Chapter 11

The Radial Equation

(10-82, P198) →

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)R_{nlm}(r) - \frac{2\mu}{\hbar^2}\left[V(r)+\frac{l(l+1)\hbar^2}{2\mu r^2}\right]R_{nlm}(r) + \frac{2\mu E}{\hbar^2}R_{nlm}(r) = 0 \quad (1)$$

We will examine the sols. to this equ. for a variety of potentials restricted by the cond. that:

$$V(r) \longrightarrow 0 \quad \text{as } r\to\infty \text{ faster than } \frac{1}{r} \quad \left(\text{except for the Coulomb pot.}\right)$$

(see eq. 12)

Also we will assume $\lim_{r\to 0} r^2 V(r) = 0$ (2) (i.e. not singular as $\frac{1}{r^2}$ at the origin) (see equ 8)

For convenience; $\mathcal{U}_{nlm}(r) = r\,R_{nlm}(r)$ (3)

Since $\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)\frac{\mathcal{U}_{nlm}(r)}{r} = \frac{1}{r}\frac{d^2}{dr^2}\mathcal{U}_{nlm}(r)$ (4)

$$\longrightarrow \frac{d^2\mathcal{U}_{nlm}(r)}{dr^2} + \frac{2\mu}{\hbar^2}\left[E - V(r) - \frac{l(l+1)\hbar^2}{2\mu r^2}\right]\mathcal{U}_{nlm}(r) = 0 \quad (5)$$

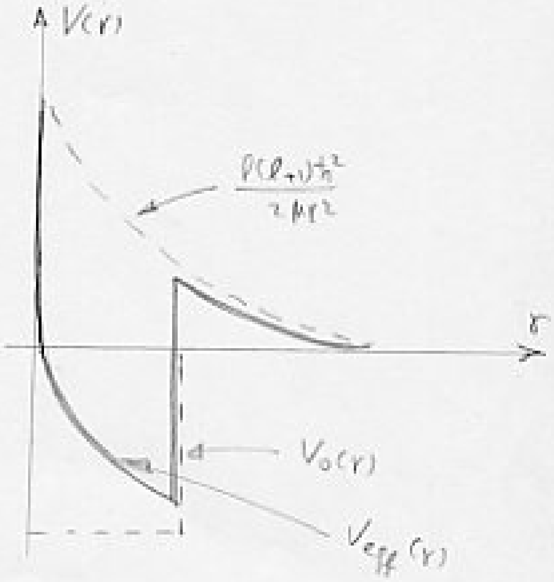
This looks like a <u>one-dim.</u> equ. except that:

a) $$V(r) \longrightarrow V(r) + \underbrace{\frac{l(l+1)\hbar^2}{2\mu r^2}}_{\text{Repulsive centrifugal barrier}} \quad (6)$$

b) the def. of $U_{n\ell m}(r)$ and the finiteness of the wave func. at the origin require that:

$$u_{n\ell m}(0) = 0 \qquad (7)$$

which makes it more like the one-dim. prob. for which $V = +\infty$ in the left-hand region.



Consider the radial equ. near the origin. Taking into account the equ(2):

$$\rightarrow \frac{d^2 u}{dr^2} - \frac{\ell(\ell+1)}{r^2} u \simeq 0 \qquad (8)$$

If we assume $u(r) \sim r^s \qquad (9)$

$$(8) \rightarrow s(s-1) r^{s-2} - \frac{\ell(\ell+1)}{r^2} r^s \simeq 0$$

$$\rightarrow s(s-1) - \ell(\ell+1) = 0 \qquad (10)$$

$$\rightarrow \begin{cases} s = \ell+1 \\ s = -\ell \end{cases}$$

$$\rightarrow \begin{cases} u(r) \sim r^{\ell+1} & \text{regular sol. } (u(0)=0) \\ u(r) \sim r^{-\ell} & \text{irregular sol. } (u(0)\neq 0) \end{cases}$$

(11)

For $r \to \infty$

$$\frac{d^2 u}{dr^2} + \frac{2\mu E}{\hbar^2} u \approx 0 \qquad (12)$$

Since $\int |\Psi(\vec{r})|^2 d\vec{r}^3 = 1$

$$\to \int_0^\infty r^2 dr \int d\Omega \, |R_{n\ell m}(r) \, Y_\ell^m(\theta,\varphi)|^2 = \int_0^\infty r^2 dr \, |R_{n\ell m}(r)|^2 = 1$$

$$\to \int_0^\infty dr \, |u_{n\ell m}(r)|^2 = 1 \qquad (13)$$

$\xrightarrow{\text{so that}}$ $u(r) \to 0$ as $r \to \infty$

a) If $E < 0$

$$\frac{2\mu E}{\hbar^2} = -\alpha^2 \qquad (14)$$

The asymptotic sol. $u(r) \sim e^{-\alpha r}$ $(r \to \infty)$ (15)

b) If $E > 0$, we have sols. that are normalizable in a box. With $\frac{2\mu E}{\hbar^2} = k^2$ (16)

$\xrightarrow{\text{sol.}}$ $a e^{ikr} + b e^{-ikr}$ (17)

A - The Free Particle

$$V(r) = 0$$

$$\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2}\right] R(r) + k^2 R(r) = 0 \qquad (18)$$

where $k^2 = \frac{2\mu E}{\hbar^2}$

$\rho \equiv kr$ change of variable

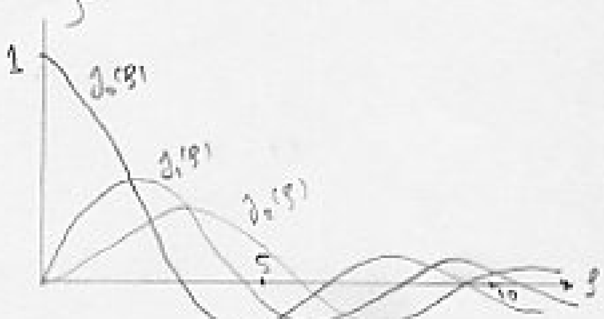
$$\longrightarrow \frac{d^2R}{d\rho^2} + \frac{2}{\rho}\frac{dR}{d\rho} - \frac{l(l+1)}{\rho^2}R + R = 0 \qquad (19)$$

$\xrightarrow{\text{sols.}}$ spherical Bessel fncs.

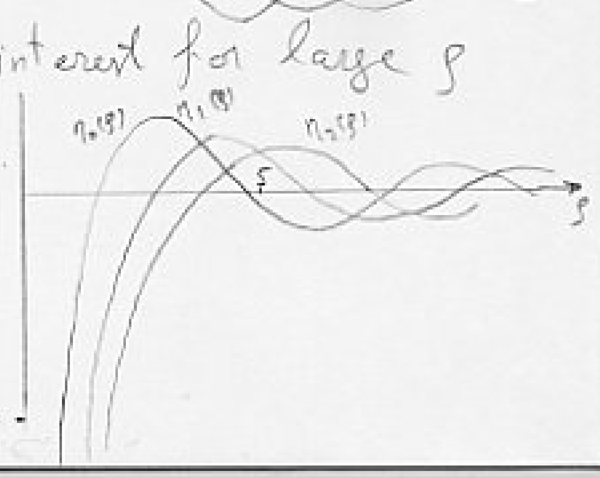
$$\begin{cases} j_l(\rho) = (-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \left(\frac{\sin\rho}{\rho}\right) & \text{(regular)} \\ n_l(\rho) = -(-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \left(\frac{\cos\rho}{\rho}\right) & \text{(irregular)} \end{cases} \qquad (20)$$

$$\begin{cases} j_0(\rho) = \frac{\sin\rho}{\rho} \\ n_0(\rho) = -\frac{\cos\rho}{\rho} \end{cases} \qquad \begin{cases} j_1(\rho) = \frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho} \\ n_1(\rho) = -\frac{\cos\rho}{\rho^2} - \frac{\sin\rho}{\rho} \end{cases}$$

$$\begin{cases} j_2(\rho) = \left(\frac{3}{\rho^3} - \frac{1}{\rho}\right)\sin\rho - \frac{3}{\rho^2}\cos\rho \\ n_2(\rho) = -\left(\frac{3}{\rho^3} - \frac{1}{\rho}\right)\cos\rho - \frac{3}{\rho^2}\sin\rho \end{cases} \qquad (21)$$



The combinations that will be of interest for large ρ are the spherical Hankel fncs.



$$h_\ell^{(1)} = j_\ell(\rho) + i n_\ell(\rho)$$

$$h_\ell^{(2)} = j_\ell(\rho) - i n_\ell(\rho) = \left(h_\ell^{(1)}(\rho)\right)^* \qquad (22)$$

$$h_0^{(1)}(\rho) = \frac{e^{i\rho}}{i\rho} \quad , \quad h_1^{(1)}(\rho) = -\frac{e^{i\rho}}{\rho}\left(1 + \frac{i}{\rho}\right) \, , \quad h_2^{(1)} = \frac{i e^{i\rho}}{\rho}\left(1 + \frac{3i}{\rho} - \frac{3}{\rho^2}\right) \qquad (23)$$

a) The behavior near the origin,

$\rho \to 0 \qquad \rho \ll \ell$

$$j_\ell(\rho) \simeq \frac{\rho^\ell}{1\cdot 3\cdot 5\cdots(2\ell+1)} = \frac{\rho^\ell}{(2\ell+1)!!} \quad , \quad n_\ell \simeq \frac{-(2\ell-1)!!}{\rho^{\ell+1}} \qquad (24)$$

b) For large ρ- asymptotic limit ;

$\rho \to$ large $\qquad \rho \gg \ell$

$$j_\ell(\rho) \simeq \frac{1}{\rho} \sin\left(\rho - \frac{\ell\pi}{2}\right) = \frac{1}{\rho} \cos\left(\rho - \frac{(\ell+1)}{2}\pi\right)$$

$$n_\ell(\rho) \simeq -\frac{1}{\rho} \cos\left(\rho - \frac{\ell\pi}{2}\right) = \frac{1}{\rho} \sin\left(\rho - \frac{(\ell+1)}{2}\pi\right) \qquad (25)$$

So that; $\quad h_\ell^{(1)}(\rho) \simeq -\frac{i}{\rho} e^{i(\rho - \ell\pi/2)} = \frac{1}{\rho} e^{i(\rho - (\ell+1)\pi/2)}$

The sol., regular at the origin:

$$R_\ell(r) = j_\ell(kr) \qquad (26)$$

(25) → Its asymptotic form; $R_\ell(kr) \simeq \frac{-1}{2ikr}\Big[\underbrace{e^{-i(kr-\ell\pi/2)}}_{\text{incoming spherical wave}} - \underbrace{e^{i(kr-\ell\pi/2)}}_{\text{outgoing spherical wave}}\Big]$ (26′)

Remarks: $\begin{cases} j_0(0)=1, \; j_1(0)=0 \; \cdots \\ n_0(0)=\infty, \; n_1(0)=\infty \; \cdots \end{cases}$

Now, the generalization of the one-dim. flux;

$$\bar{j} = \frac{\hbar}{2i\mu}\left[\psi^*(\bar{r})\,\nabla\psi(\bar{r}) - (\nabla\psi^*(\bar{r}))\psi(\bar{r})\right] \qquad (27)$$

We shall see that it is only the flux in the radial direction that is of interest for large r.

$$\int d\Omega\; \hat{e}_r\cdot \bar{j}(r) = \frac{\hbar}{2i\mu}\int d\Omega\left(\psi^*\frac{\partial}{\partial r}\psi - \frac{\partial\psi^*}{\partial r}\psi\right) \qquad (28)$$

radial flux integrated over all angles

Remark: $\nabla\psi = \hat{e}_r\frac{\partial\psi}{\partial r} + \hat{e}_\theta\frac{1}{r}\frac{\partial\psi}{\partial\theta} + \hat{e}_\varphi\frac{1}{r\sin\theta}\frac{\partial\psi}{\partial\varphi}$

For a sol. of the form; $\psi(\bar{r}) = C\,\frac{e^{\pm ikr}}{r}\,Y_\ell^m(\theta,\varphi)$

$$\int d\Omega\; j_r = \frac{\hbar}{2i\mu}|C|^2\left[\frac{e^{\mp ikr}}{r}\left(\pm ik\frac{e^{\pm ikr}}{r} - \frac{e^{\pm ikr}}{r^2}\right) - \text{Complex conjugate}\right]$$

$$= \pm\frac{\hbar k|C|^2}{\mu}\frac{1}{r^2} \qquad \left(\begin{matrix}+ \rightsquigarrow \text{outgoing flux} \\ - \rightsquigarrow \text{incoming} \;\; ''\end{matrix}\right) \qquad (29)$$

where we have used, $\int d\Omega \, |Y_\ell^m(\theta,\varphi)|^2 = 1$

Remark: $\int d\Omega \; Y_{\ell'}^{m'^*}(\theta,\varphi)\, Y_\ell^m(\theta,\varphi) = \delta_{\ell\ell'}\delta_{mm'}$ (30)

(29) $\rightarrow \int r^2 d\Omega \, J_r =$ indep. of r (31) (Total flux going through the spherical surface at radius r)

For our sol. (26)

$$\int r^2 d\Omega \, J_r = -\frac{\hbar k}{\mu}\left|\frac{i}{2k}e^{i\ell\frac{\pi}{2}}\right|^2 = -\frac{\hbar k}{\mu}\frac{1}{4k^2} \quad \text{incoming flux}$$

$$\int r^2 d\Omega \, J_r = +\frac{\hbar k}{\mu}\frac{1}{4k^2} \quad \text{outgoing flux} \qquad (40)$$

Total flux $= 0$ (Since there is no source of flux)

In general by the flux conservation, for a sol. of the form

$$\underset{r\to \text{large}}{R_\ell(r)} \simeq -\frac{1}{2ikr}\left[e^{-i(kr-\ell\frac{\pi}{2})} - S_\ell(k)\, e^{i(kr-\ell\pi/2)}\right] \quad (41) \quad (V(r)\neq 0)$$

We must have $|S_\ell(k)|^2 = 1$ (42)

$S_\ell(k)$ can be written in the form, $S_\ell(k) = e^{2i\delta_\ell(k)}$ (43)

(41) $\rightarrow$ $R_\ell(r)\, e^{-i\delta_\ell(k)} \simeq -\frac{1}{2ikr}\left[e^{-i(kr-\frac{\ell\pi}{2}+\delta_\ell(k))} - e^{i(kr-\frac{\ell\pi}{2}+\delta_\ell(k))}\right]$

$$\rightarrow \quad R_\ell(r) \simeq e^{i\delta_\ell(k)} \frac{\sin[kr - \ell\pi/2 + \delta_\ell(k)]}{kr} \qquad (44)$$

$\rightarrow$ $\delta_\ell(k)$: phase shift

Note that for free particle sol. we had:

$$j_\ell(kr) \xrightarrow[\text{asymptotic form}]{} \frac{\sin[kr - \frac{\ell\pi}{2}]}{kr} \qquad (45)$$

Now, note that the flux in the $\hat{e}_\theta$-dir involves,

$$\hat{e}_\theta \cdot J = \frac{\hbar}{2i\mu}\left(\psi^* \frac{1}{r}\frac{\partial}{\partial\theta}\psi - c.c.\right) \sim \frac{1}{r^3}$$

$$\hat{e}_\theta \cdot J\,(r^2 dr) \sim \frac{1}{r} \qquad (46)$$

$\rightarrow$ So for $r \rightarrow \infty$ the dominant term is only radial flux.

B. The Square Well, Bound State

$$V(r) = \begin{cases} -V_0 & r<a \\ 0 & r>a \end{cases} \qquad (47)$$

The radial equ;

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} - \frac{\ell(\ell+1)}{r^2}R + \frac{2\mu}{\hbar^2}(V_0+E)R = 0 \quad r<a \qquad (48)$$

$$\frac{d^2R}{dr^2}+\frac{2}{r}\frac{dR}{dr}-\frac{l(l+1)}{r^2}R+\frac{2\mu}{\hbar^2}ER=0 \qquad r>a$$

We look for bound state sols. for which $\underline{E<0}$

$$\frac{2\mu}{\hbar^2}(V_0+E)\equiv k^2 \quad , \quad \frac{2\mu}{\hbar^2}E=-\alpha^2 \qquad (49)$$

For $r<a$:

$R(r)=A\,j_l(kr)$ regular at the origin

For $r>a$

$$\underset{\text{as } r\to\infty}{R(r)\longrightarrow 0} \qquad (50)$$

The sol. : spherical Bessel func.

$$R(r)=B\,h_l^{(1)}(i\alpha r)$$

where k is replaced by $i\alpha$ in equ. (18)

Remark: $\underset{\substack{\rho\to\text{large}\\ \rho\gg l}}{h_l^{(1)}(\rho)\simeq -\frac{i}{\rho}e^{i(\rho-l\pi/2)}}$

In our case $\rho\to i\alpha r$, $\Rightarrow h_l^{(1)}(i\alpha r)\simeq -\frac{1}{\alpha r}\underbrace{e^{-\alpha r}}_{\substack{\text{decreasing}\\ \text{satisfying equ. (50)}}}e^{il\pi/2}$

(51)

i) The two sols. must match at $r = a$

ii) and so must the derivatives

$$\rightarrow \quad \left[A\, j_\ell(kr)\right]_{r=a} = \left[B\, h_\ell^{(1)}(i\alpha r)\right]_{r=a}$$

$$\left[\frac{d}{dr}\left(A\, j_\ell(kr)\right)\right]_{r=a} = \left[\frac{d}{dr}\left(B\, h_\ell^{(1)}(i\alpha r)\right)\right]_{r=a}$$

$$\rightarrow k\left[\frac{d}{d(kr)}\left(A\, j_\ell(kr)\right)\right]_{r=a} = i\alpha\left[\frac{d}{d(i\alpha r)}\left(B\, h_\ell^{(1)}(i\alpha r)\right)\right]_{r=a}$$

$$\rightarrow \quad k\left[\frac{d j_\ell(\rho)/d\rho}{j_\ell(\rho)}\right]_{\rho = ka} = i\alpha\left[\frac{d h_\ell^{(1)}(\rho)/d\rho}{h_\ell^{(1)}(\rho)}\right]_{\rho = i\alpha a} \qquad (52)$$

This is a very complicated transcendental equ. involving ℓ, V_0, and E.

Special Case: $\ell = 0$, we use the fnc. $u(r) = rR(r)$ (for simplification);

$$\left[\frac{u(r)}{r}\right]_{\substack{\text{left}\\ r=a}} = \left[\frac{u(r)}{r}\right]_{\substack{\text{right}\\ r=a}} \rightarrow \left[u(r)\right]_{\substack{L\\ r=a}} = \left[u(r)\right]_{\substack{R\\ r=a}} \qquad (53)$$

$$\left[\frac{d}{dr}\left(\frac{u}{r}\right)\right]_{\substack{L\\ r=a}} = \left[\frac{d}{dr}\left(\frac{u}{r}\right)\right]_{\substack{R\\ r=a}} \qquad (54)$$

$$\rightarrow \left[\frac{1}{r}\frac{du}{dr} - \frac{u}{r^2} \right]_{L,\ r=a} = \left[\frac{1}{r}\frac{du}{dr} - \frac{u}{r^2} \right]_{R,\ r=a} \qquad (55)$$

$$(53)\ (54) \rightarrow \left[\frac{1}{r}\frac{du}{dr} \right]_{L,\ r=a} = \left[\frac{1}{r}\frac{du}{dr} \right]_{R,\ r=a}$$

$$\rightarrow \left[\frac{du}{dr} \right]_{L,\ r=a} = \left[\frac{du}{dr} \right]_{R,\ r=a} \qquad (56)$$

$$(21) \rightarrow u(r)_L = A r j_0(kr) = \frac{A}{k} S(kr)$$

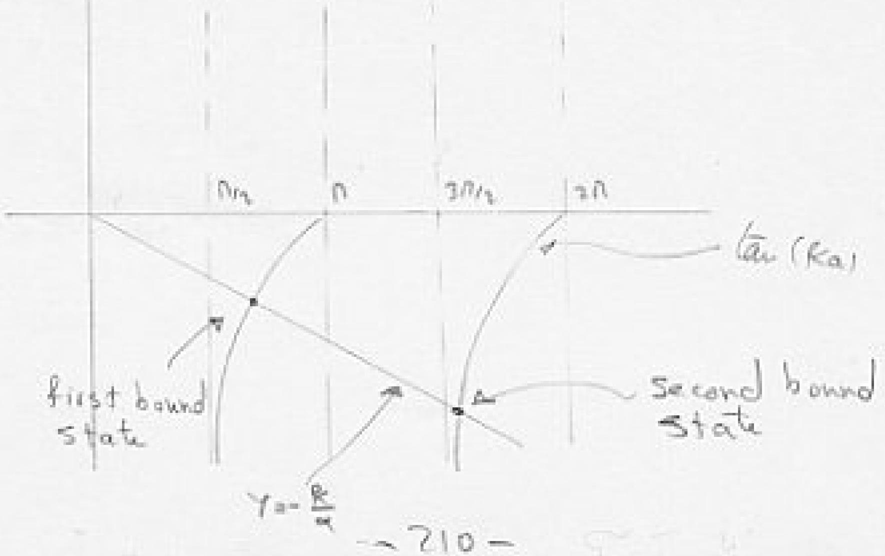
$$(23) \rightarrow u(r)_R = B r h_0^{(1)}(i\alpha r) = -\frac{B}{\alpha} e^{-\alpha r}$$

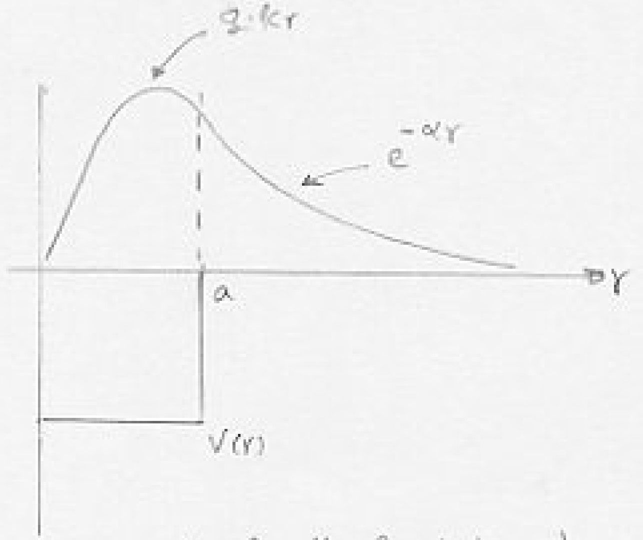
$$\left[\frac{A}{k} S(kr) \right]_{r=a} = \left[-\frac{B}{\alpha} e^{-\alpha r} \right]_{r=a}$$

$$\left[\frac{Ak}{k} C(kr) \right]_{r=a} = \left[+\frac{B\alpha}{\alpha} e^{-\alpha r} \right]_{r=a}$$

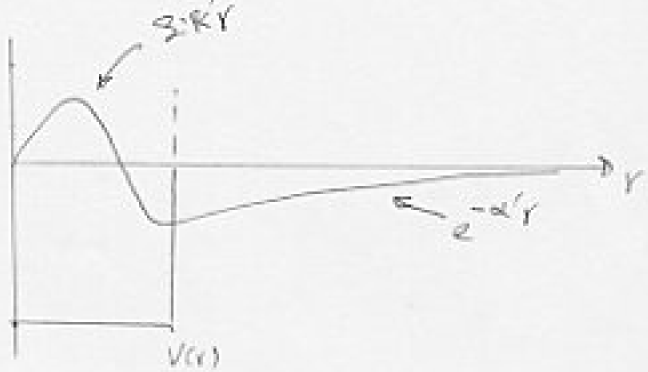
$$\rightarrow \frac{S(ka)}{k\,C(ka)} = \frac{-e^{-\alpha a}}{\alpha e^{-\alpha a}} \rightarrow \tan(ka) = -\frac{k}{\alpha}$$

Since $k > 0$, $\alpha > 0 \rightarrow -\frac{k}{\alpha} < 0$





Sol. for the first bound state ($u(r) = rR(r)$, $l=0$)



Sol. for the second bound state

Now, for very <u>deep pot.</u> for which $ka \gg l$, we are justified in using the asymptotic form of $j_l(\rho)$ (equ. 25);

$$(52) \rightarrow -\frac{1}{a} + k\cot\left(ka - \frac{l\pi}{2}\right) = \underbrace{\text{R.H.S.}}_{\text{does not contain } V_0} \quad (57)$$

$\left\{ \begin{array}{l} \text{The R.H.S. does not contain } V_0 \text{ (which is large)} \\ \text{and if } |E| \ll V_0 \end{array} \right\} \quad \cot\left(ka - \frac{l\pi}{2}\right) = \frac{\text{R.H.S.}}{k} + \frac{1}{ka}$

$\rightarrow$ the largeness of ka implies that $\cot\left(ka - \frac{l\pi}{2}\right) \approx 0$

$$\rightarrow ka - \frac{l\pi}{2} \simeq \left(n + \tfrac{1}{2}\right)\pi \quad (58)$$

Since $|E| \ll V_0$, $(49) \rightarrow k \simeq k_0\left(1 + \frac{E}{2V_0}\right)$ (59)

where $k_0 = \frac{2\mu V_0}{\hbar^2}$ (60)

(58)(59) $\Rightarrow \dfrac{E}{2V_0} = -1 + \dfrac{[n+(\ell+1)/2]\pi}{k_0 a}$ (61)

For $n \longrightarrow$ large (far from the bottom of the well)

for all $\ell \ll k_0 a$, the energy levels are approximately equally spaced;

$$\frac{\Delta E}{2V_0} \simeq \frac{\pi}{k_0 a} \quad (62)$$

A related Prob.: The infinite box in 3-dim:

$$V(r) = \begin{cases} 0 & r<a \\ \infty & r>a \end{cases} \quad (63)$$

$$\frac{2\mu E}{\hbar^2} = k^2 \quad (64)$$

$R(r) = A j_\ell(r)$ regular at $r=0$ $(r<a)$

$R(r) = 0$ $r \geqslant a$ (65)

$\longrightarrow j_\ell(ka) = 0$ (66)

Roots

$ka \backslash \ell$	0	1	2	3	4	5	
	3.14	4.49	5.76	6.99	8.18	9.36	n=1 first root
	6.28	7.73	9.10	10.42			n=2 Second "
	9.42						n=3 - - -

Using the spectroscopic notation;

$$
\begin{aligned}
S &: l=0 \\
P &: l=1 \\
D &: l=2 \\
F &: l=3 \\
G &: l=4
\end{aligned}
\qquad (67)
$$

Then the order of the levels are;

1S, 1P, 1D, 2S, 1F, 2P, 1G, 2D, 1H, 3S

A model of nucleus:

Protons and Neutrons inside such an ifinite box.

For spin $\frac{1}{2}$ particles (fermions) each level is occupied only with 2-particles.

Consider Protons;

1S:	2-protons	($l=0$)
1P:	6 - "	($l=1$, $m=-1, 0, +1$)
1D:	10 - "	($l=2$ - - -)
2S:	2 - "	($l=0$)
1F:	14 - "	($l=3$)
2P:	6 - "	($l=1$)
1G:	18 - "	($l=4$)
2D:	10 - "	($l=2$)
1H:	22 - "	($l=5$)
3S:	2 - "	($l=0$)

(68)

Thus the levels will be filled when the number of protons is ;

$$2, 8(=2+6), 18(2+6+10), 20(=18+2), 34(=20+14),$$

$$40, 58, 68, 90, 92, 106 \qquad (69)$$

and similarly for neutrons.

In real nuclei ; the magic numbers are :

$$2, 8, 20, 28, 50, 82, 126, \ldots \qquad (70)$$

The nuclei having these number of protons or neutrons exhibit special characteristics.

C. The Square Well Continuum Sols.

With $E > 0$, we write $\quad \frac{2ME}{\hbar^2} = K^2 \qquad (71)$

For $r > a$, the sol. will be a combination of the regular and irregular sols. of the free field eqn.

$$R_\ell(r) = B j_\ell(Kr) + C n_\ell(Kr) \qquad (72)$$

For $r < a$ $\quad R_\ell(r) = A\, j_\ell(kr)$ (73)

where $k^2 = \dfrac{2\mu(E+V_0)}{\hbar^2}$ (74) $\quad (V_0 > 0$ for attractive pot.$)$

Matching: $\quad k\left[\dfrac{dj_\ell(\rho)/d\rho}{j_\ell(\rho)}\right]_{\rho=ka} = k\left[\dfrac{B\, dj_\ell(\rho)/d\rho + C\, dn_\ell/d\rho}{B j_\ell(\rho) + C n_\ell(\rho)}\right]_{\rho=ka}$

(75)

The asymptotic form of (72);

$$R_\ell(r) \simeq \frac{B}{kr}\left[\sin\left(kr - \frac{\ell\pi}{2}\right) - \frac{C}{B}\cos\left(kr - \frac{\ell\pi}{2}\right)\right] \quad (76)$$

$$(44) \rightarrow R_\ell(r) \simeq \frac{e^{i\delta_\ell(k)}}{kr}\left[\sin\left(kr - \frac{\ell\pi}{2}\right)\cos\delta_\ell(k) + \cos\left(kr - \frac{\ell\pi}{2}\right)\sin\delta_\ell(k)\right]$$

(77)

With the assumption $e^{i\delta_\ell(k)} \simeq 1$ $\quad$ (for $\delta_\ell(k) \simeq$ small) (78)

$(76)(77) \rightarrow \dfrac{C}{B} = -\tan\delta_\ell(k)$ (79)

The actual computation of C/B from (75) is tedious, except for $\ell = 0$

Once again $u(r) = r R(r)$

for $\ell = 0$

$$\begin{aligned} rR(r) &= B\sin kr + C\cos kr & r > a \\ rR(r) &= A\sin kr & r < a \end{aligned} \quad (80)$$

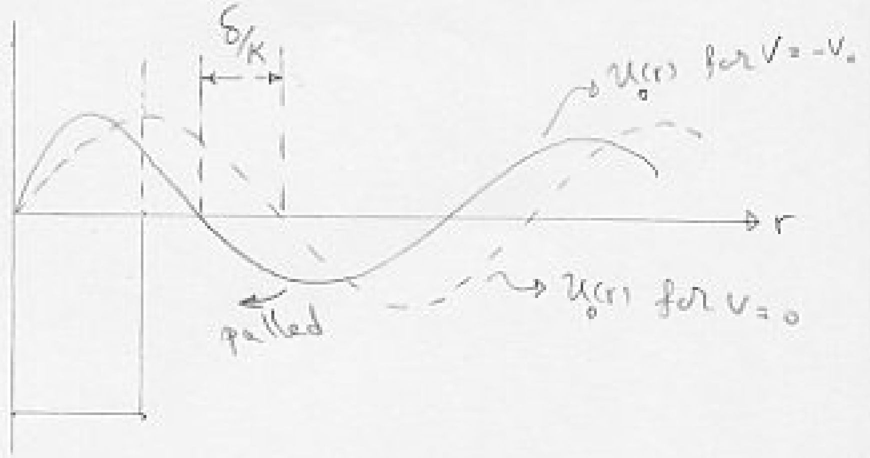
$$(53)(56) \rightarrow \begin{cases} A \sin Ka = B \sin ka + C \cos ka \\ KA \cos Ka = Bk \cos ka - Ck \sin ka \end{cases} \quad (81)$$

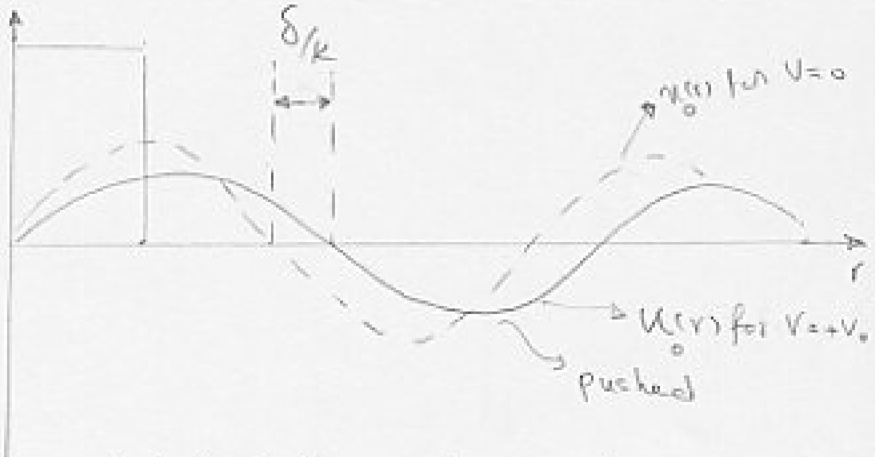
$$\rightarrow \quad \frac{1}{K} \tan Ka = \frac{B \sin ka + C \cos ka}{Bk \cos ka - Ck \sin ka} \quad (82)$$

Using (79) and (82) $\delta_{\ell=0}(k)$ can be obtained

Indeed in general

$$(75)(79) \rightarrow \tan \delta_\ell(k) = \frac{k\, j'_\ell(ka)\, j_\ell(Ka) - K\, j_\ell(ka)\, j'_\ell(Ka)}{k\, n'_\ell(ka)\, j_\ell(Ka) - K\, n_\ell(ka)\, j'_\ell(Ka)} \quad (83)$$





Note that for repulsive pot. equ. (74) must be changed to $K^2 = \frac{2\mu(E-V_0)}{\hbar^2}$, where $V_0 > 0$ and K may or may not be real.

Important relation :

By superposition principle we have the following sol. for the free-particle equ. (using equ. (26));

$$\psi(\bar{r}) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} A_{\ell m}\, j_\ell(kr)\, Y_{\ell m}(\theta,\varphi) \qquad (84)$$

Another sol. of the free-particle equ., which reads

$$(\nabla^2 + k^2)\,\psi(r) = 0 \qquad (85)$$

before the separation into angular and radial part is made, is the plane wave;

$$\psi(r) = e^{ik\cdot r} \qquad (86)$$

Now if we define the z-axis by the dir. of $\bar{k}$;

$$\rightarrow \quad e^{ik\cdot r} = e^{ikr\cos\theta} \qquad (87)$$

$\rightarrow$ $\psi(\bar{r})$ has no φ-dependence

$\rightarrow$ $m=0$ only in (84)

Using $\quad Y_\ell^0(\theta,\varphi) = \left(\frac{2\ell+1}{4\pi}\right)^{1/2} P_\ell(\cos\theta) \qquad (88)$

$\rightarrow$ Legendre polynomial,

$$\rightarrow e^{ik\cos\theta} = \sum_{\ell=0}^{\infty} \left(\frac{2\ell+1}{4\pi}\right)^{1/2} A_\ell j_\ell(kr) P_\ell(\cos\theta) \quad (89)$$

Now using the $\frac{1}{2}\int_{-1}^{1} d(\cos\theta) P_\ell(\cos\theta) P_{\ell'}(\cos\theta) = \frac{\delta_{\ell\ell'}}{2\ell+1}$ (90)

$$\rightarrow A_\ell j_\ell(kr) = \frac{1}{2}\left[4\pi(2\ell+1)\right]^{1/2} \int_{-1}^{1} dz\, P_\ell(z)\, e^{ikrz}$$

(91)

Now using: $j_\ell(\rho) = \frac{1}{2i^\ell}\int_{-1}^{+1} ds\, e^{i\rho s} P_\ell(s)$ (92)

$$\rightarrow A_\ell j_\ell(kr) = \frac{1}{2}\left[4\pi(2\ell+1)\right]^{1/2} \left(2i^\ell j_\ell(kr)\right) \quad (92)$$

$$\rightarrow A_\ell = i^\ell \left[4\pi(2\ell+1)\right]^{1/2} \quad (93)$$

(84) (88) (87)(93) $\rightarrow$ $e^{ikr\cos\theta} = \sum_{\ell=0}^{\infty} (2\ell+1)\, i^\ell j_\ell(kr) P_\ell(\cos\theta)$

(94)