

19

165

$$(1-2xt+t^2)^{-1} = \left[ \sum_{n=0}^{\infty} P_n(x) t^n \right]^2$$

$$\int_{-1}^1 dx \frac{1}{(1-2xt+t^2)^{-1}} = \sum_{n=0}^{\infty} \int_{-1}^1 dx P_n^2(x) t^{2n}$$

$$\Rightarrow \frac{-1}{2t} \ln \left[ \frac{1-2t+t^2}{1+2t+t^2} \right] = \sum_{n=0}^{\infty} \int_{-1}^1 dx P_n^2(x) t^{2n}$$

$$\Rightarrow \frac{-1}{t} \left( \ln |1-t| - \ln |1+t| \right)$$

← doubles odd terms

$$= \frac{1}{t} \sum_{n=1}^{\infty} \left( \frac{t^n}{n} + (-1) \frac{t^n}{n} \right)$$

$$= 2 \sum_{n=0}^{\infty} \left( \frac{t^{2n}}{2n+1} \right)$$

$$\int_{-1}^1 dx P_n^2(x) = \frac{2}{2n+1}$$

One more relation I would like below. First I need a result about sums double

$$\sum_{n=0}^{\infty} \sum_{k=0}^n a_{n,k} = \sum_{n=0}^{\infty} \sum_{k=0}^{\lfloor n/2 \rfloor} a_{n-k,k}$$

LHS

$$a_{0,0} + (a_{1,0} + a_{1,1}) + (a_{2,0} + a_{2,1} + a_{2,2}) + (a_{3,0} + a_{3,1} + a_{3,2} + a_{3,3}) + \dots$$

(n=0)                      (n=1)                      (n=2)                      (n=3)

RHS

$$a_{0,0} + (a_{1,0}) + (a_{2,0} + a_{1,1}) + (a_{3,0} + a_{2,1}) + (a_{4,0} + a_{3,1} + a_{2,2}) + \dots$$

(n=0)                      n=1                      n=2                      (n=3)                      (n=4)

166

Nach

$$(1-2xt+t^2)^{-1/2}$$

$$= 1 + \frac{1}{2}(2xt-t^2) + \frac{\frac{1}{2}(\frac{1}{2}+1)}{2!}(2xt-t^2)^2 + \frac{\frac{1}{2}(\frac{1}{2}+1)(\frac{1}{2}+2)}{3!}(2xt-t^2)^3$$

$$\frac{\frac{1}{2}(\frac{1}{2}+1)}{2!} = \frac{1 \cdot 3}{2! \cdot 2^2} = \frac{4!}{2^4 \cdot 2! \cdot 2}$$

$$\frac{\frac{1}{2}(\frac{1}{2}+1)(\frac{1}{2}+2)}{3!} = \frac{1 \cdot 3 \cdot 5}{2^3 \cdot 3!} = \frac{6!}{2^6 \cdot (3!)^2}$$

$$(1-2xt+t^2)^{-1/2} = \sum_{n=0}^{\infty} \frac{(2n)!}{2^{2n} (n!)^2} (2xt-t^2)^n$$

$$= \sum_{n=0}^{\infty} \frac{(2n)! t^n}{2^{2n} (n!)^2} \sum_{k=0}^n (-1)^k \frac{n!}{k!(n-k)!} (2x)^{n-k} t^k$$

$$= \sum_{n=0}^{\infty} \sum_{k=0}^n \frac{(2n)!}{2^{2n} n! k!(n-k)!} (-1)^k (2x)^{n-k} t^k t^n$$

$$= \sum_{n=0}^{\infty} t \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{(2n-2k)!}{2^{2n-2k} k!(n-k)!(n-2k)!} (-2x)^{n-2k}$$

$$P_n(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{(2n-2k)!}{2^{2n-2k} k!(n-k)!(n-2k)!} (-2x)^{n-2k}$$

Beit

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

$$\frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n$$

$$= \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{1}{2^n n!} \frac{(-1)^k k!}{k! (n-k)!} \frac{(2n-2k)!}{(n-2k)!} x^{n-2k}$$

$$= P_n(x)$$

Now orthonormality of  $P_n$  follows just let  $P_n$  from de. Gegen normalisation is a little harder, I will just give result  $m \geq 0$

$$\int_{-1}^1 dx P_l^m(x) P_l^m(x) = \frac{2}{2l+1} \frac{(l+m)!}{(l-m)!} \delta_{ll} \quad *$$

For  $l \leq m \leq l$

$$Y_l^m(\theta, \phi) = \left[ \frac{(2l+1)(l-m)!}{4\pi(l+m)!} \right]^{1/2} (-i)^m e^{im\phi} P_l^m(\cos\theta)$$

$$Y_l^{-m} = (-1)^m (Y_l^m)^*$$

### Solution To Rotationally Invariant Problems

Particle of mass  $\mu$  moving in spherically sym potential  $V(r)$

$$\left[ \frac{-\hbar^2}{2\mu} \left( \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2} \left( \frac{1}{\sin^2\theta} \frac{\partial}{\partial \theta} \sin^2\theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2} \right) \right) + V(r) \right] \Psi_E(r, \theta, \phi) = E \Psi_E(r, \theta, \phi)$$

See that every eigenfunction is also eigenfunction of  $L^2, L_z$

$$\Psi_{Elm}(r, \theta, \phi) = R_{Elm}(r) Y_l^m(\theta, \phi)$$

$$\left[ \frac{-\hbar^2}{2m} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - \frac{l(l+1)}{r^2} \right] + V(r) \right] R_{El}(r) = E R_{El}(r)$$

Note can drop subscript  $m$  since radial wt's don't depend on  $m$ . We have  $2l+1$  degeneracy for each  $l$

Convenient to rewrite in terms of  $U_{El}$  def:

$$R_{El} = \frac{U_{El}}{r}$$

$$\frac{\partial}{\partial r} R_{El} = -\frac{1}{r^2} U_{El}(r) + \frac{U_{El}'(r)}{r}$$

$$r^2 \frac{\partial}{\partial r} R_{El} = -U_{El}(r) + r U_{El}'(r)$$

$$\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} R_{El}(r) = -U_{El}'(r) + U_{El}'(r) + r U_{El}''(r)$$

$$\left\{ \frac{-\hbar^2}{2m} \left[ \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} \right] + V(r) \right\} U_{El}(r) = E U_{El}(r)$$

$$\left\{ \frac{d^2}{dr^2} + \frac{2m}{\hbar^2} \left[ E - V(r) - \frac{l(l+1)\hbar^2}{2mr^2} \right] \right\} U_{El}(r) = 0$$

Look like 1-dim Schrödinger eq. after

- (i) Coordinate variable  $r$  goes from  $0 \rightarrow \infty$  instead of  $-\infty$  to  $\infty$
- (ii) In addition to potential a repulsive centrifugal barrier  $\frac{l(l+1)\hbar^2}{2mr^2}$  in all but  $l=0$  states
- (iii) Boundary conditions on  $U$  different than 1-d case



$$U(r) \xrightarrow{r \rightarrow \infty} C \Rightarrow R \sim \frac{U}{r} \sim \frac{C}{r}$$

So the wt diverges. Not a problem  $R$  still square integrable. But it actually doesn't satisfy the Schrödinger eq  $\psi \sim e^{-\kappa r}$   $\psi' \sim e^{-\kappa r}$

$$\nabla^2 \left( \frac{1}{r} \right) = 4\pi \delta^3(\vec{r})$$

→ need the  $\delta$  term

Soln  $\psi(r)$  doesn't contain a  $\delta$ -function at orig must have

$$U(r) \rightarrow 0 \quad \text{as } r \rightarrow 0$$

We can derive more properties by examining the equation it satisfies without using explicit form of the potential  $V(r)$ . Consider limit  $r \rightarrow 0$ , and assume  $V(r)$  is less singular than  $r^{-2}$ . Then for small  $r$  equation is dominated by the centrifugal term

$$U_2'' \approx \frac{l(l+1)}{r^2} U_2$$

We have dropped subscript to note it is inconsequential for dominant behavior near  $r \rightarrow 0$ . Try soln

$$U_2 \sim r^\alpha$$

$$\alpha(\alpha-1) = l(l+1)$$

$$\alpha = l+1 \quad \text{or} \quad \alpha = -l$$

$$U_2 \sim \begin{cases} r^{l+1} & \text{regular soln} \\ r^{-l} & \text{irregular soln} \end{cases}$$

$$d_x^+ d_x^+ (d_x^+ U_e) = d_x^+ U_e$$

$$d_{x+1} d_{x+1} (d_x^+ U_e) = d_x^+ U_e$$

So 
$$d_x^+ U_e = C_2 U_{x+1}$$

where  $C_2$  is a constant. If  $k=0$  then there are two solutions

$$U_0^A(\rho) = \sin \rho, \quad U_0^B(\rho) = \cos \rho$$

if oxygen included in region considered the  $U_0^B(\rho)$  is forbidden. Now lets see explicitly how other solns are found

$$\begin{aligned} \rho R_{x+1} &= d_x^+ \rho R_x \\ &= \left( -\frac{d}{d\rho} + \frac{k+1}{\rho} \right) (\rho R_x) \end{aligned}$$

$$\Rightarrow R_{x+1} = \left( -\frac{d}{d\rho} + \frac{k}{\rho} \right) R_x$$

$$\Rightarrow R_{x+1} = \rho^k \left( -\frac{d}{d\rho} \right) \frac{R_x}{\rho^k}$$

Now let

$$\frac{R_{x+1}}{\rho^{k+1}} = -\frac{1}{\rho} \frac{d}{d\rho} \frac{R_x}{\rho^k} = \left( -\frac{1}{\rho} \frac{d}{d\rho} \right)^2 \frac{R_{x-1}}{\rho^{k-1}}$$

$$= \left( -\frac{1}{\rho} \frac{d}{d\rho} \right)^{k+1} \frac{R_0}{\rho^0} \leftarrow \text{overall minus sign - function}$$

$$\Rightarrow R_x = (-\rho)^k \left( \frac{1}{\rho} \frac{d}{d\rho} \right)^k R_0$$

$$R_0^A = \sin \rho / \rho, \quad R_0^B = -\cos \rho / \rho$$

Spherical Bessel Functions

$$R_e^A \equiv j_e = (-p)^e \left( \frac{1}{p} \frac{d}{dp} \right)^e \left( \frac{\sin p}{p} \right)$$

Spherical Neuman Functions of order  $l$

$$R_e^B \equiv n_e = (-p)^e \left( \frac{1}{p} \frac{d}{dp} \right)^e \left( \frac{\cos p}{p} \right)$$

$$j_0(p) = \frac{\sin p}{p}$$

$$n_0(p) = -\frac{\cos p}{p}$$

$$j_1(p) = \frac{\sin p}{p^2} - \frac{\cos p}{p}$$

$$n_1(p) = -\frac{\cos p}{p} - \frac{\sin p}{p^2}$$

Can show as  $p \rightarrow \infty$  then behave  $\sim$

$$j_e \rightarrow \frac{1}{p} \sin \left( p - \frac{(2l+1)\pi}{2} \right)$$

$$n_e \rightarrow \frac{1}{p} \cos \left( p - \frac{(2l+1)\pi}{2} \right)$$

$j_e(p)$  find as  $p \rightarrow 0$

$$j_e(p) \xrightarrow{p \rightarrow 0} \frac{p^e}{(2e+1)!!}$$

$$(2e+1)!! = (2e+1)(2e-1)\dots(5)(3)(1)$$

But

$$n_e(p) \xrightarrow{p \rightarrow 0} \frac{-(2e-1)!!}{p^{2e+1}}$$

Free particle wt's choose regular small sphere

$$\Psi_{E,m}(r, \theta, \phi) = j_l(kr) Y_l^m(\theta, \phi)$$

Connection to Soln in Cartesian Coord

$$\Psi_E(x, y, z) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{p}\cdot\vec{r}/\hbar} \quad E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$
$$\vec{p} = \hbar \vec{k}$$

$$\frac{\vec{p}\cdot\vec{r}}{\hbar} = kr \cos\theta$$

$$\Psi_E(r, \theta, \phi) = \frac{e^{ikr \cos\theta}}{(2\pi\hbar)^{3/2}}$$

Now can expand in spherical harmonics

$$e^{ikr \cos\theta} = \sum_{l=0}^{\infty} \sum_{m=-l}^l C_l^m j_l(kr) Y_l^m(\theta, \phi)$$

LHS independent of m so all m=0 contribute

$$e^{ikr \cos\theta} = \sum_{l=0}^{\infty} C_l^0 j_l(kr) Y_l^0(\theta, \phi)$$

$$Y_l^0 = \left(\frac{2l+1}{4\pi}\right)^{1/2} P_l(\cos\theta)$$

$$e^{ikr \cos\theta} = \sum_{l=0}^{\infty} C_l^0 j_l(kr) P_l(\cos\theta)$$

Constant  $C_l^0 = i^l (2l+1)$

$$e^{ikr \cos\theta} = \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos\theta) j_l(kr)$$

### Free Particle in Spherical Coordinates

Write  $\psi$

$$\psi_{l,m}(r, \theta, \phi) = R_{l,m}(r) Y_{l,m}(\theta, \phi)$$

$$\left[ \frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} \right] U_{l,m}(r) = 0 \quad k^2 = \frac{2mE}{\hbar^2} \quad \text{mass}$$

Divides by  $k^2$  + introducing  $\rho = kr$

$$\left[ -\frac{d^2}{d\rho^2} + \frac{l(l+1)}{\rho^2} \right] U_l = U_l$$

Define operators analogous to raising & lowering operators

$$d_l = \frac{d}{d\rho} + \frac{l+1}{\rho}, \quad d_l^\dagger = -\frac{d}{d\rho} + \frac{l+1}{\rho}$$

The differential equation is

$$d_l d_l^\dagger U_l = U_l \quad *$$

$$\text{Now: } d_l d_l^\dagger U = \left( \frac{d}{d\rho} + \frac{l+1}{\rho} \right) \left( -\frac{d}{d\rho} + \frac{l+1}{\rho} \right) U$$

$$= -\frac{d^2}{d\rho^2} U + \left( \frac{l+1}{\rho} \right) \left( \frac{l+1}{\rho} \right) U + \left[ \frac{d}{d\rho}, \frac{l+1}{\rho} \right] U$$

$$= -\frac{d^2}{d\rho^2} U + \frac{(l+1)(l+1)U}{\rho^2} - \frac{l+1}{\rho^2} U$$

$$= -\frac{d^2}{d\rho^2} + \frac{l^2 + 2l + 1 - l - 1}{\rho^2} U = d_l^\dagger d_l U$$

$$\Rightarrow d_l d_l^\dagger = d_l^\dagger d_l \quad \rho^{-2}$$

So \* multiply both sides by  $d_l^\dagger$

We expect irregular solution if doesn't satisfy condition  $U_{E,l}(r) \rightarrow 0$  as  $r \rightarrow 0$ . Note this only holds for  $l > 0$ . For  $l = 0$  centrifugal barrier is irrelevant. Although  $U_0(r) \rightarrow 0$  as  $r \rightarrow 0$ , particle has non zero amplitude to be at the origin because  $R_0(r) = U_0(r)/r \neq 0$  at  $r = 0$ . For non problem we consider  $U_0(r) \sim r$  as  $r \rightarrow 0$  so behavior even holds for  $l = 0$ .

Next consider the behavior of  $U_{E,l}(r)$  as  $r \rightarrow \infty$ . If  $V(r)$  does not vanish as  $r \rightarrow \infty$  it will dominate the result. So lets consider case  $rV(r) \rightarrow 0$  as  $r \rightarrow \infty$ . At large  $r$  is become.

$$\frac{d^2 U_E}{dr^2} = -\frac{2mE}{\hbar^2} U_E$$

- 1)  $E > 0$  the particle is allowed to scatter to classically. We expect  $U_{E,l}(r)$  to oscillate as  $r \rightarrow \infty$
- 2)  $E < 0$  the particle is bound. The region  $r \rightarrow \infty$  is forbidden classically and we expect  $U_{E,l}(r)$  to fall off exponentially slow

For case  $E > 0$

$$U_E = A e^{ikr} + B e^{-ikr} \quad k = \left(\frac{2mE}{\hbar^2}\right)^{1/2}$$

Probably better as a free particle far from origin. Lets write solution in the case for particle  $r$

$$U_E = f(r) e^{\pm ikr}$$

and ignore centrifugal barrier

$$f'' \pm 2ik f' - \frac{2m}{\hbar^2} V(r) f = 0$$

We expect for very large  $r$  that  $f(r)$  is slowly varying so we ignore  $f''(r)$

$$\frac{df}{f} = \pm \frac{i}{k} \frac{\mu}{\hbar^2} V(r) dr$$

$$f(r) = f(r_0) \exp \left[ \pm \frac{i\mu}{\hbar^2} \int_{r_0}^r V(r) dr \right]$$

where  $r_0$  is some constant. If  $rV(r) \rightarrow 0$  as  $r \rightarrow \infty$  can do integral as  $r \rightarrow \infty$  if approaches a constant given behaviour we want. But if instead

$$V(r) = -\frac{e^2}{r}$$

$$f(r) = f(r_0) \exp \left[ \pm \frac{i\mu e^2}{\hbar^2} \ln \left( \frac{r}{r_0} \right) \right]$$

$$U_E(r) \sim \exp \left[ \pm i \left( kr + \frac{\mu e^2}{\hbar^2} \ln r \right) \right]$$

If  $V(r)$  falls faster the  $Y_r$  problem is even worse.

Next consider case  $E < 0$ . All the results with  $E > 0$  carry over with changes

$$k \rightarrow i\kappa \quad \chi = \left( \frac{2\mu|E|}{\hbar^2} \right)^{1/2}$$

$$U_E \xrightarrow{r \rightarrow \infty} A e^{-\kappa r} + B e^{\kappa r}$$

$A$  &  $B$  as not arbitrary since  $U_E$  continued inward to  $r \rightarrow 0$  must vanish. The growing exponential must vanish for normalizability. So even only get soln for certain discrete values of  $E$ . (All  $A$  &  $B$  are arbitrary just set  $B=0$  without disturbing  $E$ )

Note as before plus analyze  $rV(r) \rightarrow 0$  as  $r \rightarrow \infty$   
 as before with  $k = i\kappa$

$$U_E(r) \sim \exp[-\kappa r] \exp\left[\frac{+ucl}{\hbar^2} \ln r\right]$$

$$\sim r^{(me^2/\hbar^2\kappa^2)} e^{-\kappa r}$$

When ELO eigenfunctions are normalized to unit

$$\int_0^\infty U_{E'l}^*(r) U_{El}(r) dr = \delta_{EE'}$$

$$\Psi_{E'lm}^*(r, \theta, \phi) = R_{E'l}(r) Y_{lm}(\theta, \phi)$$

$$\iiint \Psi_{E'lm}^*(r, \theta, \phi) \Psi_{Elm}(r, \theta, \phi) r^2 d\Omega$$

$$= \delta_{EE'} \delta_{ll'} \delta_{mm'}$$