**3D PROBLEMS in (r, θ, φ)**

For Central Potentials $V(r)$: When seeking eigenstates of Hamiltonians with $V(r)$, always separate $\Psi_E(r, θ, φ) = R(r) Y(θ, φ)$.

$Y(θ, φ)$ is universal for all central potentials....

**Spherical Harmonics** $Y_{lm}(θ, φ)$

Further, separate $Y(θ, φ) = F(φ) T(θ)$.

$\hat{L}^2 Y(θ, φ) = \lambda^2 Y(θ, φ)$

Further, separate $Y(θ, φ) = F(φ) T(θ)$.

$\hat{L}^2 = \text{angle-dep. part of Laplacian } \nabla^2 (-\frac{r^2}{\hbar^2})$

= much easier than $\hat{L} \hat{L} \hat{L}^2 !$

$Y(θ, φ)$ are the e-funcs of $\hat{L}^2 ! (\ldots \text{and } \hat{L}_z \ldots)$
\[ \Phi \text{-part: done in Disc 10, yielded sep. constant } m^2 \] 

\[ F(\phi) \] 

\[ \Theta \text{ part, } T(\theta): \]

\[ (m^2 - \lambda^2 \sin^2 \theta) T(\theta) = \sin \theta \frac{d}{d\theta} \left( \sin \theta \frac{dT}{d\theta} \right) \] 

\[ \Rightarrow \text{ solve this ODE} \]

**Case m=0:**

Derivation will give us

\[ T(\theta) = \text{Legendre polynomials} \]

for \( m \neq 0 \), Legendre polynomials

change variables in ODE:

\[ x = \cos \theta \]

\[ dx = -\sin \theta \, d\theta \]

\[ \sin \theta = \sqrt{1-x^2} \]

\[ \therefore \frac{d\theta}{d\theta} = -\frac{dx}{\sin \theta \sqrt{1-x^2}} \]

\[ \sin \theta = -\frac{1-x^2}{d\theta} \frac{dx}{d\theta} \]

ODE becomes:

\[ -\lambda^2 (1-x^2) P(x) = -(1-x^2) \frac{d}{dx} \left( -\frac{1-x^2}{dx} \frac{dP(x)}{dx} \right) \]

\[ -\lambda^2 P(x) = \frac{d}{dx} \left( (1-x^2) \frac{dP}{dx} \right) = -2x P' + (1-x^2) P'' \]

\[ 0 = \lambda^2 P - 2x P' + (1-x^2) P'' \] 

Legendre ODE

Separation constant

... will get quantized \( \equiv \) restricted to \( \{ \text{discrete values} \} \)

... how?
Solve using **POLYNOMIAL METHOD** (Frobenius method; truncated power series) for Legendre's ode

**Guess:** \( P(x) = \sum_{j=0}^{\infty} a_j x^j \)

**Plug:** \( 0 = \sum_{j=0}^{\infty} \lambda^2 a_j x^j - \sum_{j=0}^{\infty} 2x a_j j x^{j-1} + \sum_{j=0}^{\infty} (1-x^2) a_j j(j-1) x^{j-2} \)

\( 0 = \sum_{j=0}^{\infty} x^j a_j (\lambda^2 - 2j - j(j-1)) + \sum_{j=0}^{\infty} j(j-1) a_j x^{j-2} \)

**GROUP terms w SAME POWER of \( x \)**

in order to produce \( a + bx + cx^2 + \ldots = 0 \)

True for all \( x \) : EACH coeffic \( a, b, c \ldots \) individually = 0

\( \Rightarrow \) In term 2, **SHIFT INDICES**: replace all \( j \) w \( j+2 \)

\( 0 = \sum_{j=0}^{\infty} x^j + \sum_{j+2=0}^{j+2=\infty} (j+2)(j+1) a_{j+2} x^j \)

**deal w OUTLIER TERMS** \( j = -2 \neq j = -1 \)

i.e. terms that are not present in all summations
Term \( \circled{2} \): \((j+2)(j+1)q_{j+2}x^j \rightarrow \) @ \( j = -2 : \) \text{ZERO}  
\rightarrow @ \( j = -1 : \) \text{ZERO}

\text{ODE is } \quad 0 = \sum_{j=0}^{\infty} x^j \left[ a_j (x^2 - 2j - j(j-1)) + a_{j+2} (j+2)(j+1) \right] 
\quad = 0 \text{ for each } j

\text{for each} \quad j = 0 \rightarrow \infty, \quad 0 = a_j (x^2 - j^2 - j) + a_{j+2} (j+2)(j+1)

\text{RECURSION RELATION} \quad a_{j+2} = a_j \quad \frac{j(j+1) - x^2}{(j+2)(j+1)} \quad \text{for} \quad j = 0, 1, 2, ...

\text{If you know}

\( a_0 \rightarrow \text{get } a_2, a_4, a_6, ... \)

\( a_1 \rightarrow \text{get } a_3, a_5, a_7, ... \)

\( \uparrow \) The 2 free params that you always get from second order ODE

- pick \( a_i = 0 \) : generates \( P(x) = q_o + a_2 x^2 + a_4 x^4 + ... \text{EVEN series} \)
- pick \( a_o = 0 \) : generates \( P(x) = a_1 x + a_3 x^3 + a_5 x^5 + ... \text{ODD series} \)

\( \Rightarrow \) These 2 choices give 2 indep. power series, which will give us \{ complete set \} of \( P(x) \) solu's
TRUNCATE SERIES after convergence check

\[ P(x) = \begin{cases} a_0 + a_2x^2 + \ldots & \text{Even series doesn't diverge!} \\ a_1x + a_3x^3 + \ldots & \text{Odd series diverge!} \end{cases} \]

Represents \( T(\theta) = \theta \)-dep part of \( V_E(r, \theta, \phi) \) for central potentials \( \ldots \) must be \text{NORMALIZABLE}.

**Convergence Tests** for \( \sum_{n=1}^{\infty} u_n \):

1. **Fastest - Ratio Test**
   \[ \lim_{n \to \infty} \left| \frac{u_{n+1}}{u_n} \right| = p \Rightarrow \]
   \( p < 1 \): Converges
   \( p > 1 \): Diverges
   \( p = 1 \): No information

2. **Most - Gauss' Sensitive Test**
   \( \frac{u_n}{u_{n+1}} = \frac{1 + \frac{h}{n} + \text{Bounded}(h)}{n^2} \) as \( n \to \infty \)
   \( \Rightarrow h > 1 \): Converges
   \( h \leq 1 \): Diverges

\( (b) \) \( u_n \) equiv \( \frac{n^2 + a_n n + a_0}{n^{2+b} n + b_0} \)

\( \Rightarrow a_n > b_n + 1 \) Conv
\( a_n \leq b_n + 1 \) DIV

**Try it out for our**

\[ a_{j+2} = a_j + \frac{j(j+1) - x^2}{(j+2)(j+1)} \]

\[ P(x) = \sum_{j=0,2,4,\ldots}^{\infty} a_j x^j \]

**Ratio Test**:
\[ \frac{a_{j+2}}{a_j} \quad j \to \infty \]
\[ \frac{j(j+1) - x^2}{(j+2)(j+1)} \quad \frac{j^2 + 1}{j^2 + 2j} \quad 1 \quad \text{no info.} \]
GAUSS’ TEST: \( \frac{U_n}{U_{n+1}} = \frac{q_j x^2}{(j+2)(j+1)} \), where \( x = \cos \theta \leq 1 \), take \( x = 1 \) for worst case for convergence.

Take \( n = j/2 \) so that \( \frac{U_n}{U_{n+1}} = \frac{(2n)^2 + 3(2n) + 1}{(2n)^2 + (2n) - \lambda^2} \).

So that \( a_i = \frac{3}{2} \), \( b_i = \frac{1}{2} \), \( b_{i+1} = \frac{3}{2} \), \( a_i \leq b_{i+1} \), \( \therefore \) SERIES DIVERGES!

:: TRUNCATE SERIES:

Force series to stop @ some finite \( j \) by judicious choice of SEPARATION CONSTANT \( \lambda^2 \).

\( \therefore \) SET \( a_{j+2} = q_j \cdot ZERO \) for each \( j \) in turn;

:: set numerator \( j(j+1) - \lambda^2 = 0 \) for each \( j = 0, 1, 2, 3, \ldots \) in turn

\( \lambda^2 = l(l+1) \) where \( l = \text{INTEGER} \)

\( \therefore \) constrained \( \lambda^2 = l^2/2\pi^2 \), \( 0, 1, 2, 3, \ldots \),

\( \therefore \) Produces \( \{ \text{polynomials } P_j(x) \} \text{ of order } l \) \( \therefore \) QUANTIZATION CONDITION (will quantize \( \lambda^2 \) into \( l^2/2\pi^2 \)).
POLYNOMIAL METHOD: for 1D SHO

4 STEPS

Find e-things of $\hat{H}_{\text{SHO}}^{1D} = -\hbar^2 \frac{d^2}{2m \, dx^2} + \frac{mw^2 \, x^2}{2}$

:. Solve ODE: $\hat{H} \Psi_E = E \Psi_E \Rightarrow \frac{-\hbar^2}{m} \Psi'' + \frac{mw^2}{m} \Psi = 2E \Psi$

1. Use DIMENSIONLESS QUANTITIES to simplify ODE

OPTIONAL

* Group parameters of problem into dimensionless combinations → always helps to simplify

E.g. dimensionless combos can be compared with 1, "big" & "small" & Taylor approx are clarified

Dimensionless energy: have $E \approx \hbar w$

both with dimensions of energy

$\Rightarrow$ define $\left[ K = \frac{2E}{\hbar w} \right]$ "dimensionless energy" 

$\frac{-\hbar}{mw} \frac{d^2 \Psi}{dx^2} + \frac{mw \, x^2 \Psi}{\hbar} = K \Psi$

both [1]
③ Dimensionless position: have coord. \( x \) & with position units

\[ \psi = \frac{x}{x_0} \]

"dimensionless x" = coord / natural distance

scale of \( \text{SHO} \)

ODE is now \(-x_0^2 \frac{d^2\psi}{dx^2} + \frac{x^2}{x_0^2} \psi = K \psi\)

ie. \[ \frac{d^2\psi}{d\xi^2} = \left( \xi^2 - K \right) \psi \]

\[ ODE \]

2. Asymptotic Behaviour

Find approx solution \( \psi_\infty \) to the approx ODE when \( \xi \to \pm \infty \):

\[ \frac{d^2 \psi}{d\xi^2} = \psi'' = (\xi^2 - K) \psi \approx \xi^2 \psi \]

Asymptotic ODE is \( \psi'' \approx \xi^2 \psi_\infty \) in \( \xi \to \pm \infty \) limit

SOLUTION: \( \psi_\infty (\xi) = Ae^{\pm 5^{1/2}} \cdots \text{Toss } e^{\pm 5^{1/2}} \) in \( \xi \to \infty \) limit

\[ : \text{unphysical!} \]
\[ \psi_\infty (\xi) = A e^{-\xi^2/2} \]

\[ \psi'_\infty = A(-\xi) e^{-\xi^2/2} \]

\[ \psi''_\infty = A \left[ -1 + (-\xi)(-\xi) \right] e^{-\xi^2/2} = A \left[ -1 + \xi^2 \right] e^{-\xi^2/2} \approx A \xi^2 e^{-\xi^2/2} \quad \xi \to \pm \infty = \frac{\xi^2}{2} \psi_\infty \]

\[ \Rightarrow \text{From now on, factor out the known asymptotic behaviour; solve for what's left over: } \psi_\xi = \psi_\infty \cdot h(\xi) \]

\( \psi_\infty = A e^{-\xi^2/2} \): DOMINANT BEHAVIOUR of \( \psi(\xi) \) in asymptotic \( \xi \to \pm \infty \) regime

\[ h(\xi) = \text{what's left over} \Rightarrow \text{now we solve for this using power series} \]

\[ \psi(\xi) = e^{-\xi^2/2} \cdot h(\xi) \]

\[ \psi' = -\frac{\xi}{2} e^{-\xi^2/2} h(\xi) + h'(\xi) e^{-\xi^2/2} \]

\[ \psi'' = \ldots \]

\[ \psi'' = (\xi^2 - K) \psi \Rightarrow \text{ODE for } h(\xi) \]

\[ h'' - 2\xi h' + (K-1)h = 0 \]
3. Guess POWER SERIES for “left-over” $h(\delta)$:

$$h(\delta) = \sum_{j} a_j \delta^j$$

... plug into ... follow same technique as Legendre ODE example:

- group by powers, take care of outliers, ...
- (shift indices)

$\implies$ get recursion relation

$$a_{j+2} = \frac{(2j+1-k)}{(j+1)(j+2)} a_j$$

4. TRUNCATE series if $h(\delta)$ competes with $\Psi_\infty(\delta)$ in asymptotic regime $\delta \to \pm \infty$

First, see if $h(\delta)$ power series diverges:

**RATIO TEST**: 

$$\left| \frac{a_{j+2}}{a_j} \right| = \frac{2j+1-k}{j^2+3j+2} \quad j \gg 1, j \to \infty$$

- converges

... compare $h(\delta)$ with $\Psi_\infty(\delta) \sim e^{-\delta^2/2}$ at large $\delta$:

- $h(\delta)$ must fall off FASTER than $e^{-\delta^2/2}$

$h(\delta)$: using power series $\delta = 1/2$,

$$\frac{U_{n+1}}{U_n} = \frac{2(2n+1-k)}{(2n)^2+3(2n)+2} \quad \delta \to \infty$$

$$n \to \infty \quad \frac{4n}{4n^2} \cdot \frac{\delta^2}{n} = \frac{\delta^2}{n}$$

compare to ...
• $\Psi_\infty (\xi) = e^{-\frac{\xi^2}{2}} = \sum_{n=0}^{\infty} (-\frac{\xi^2}{2})^n / n! \cdot \frac{1}{U_n + 1/2} \rightarrow \frac{-\xi^2}{2n}$
  asymptotic behaviour
  
  VERY SIMILAR!... can see that
  
  @ large $n$, $h(\xi)$ matches expansion of
  
  $e^{+\xi^2} = \sum_{n=0}^{\infty} (\frac{\xi^2}{n!}) \cdot \frac{1}{U_n + 1/2} \rightarrow \frac{\xi^2}{n}$
  
  Thus $h(\xi)$ we found has same large $\xi$ behaviour
  as $e^{+\xi^2}$, which matches with $\Psi_\infty = e^{-\frac{\xi^2}{2}}$
  
  blows up as $\xi \rightarrow \infty$!
  
  $\Rightarrow$ MOST TRUNCATE $h(\xi)$ to prevent this
  
  $\Rightarrow a_{j+2} = q_j \frac{(2j+1-K)}{(j+1)(j+2)} \quad \text{set to zero}\quad \text{at various:} \quad K = 2j_{\text{max}} + 1$
  
  for $j_{\text{max}} = 0, 1, 2, \ldots$
  
  and $K$: dimensionless $= \frac{2E}{\hbar w}$
  
  $E = \hbar w K = \hbar w (j_{\text{max}} + \frac{1}{2}) \Rightarrow$ STO spectrum
  
  $E_n = \hbar w (n + \frac{1}{2})$
  
  $n = j_{\text{max}} = 0, 1, 2, \ldots$
  
  Polynomial Method: mastered! :)

RETURN TO SPHERICAL HARMONICS
\[ \phi - \text{part}: F''(\phi) = -\mu^2 F(\phi) \] from Disc 10, separation constant

Solution: \( F(\phi) \sim e^{im\phi} \) physically, angles \( \phi \pm \phi + 2\pi \) are THE SAME ANGLE!

\[ e^{im \cdot 2\pi} = e^{i0} = 1 \quad \therefore F(\phi + 2\pi) = F(\phi) \]

\[ \mu \cdot 2\pi = m \cdot 2\pi \quad \text{integer} \]

\[ \mu = m = 0, \pm 1, \pm 2, \ldots \]

and \[ F_m(\phi) \sim e^{im\phi} \]

Quantization again, due to boundary conditions/physical considerations

Significance of \( \mu = m \): \( F_m(\phi) \) are e-functions of
with e-values \[ \mu \hbar \]

Recall, from \( \Theta \)-part, e-values of \( \hat{L}_z \) are \[ \ell (\ell + 1) \hbar^2 \]

\[ \rightarrow \text{Spherical Harmonics} \quad Y_{\ell m}(\theta, \phi) = T_{\ell}(\theta) F_m(\phi) \] simultaneously e-functions of \( \hat{L}_z \) and \( \hat{L}_z \)

Simultaneous e-functions of \( \hat{L}_z \) and \( \hat{L}_z \)
Significance of $Y_m(\theta, \phi)$ on allowed angular mom vectors $L$

\[ |L| = \sqrt{\sum_{m=-l}^{l} m^2} \]

\[ L_z = \hbar m \quad m = -l, -l+1, \ldots, 0, \ldots, l-1, l \]

\[ |L_z| \text{ can't be larger than } |L|! \quad : \quad |m| \leq l \]

\[ |L| = \sqrt{l(l+1)} \hbar \]

\[ |L_z| = |\hbar m| \]

\[ \text{Strange feature: } |L| = \sqrt{l(l+1)} > \hbar |L_z| \]

\[ \text{for } m = 2 \]

\[ \text{Each } e\text{-state of } L^2 \pm L_z \text{ is a cone of vectors } L \text{ of equal prob.} \]

\[ [L^2, L_z] = 0 \]

\[ [L_x, L_z] \neq 0 \quad \text{but } [L_y, L_z] = 0 \]
If we could have \( L_z = L \) then we would know \( L_x = L_y = 0 \) which would violate the uncertainty principle associated with \([L_x, L_z] = -i\hbar \neq 0 \) \([L_y, L_z] = i\hbar \neq 0 \).