$\Rightarrow$ Uniform weight over volume element.

2. Zeros of spherical Bessel functions be used to match spherical boundary conditions in the usual way.

F. Ex: Particle in a Spherical Potential Well

1. Schrödinger Eq: $-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi$ ← Find Ground State Energy, E_{min}

2. Potential $V(r) = \begin{cases} 0 & r \leq a \\ \infty & r > a \end{cases}$ $\Rightarrow$ Boundary Condition. $\psi(r=a) = 0$.

3. Applying Separation of Variables $\psi(r,\theta,\phi) = R(r)\,\Theta(\theta)\,\Phi(\phi)$,

$$\boxed{\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left[k^2 - \frac{l(l+1)}{r^2}\right]R = 0} \quad \text{where } k^2 = \frac{2mE}{\hbar^2}$$

4. General Solution: $R(r) = A\, j_l(kr) + \cancel{B}^{\,0}\, y_l(kr)$
since $y_l(kr)$ is irregular at $r=0$!

5. Apply BC: $R(r=a) = 0$

a. $ka = \underset{\text{zero}}{\alpha_{li}} \Rightarrow \boxed{k = \frac{\alpha_{li}}{a}}$

6. Ground state energy corresponds to $l=0$, $\Rightarrow \alpha_{01} = \pi$ ← Look up in Table 14.2

$\Rightarrow \boxed{E_{min} = \frac{\hbar^2}{2m}\frac{\pi^2}{a^2}}$

I. (Continued)

G. Modified Spherical Bessel Functions

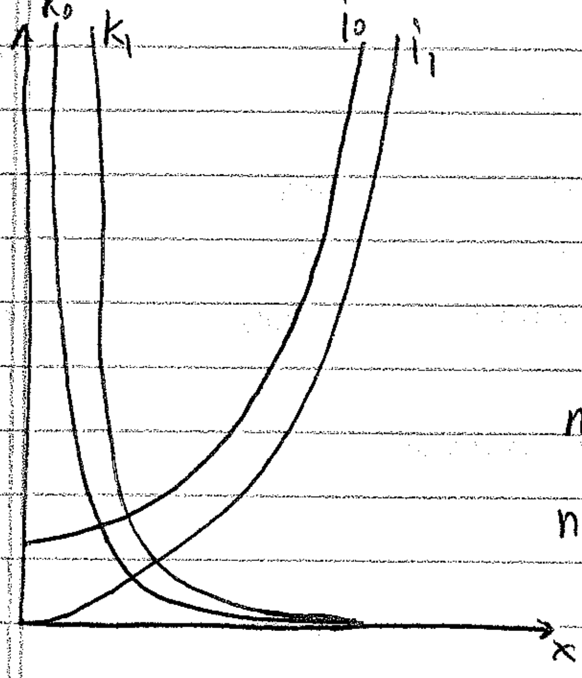
1. $$\boxed{r^2 \frac{d^2R}{dr^2} + 2r\frac{dR}{dr} - [\underbrace{k^2r^2}_{\text{change in sign!}} + \ell(\ell+1)]R = 0}$$

2. Solutions: <u>Modified Spherical Bessel Functions</u>

$$i_n(x) = \sqrt{\frac{\pi}{2x}}\, I_{n+\frac{1}{2}}(x), \quad k_n(x) = \sqrt{\frac{2}{\pi x}}\, K_{n+\frac{1}{2}}(x)$$

Different normalization.

3. $i_n, k_n(x)$



4. <u>Recurrence Relations</u>

$$i_{n-1}(x) - i_{n+1}(x) = \frac{2n+1}{x}\, i_n(x)$$

$$k_{n-1}(x) - k_{n+1}(x) = -\frac{2n+1}{x}\, k_n(x)$$

$$n\, i_{n-1}(x) + (n+1)\, i_{n+1}(x) = (2n+1)\, i_n'(x)$$

$$n\, k_{n-1}(x) + (n+1) k_{n+1}(x) = -(2n+1)\, k_n'(x)$$

5. <u>Closed Forms:</u>

$$i_0(x) = \frac{\sinh x}{x} \qquad k_0(x) = \frac{e^{-x}}{x}$$

$$i_1(x) = \frac{\cosh x}{x} - \frac{\sinh x}{x^2} \qquad k_1(x) = e^{-x}\left(\frac{1}{x} + \frac{1}{x^2}\right)$$

6. <u>Limiting Values:</u>

a. <u>$x \ll 1$:</u> $\quad i_n(x) \simeq \dfrac{x^n}{(2n+1)!!} \qquad k_n(x) \simeq \dfrac{(2n-1)!!}{x^{n+1}}$

b. Asymptotic: $(x \gg 1)$ $\quad i_n(x) \sim \dfrac{e^x}{2x} \qquad k_n(x) \sim \dfrac{e^{-x}}{x}$

I. G. (Continued)

7. Modified spherical Bessel functions arise in regions where wavefunction is evanescent ($E < V$).
   a. In the case of a spherical well of finite depth,
   $$V(r) = \begin{cases} 0 & 0 < r \leq a \\ V_0 & r > a \end{cases}$$
   b. Solutions at $r > a$ (for $E < V_0$), will consist of
   $$k_\ell(k'r)$$
   c. Solutions within ($r < a$) and without ($r > a$) must share same energy eigenvalue E and match smoothly at $r = a$.

II. Legendre Functions

A. Central Force Problem in Spherical Geometry

1. $$-\nabla^2 \psi + V(r)\psi = \lambda \psi$$
   a. Region is spherically symmetric
   b. Potential $V(r)$ is a function of radius only

2. Separation of Variables: $\psi(r,\theta,\phi) = R(r)\,\Theta(\theta)\,\Phi(\phi)$ yields
$$\frac{d^2\Phi}{d\phi^2} = -m^2\Phi$$
Legendre Polynomials $\left\{ \frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) - \frac{m^2\,\Theta}{\sin^2\theta} + \ell(\ell+1)\,\Theta = 0 \right.$

Spherical Bessel Functions $\left\{ \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + [\lambda - V(r)]R - \frac{\ell(\ell+1)\,R}{r^2} = 0 \right.$

3. Substituting $x = \cos\theta$
$$\boxed{(1-x^2)\,P''(x) - 2x\,P'(x) - \frac{m^2}{1-x^2}P(x) + \ell(\ell+1)\,P(x) = 0}$$
Associated Legendre Equation

B. Legendre Polynomials

1. Legendre Equation ($m=0$)

$$\boxed{(1-x^2)P''(x) - 2xP'(x) + \lambda P(x) = 0}$$

a. Regular singular points at $x = \pm 1$ and $x = \infty$

b. Series solution of radius of convergence $r=1$ about $x=0$.

c. Series solutions diverge at $x = \pm 1$ unless $\boxed{\lambda = \ell(\ell+1)}$

i. In this case, series is truncated at polynomial of degree ℓ.

2. Generating Function: $\boxed{g(x,t) = \dfrac{1}{\sqrt{1-2xt+t^2}} = \displaystyle\sum_{n=0}^{\infty} P_n(x)t^n}$

a. Scale: Taking $x=1$, $g(1,t) = \dfrac{1}{\sqrt{1-2t+t^2}} = \dfrac{1}{1-t} = \displaystyle\sum_{n=0}^{\infty} t^n \Rightarrow \boxed{P_n(1) = 1}$

b. Symmetry: Exchanging $x \to -x$ and $t \to -t$, we obtain

$\boxed{P_n(-x) = (-1)^n P_n(x)}$ odd n $\to$ odd parity, even n $\to$ even parity

c. Value at $x=0$: i. By symmetry, $P_{2n+1}(0) = 0$

ii. $P_{2n}(0) = (-1)^n \dfrac{(2n-1)!!}{(2n)!!}$

3. Leading Term: Coefficient of x^n in $P_n(x)$ is $\dfrac{(2n-1)!!}{n!}$

4. Closed Form Expression (Not as useful as recurrence)

$$P_n(x) = \sum_{k=0}^{[n/2]} (-1)^k \frac{(2n-2k)!}{2^n k!(n-k)!(n-2k)!} x^{n-2k}$$

$[n/2]$ is largest integer $\leq \frac{n}{2}$

II. C. Recurrence Formulas:

1. Using $\frac{\partial g(x,t)}{\partial t}$, we obtain

$$\boxed{(2n+1)\,x P_n(x) = (n+1)P_{n+1}(x) + n P_{n-1}(x)} \quad n \geq 1$$

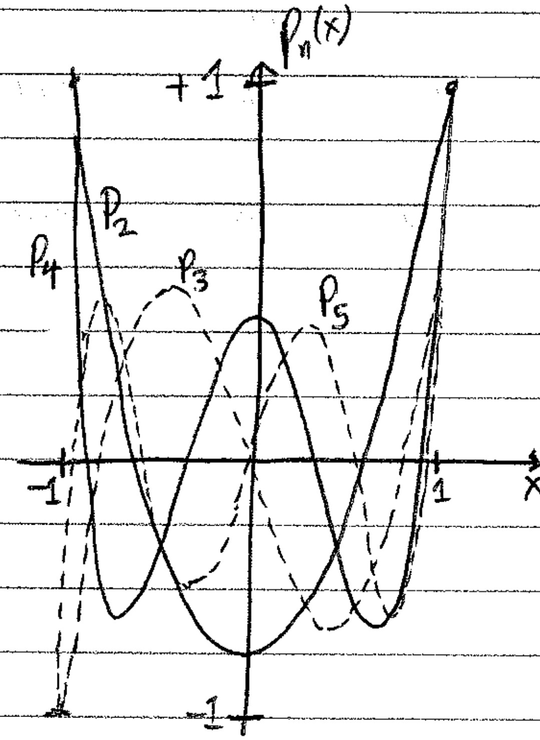
a. Can generate all P_n from $P_0(x) = 1$ and $P_1(x) = x$.

2. Using $\frac{\partial g(x,t)}{\partial x}$, we obtain (after some additional manipulations, see text)

$$\boxed{P'_{n+1}(x) - P'_{n-1}(x) = (2n+1)P_n(x)}$$

a. Numerous additional derivative relations can be developed (see text).

D. Bounds and Form of $P_n(\cos\theta)$



1. Forms of $P_n(x)$ on $[-1, 1]$ are plotted at right

2. a. $P_n(x)$ has global maximum $P_n(1) = 1$ at $x = 1$ for all n and $P_n(-1) = 1$ at $x = -1$ for even n

b. $P_n(x)$ has global minimum $P_n(-1) = -1$ at $x = -1$ if n is odd.

E. Rodrigues Formula:

1. $$\boxed{P_n(x) = \frac{1}{2^n n!}\left(\frac{d}{dx}\right)^n (x^2-1)^n}$$