Lecture 9b: Spherical Wells

In this lecture we consider piecewise constant potentials ~~[illegible]~~ which are spherically symmetric, that is

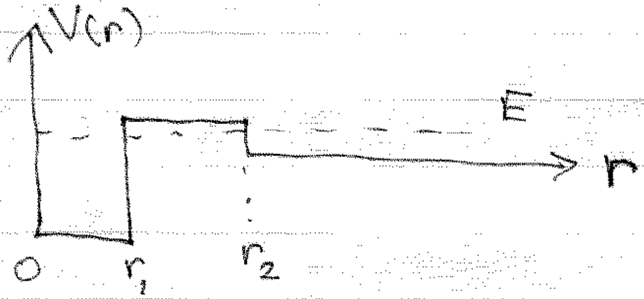
$$V = V(r) = \begin{cases} V_0 & 0 < r < r_1 \\ V_1 & r_1 < r < r_2 \\ \vdots & \end{cases}$$

The solutions to the T.I.S.E. are of the form

$$\psi_{k,\ell,m}(r,\theta,\phi) = R_{k,\ell}(r)\, Y_\ell^m(\theta,\phi)$$

Where
$$-\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}\big(R(r)\big) + \left(\frac{\hbar^2 \ell(\ell+1)}{2mr^2} + V(r)\right) R(r) = E\, R(r)$$

Eg.



In the region $r_1 < r < r_2$ Classically forbidden

otherwise classically allowed

In a given region, let $k^2 = \frac{2m}{\hbar^2}(E - V)$

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

General Solutions for constant V as a function of r

$$R_{k,\ell}(r) = A\, j_\ell(kr) + B\, n_\ell(kr)$$

$j_\ell(kr)$ like spherical generalization of sine

$n_\ell(kr)$ " " " of cosine

Also $h^{(1)}(kr) \equiv j_\ell(kr) + i\, n_\ell(kr)$

$$h^{(2)}(kr) \equiv j_\ell(kr) - i\, n_\ell(kr)$$

Like spherical versions of exponentials

$h_0^{(1)}(kr) = -i \dfrac{e^{ikr}}{kr}$ $\qquad$ $h_0^{(2)} = i \dfrac{e^{-ikr}}{kr}$

$\underbrace{h_1^{(1)}(kr) = -\left(\dfrac{i}{(kr)^2} + \dfrac{1}{kr}\right) e^{ikr}}_{\text{outgoing waves}}$ $\qquad$ $\underbrace{h_1^{(2)} = -\left(\dfrac{-i}{kr} + \dfrac{1}{kr}\right) e^{-ikr}}_{\text{incoming waves}}$

Note $\quad h_n^{(2)}(kr) = h_n^{(1)*}(kr)$

Alternate solution

$$R_{k,\ell}(r) = A\, h_\ell^{(1)}(kr) + B\, h_\ell^{(2)}(kr)$$

Infinite Spherical Well

Consider a potential $V(r) = \begin{cases} 0 & 0<r<a \\ \infty & r>a \end{cases}$

Inside the well the solution is

$$R(r) = A j_\ell(kr) + B n_\ell(kr)$$

we must have $B = 0$ since n_ℓ blows up at the origin.

Finally we have the boundary condition

$$R(a) = 0 \implies j_\ell(ka) = 0$$

Let $x_{n,\ell}$ be the n^{th} root of $j_\ell(x)$

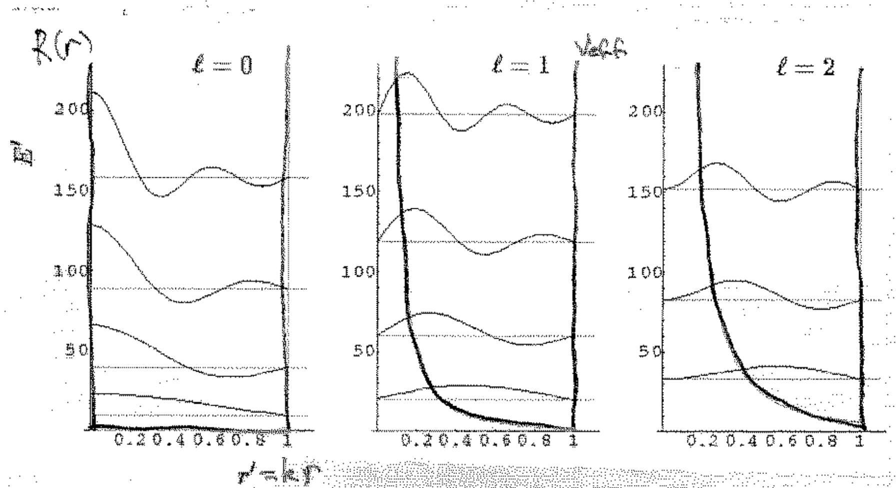
i.e. $j_\ell(\chi^{(\ell)}_{n_r}) = 0 \implies k_{n_r \ell} = \dfrac{\chi^{(\ell)}_{n_r}}{a}$

$$\Rightarrow \boxed{\begin{array}{l} \text{Eigenvalues: } E_{n_r\ell} = \dfrac{(\hbar k_{n_r\ell})^2}{2m} = \dfrac{\hbar^2}{2ma^2}\left(\chi^{(\ell)}_{n_r}\right)^2 \\ \text{Eigenfunctions: } \psi_{n,\ell,m}(r,\theta,\phi) = A_{n,\ell}\, j_\ell(k_{n\ell} r)\, Y_\ell^m(\theta,\phi) \end{array}}$$

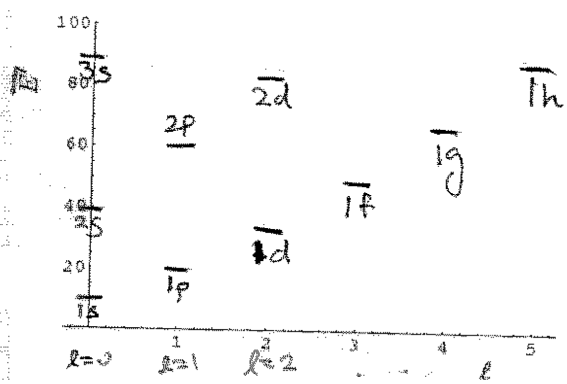
Note: Because of the symmetry (rotational) the energy depends only on two Quantum Numbers n_r, ℓ. Each level is $2\ell+1$ degenerate.

From http://www.physics.csbju.edu/QM

l,n_r	root	E'
0,0	3.1	9.87
1,0	4.5	20.19
2,0	5.8	33.22
0,1	6.3	39.48
3,0	7.0	48.83
1,1	7.7	59.68
4,0	8.2	66.95
2,1	9.1	82.72
5,0	9.4	87.53



Energy level diagram, let $\overline{E} = \dfrac{E}{\frac{\hbar^2}{2ma^2}}$



Here we have introduced "spectroscopic notation" $(n_r\, l)$

$l=0 \equiv$ s-state (s = "sharp")

$l=1 \equiv$ p-state (p = "principle")

$l=2 \equiv$ d-state (d = "diffuse")

$l=3 \equiv$ f-state (f = "fine")

$l=4 \sim g$

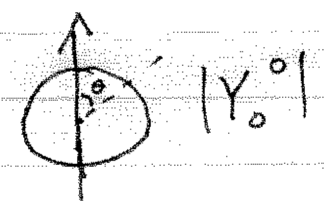
$\quad 5 = h$

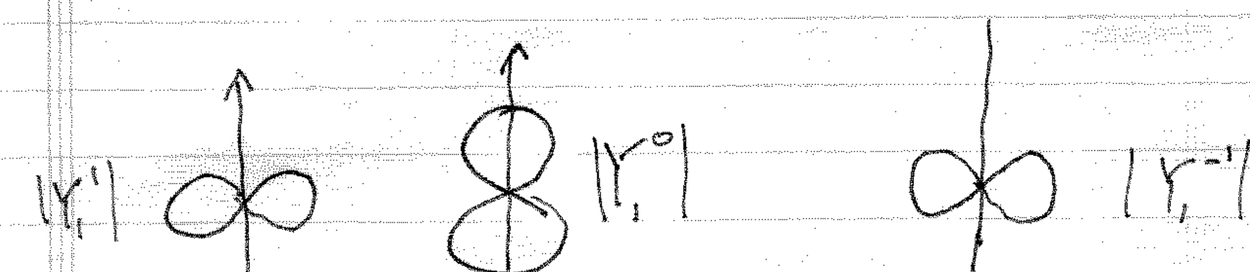
$\quad 6 = \vdots$

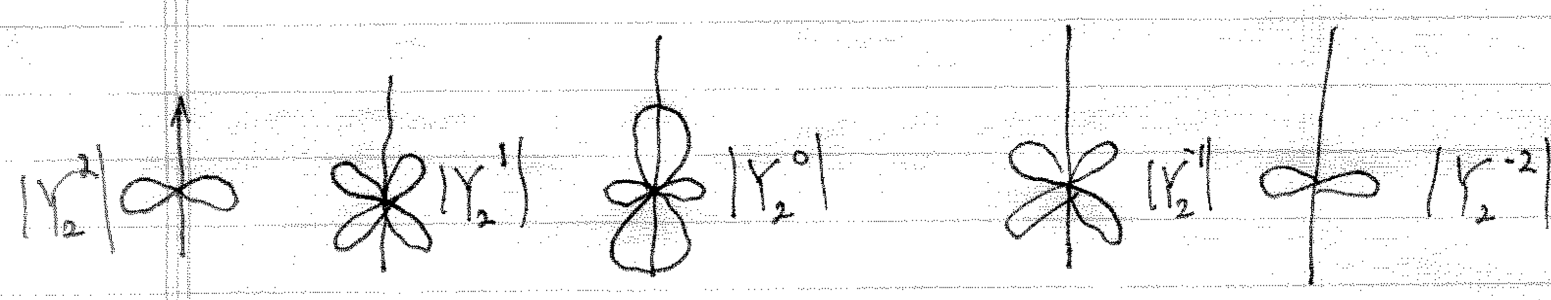
We have plotted the radial wave functions on the previous page. What about the angular wave functions?

<u>Polar Plot:</u> We seek the prob density $|Y_\ell^m(\theta,\phi)|^2$

Typically we show the $|Y_\ell^m(\theta,\phi)| = N|P_\ell^m(\theta)|$ in ~~through~~ any plane through the z-axis, understanding that the distribution is azimuthally symmetry





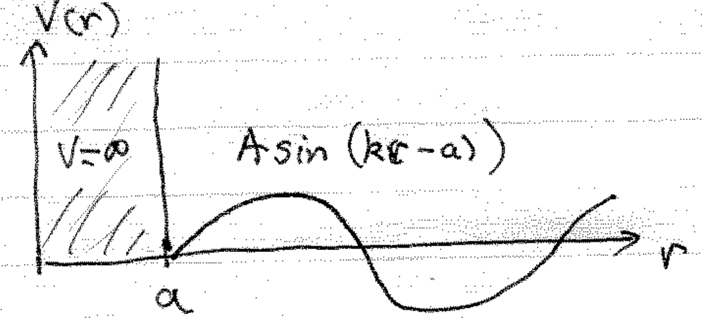


We see explicity $|Y_\ell^m| = |Y_\ell^{-m}|$

Unbound States: Hard Sphere Potential

Consider now an infinite spherical barrier of radius a

($V = 0$ outside)

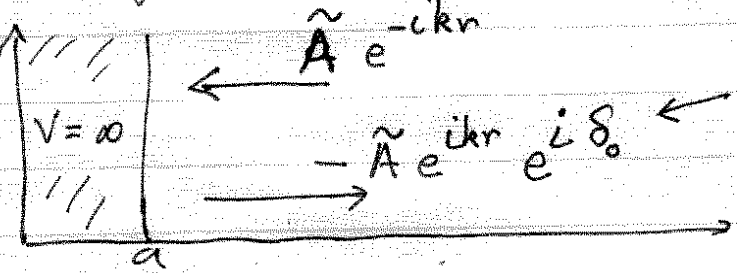


Consider $l = 0$ first

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + V(r)\,u(r) = E\,u(r)$$

Compared to the free particle, the wave function is phase shifted.

Scattering picture



← Scattering phase shift

$$u(r) = \tilde{A}\left(e^{-ikr} - e^{ikr}\, e^{i\delta_0}\right)$$

$$= -2i\,\tilde{A}\, e^{i\frac{\delta_0}{2}}\left(\frac{e^{i\left(kr+\frac{\delta_0}{2}\right)} - e^{-i\left(kr+\frac{\delta_0}{2}\right)}}{2i}\right)$$

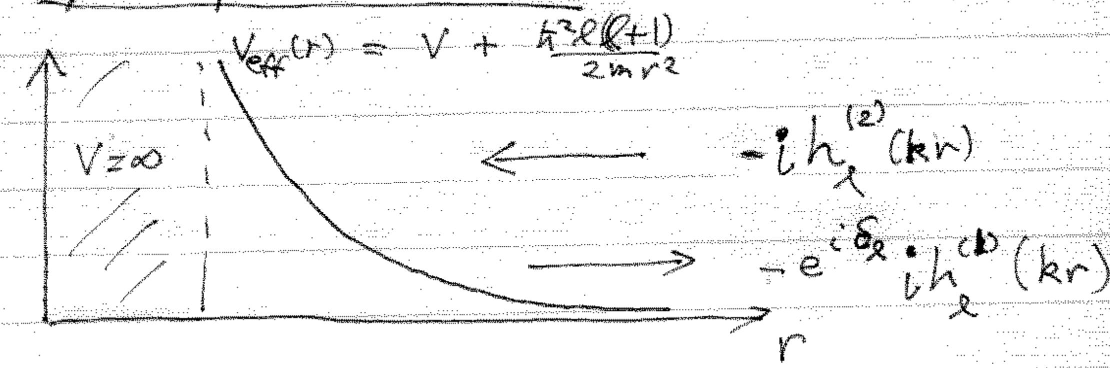
$$= A \sin\left(kr + \frac{\delta_0}{2}\right)$$

Boundary condition : $u(a) = 0$

$$\Rightarrow \sin\left(ka + \frac{\delta_0}{2}\right) = 0$$

$$\Rightarrow \boxed{\delta_0 = -2ka} \quad ✓$$

<u>Higher partial waves</u>



$$u_\ell(r) = r\left(-i\, h_\ell^{(2)}(kr) + e^{i\delta_\ell} i h_\ell^{(1)}(kr)\right)$$

$$u_\ell(a) = 0 \Rightarrow -i h_\ell^{(2)}(ka) - i e^{i\delta_\ell}\, h_\ell^{(1)}(ka) = 0$$

$$\Rightarrow \boxed{e^{i\delta_\ell} = \frac{i h_\ell^{(2)}(ka)}{-i\, h_\ell^{(1)}(ka)} = \frac{+i j_\ell(ka) + n_\ell(ka)}{-i j_\ell(ka) + n_\ell(ka)}}$$

$$\Rightarrow \delta_\ell = 2 \tan^{-1}\left(\frac{j_\ell(ka)}{n_\ell(ka)}\right)$$

Check $\ell = 0$ $\quad \delta_\ell = 2\tan^{-1}\left(\frac{\sin ka}{-\cos ka}\right) = -2ka$ ✓