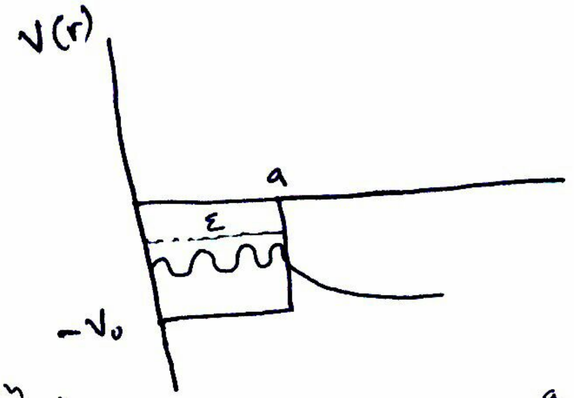
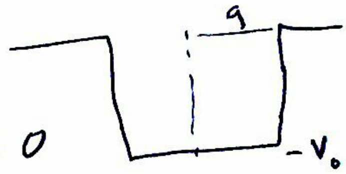
Section 6.3.3: The 3d spherical square well

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



solve for the bound states

for $0 \leq r \leq a$, the radial eq^n is $\Longleftrightarrow$



3d cylinder

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

for Bound states $E<0$, let $E = -\mathcal{E}$; $\mathcal{E} > 0$

$$\Rightarrow \quad \frac{2m}{\hbar^2}(V_0 - \mathcal{E}) = \beta^2$$

$$\Rightarrow \frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \left[\beta^2 - \frac{l(l+1)}{r^2}\right]R = 0$$

and then divide by β^2

introduce $\rho = \beta r$; when $\frac{\partial}{\partial r} = \frac{\partial \rho}{\partial r}\frac{\partial}{\partial \rho} = \beta \frac{\partial}{\partial \rho}$

$$\frac{\partial^2}{\partial r^2} = \beta^2 \frac{\partial^2}{\partial \rho^2}$$

$$\Rightarrow \frac{d^2R}{d\rho^2} + \frac{2}{\rho}\frac{dR}{d\rho} + \left[1 - \frac{l(l+1)}{\rho^2}\right]\rho = 0 \longrightarrow \text{Bessel eq}^n$$

the general solution is

$$R(\rho) = A_l\, j_l(\rho) + B_l\, n_l(\rho)$$

j_l: finite as $\rho \to 0$; n_l: diverges as $\rho \to 0$

$$\Rightarrow R_l(\rho) = A_l\, j_l(\rho) = A_l\, j_l(\beta r) \text{ only}$$

check! $j_0 = \frac{\sin\rho}{\rho}$, $j_1 = \frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho}$

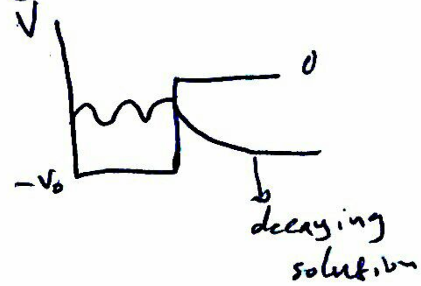
as $\rho \to 0$ $\quad j_0 \to 1$ and $j_1 \approx \frac{\rho - \rho^3/6}{\rho^2} - \frac{1-\rho^2/2}{\rho} \approx -\frac{1}{6}\rho + \frac{1}{2}\rho \approx \frac{\rho}{3}$ converges

$n_0 = -\frac{\cos\rho}{\rho}$, $n_1 = -\frac{\cos\rho}{\rho^2} - \frac{\sin\rho}{\rho}$

$\Rightarrow$ as $\rho \to 0$ $\quad n_0 \to -\frac{1}{\rho}$ and $n_1 \to -\frac{1}{\rho^2}$ diverges in general as $\rho \to 0$

$$j_\ell(\rho) \approx \frac{\rho^\ell}{(2\ell+1)!!} \quad \text{and} \quad n_\ell(\rho) \approx \frac{(2\ell-1)!!}{\rho^{\ell+1}}$$ good approximation

now for $r \geq a$, the solution is a combination of j_ℓ and n_ℓ but with imaginary argument.



$$\frac{2m}{\hbar^2}(\overset{\text{zero outside}}{\cancel{V_0}} - \mathcal{E}) = \beta^2$$

$$-\frac{2m\mathcal{E}}{\hbar^2} = \beta^2 \quad ; \text{ with } \varkappa^2 = \frac{2m\mathcal{E}}{\hbar^2}$$

$$-\varkappa^2 = \beta^2 \Rightarrow \beta = i\varkappa \Rightarrow \rho = i\varkappa r$$
$$\rho^2 = -\varkappa^2 r^2$$

$$\Rightarrow R_\ell(\rho) = C j_\ell(i\varkappa r) + D_\ell n_\ell(i\varkappa r)$$

This solution can be expressed in terms of Hankel functions as follows:

$h_\ell^{(1)} = j_\ell + i n_\ell$ Hankel function of first kind

$h_\ell^{(2)} = j_\ell - i n_\ell = (h_\ell^{(1)})^*$ Hankel function of second kind.

again for these functions to be physical, they must converge as $\rho \to \infty$

let us check ?

$$h_\ell^{(1)} = j_\ell + i n_\ell \overset{\rho\to\infty}{\simeq} \frac{\sin(\rho - \frac{\ell\pi}{2}) - i\cos(\rho - \ell\pi/2)}{\rho}$$

$$= \frac{-i}{\rho}\left[\cos(\rho - \ell\pi/2) + i\sin(\rho - \ell\pi/2)\right]$$

$$= \frac{-i}{\rho} e^{+i(\rho - \ell\pi/2)}$$

for $l=0$ (for instance)

$$h_0^{(1)} \simeq \frac{-i}{\rho} e^{i\rho} = \frac{-i}{i\chi r} e^{i^2\chi r} = -\frac{1}{\chi r} e^{-\chi r} \longrightarrow 0 \text{ as } \rho \longrightarrow \infty$$

converges
acceptable

Now for $h_l^{(2)}$

$$h_l^{(2)} = j_l - i n_l = \frac{\sin(\rho - l\pi/2) + i\cos(\rho - l\pi/2)}{\rho}$$

$$= \frac{i}{\rho}\left[\cos(\rho - l\pi/2) - i\sin(\rho - l\pi/2)\right] = \frac{i}{\rho} e^{-i(\rho - l\pi/2)}$$

for $l=0$ (for instance) $h_0^{(2)} \propto \frac{i}{\rho} e^{-i\rho} = \frac{i}{i\chi r} e^{-i^2\chi r} = \frac{1}{\chi r} e^{\chi r}$

blow up as $\rho \to \infty$
Not acceptable

$\Rightarrow$ only $h_l^{(1)}$ is acceptable

$$\Rightarrow R_l(\rho) = B\, h_l^{(1)}(\rho)$$

$$\therefore R_l(\rho) = \begin{cases} A_l\, j_l(\rho) & ; r < a \\ B_l\, h_l^{(1)}(\rho) & ; r > a \end{cases}$$

or using $u_l(\rho) = \rho R_l(\rho)$ and for $l=0$

$$u_0(\rho) = \rho R_0(\rho) = \rho A j_0(\rho) \Rightarrow \text{let us call it } u_<$$

$$u_<(r) = \cancel{\beta r} A \frac{\sin \beta r}{\cancel{\beta r}} = A \sin\beta r \quad \text{for } r < a$$

and $h_0^{(1)}(\rho) = j_0 + i n_0 = \dfrac{\sin\rho}{\rho} - i\dfrac{\cos\rho}{\rho} = \dfrac{-i}{\rho}\left[\cos\rho + i\sin\rho\right]$

$$= \frac{-i}{\rho} e^{i\rho}$$

$$\Rightarrow u_0(\rho) = \rho B h_0^{(1)}(\rho) = \rho B\left(\frac{-i}{\rho} e^{i\rho}\right)$$

$$= -iB\, e^{+i\rho} \equiv u_>$$

call it D

$$\Rightarrow u_>(r) = D e^{i^2\chi r}$$

$$= D e^{-\chi r} \quad \text{for } r > a$$

$$\therefore \quad u(r) = \begin{cases} u_<(r) = A \sin\beta r & ; r<a \quad \text{where } \beta^2 = \frac{2m}{\hbar^2}(V_0-\varepsilon) \\ u_>(r) = De^{-\varkappa r} & ; r>a \quad \text{where } \varkappa^2 = \frac{2m\varepsilon}{\hbar^2} \end{cases}$$

B.Cs: first $\beta^2 = \frac{2m}{\hbar^2}(V_0-\varepsilon) = \frac{2mV_0}{\hbar^2} - \frac{2m\varepsilon}{\hbar^2} = \frac{2mV_0}{\hbar^2} - \varkappa^2$

$\Rightarrow \quad \beta^2+\varkappa^2 = \frac{2mV_0}{\hbar^2}$, circle of radius $\sqrt{\frac{2mV_0}{\hbar^2}}$

Now matching the log derivative at $r=a$ yields

$u_< = A\sin\beta r \quad ; \quad u_<' = A\beta\cos\beta r$

$u_> = De^{-\varkappa r} \quad ; \quad u_>' = -\varkappa De^{-\varkappa r}$

$\Rightarrow \left(\frac{u'}{u}\right)_< = \left(\frac{u'}{u}\right)_> \Rightarrow \frac{\beta \cancel{A} \cos\beta a}{\cancel{A}\sin\beta a} = \frac{-\cancel{D}\varkappa \cancel{e^{-\varkappa a}}}{\cancel{De^{-\varkappa a}}} = -\varkappa$

$\beta\cot(\beta a) = -\varkappa \quad \Rightarrow \cot(\beta a) = -\varkappa/\beta$

or $\tan(\beta a) = -\beta/\varkappa$

transcendental eq^n

$\therefore \quad \beta\cot(\beta a) = -\varkappa$

$\beta a\cot(\beta a) = -\varkappa a \quad$, let $y = \beta a$

$y\cot y = -\varkappa a \quad$, but $\beta^2+\varkappa^2 = \frac{2mV_0}{\hbar^2}$

$\beta^2a^2+\varkappa^2a^2 = \frac{2ma^2V_0}{\hbar^2} = \lambda^2$

$y^2+\varkappa^2a^2 = \lambda^2$

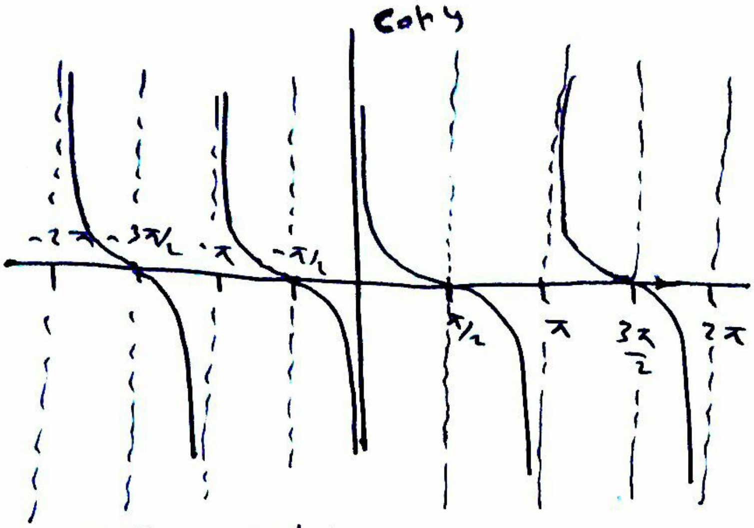
$\varkappa^2a^2 = \lambda^2-y^2$

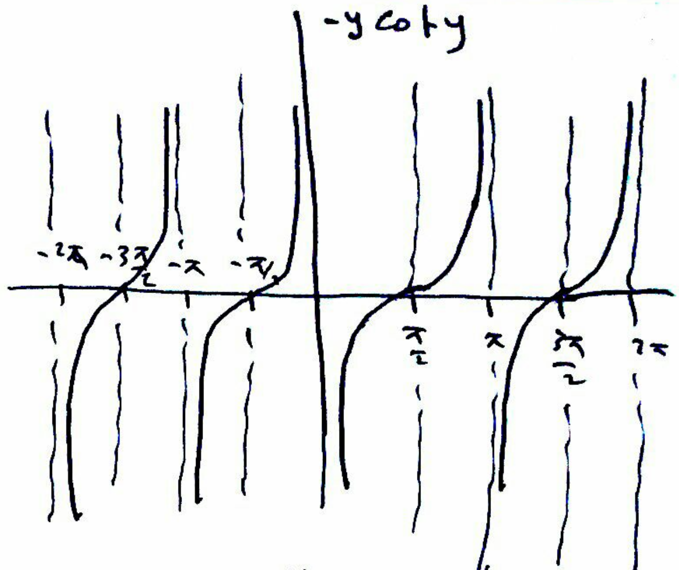
$\varkappa a = \sqrt{\lambda^2-y^2}$

$\Rightarrow y\cot y = -\sqrt{\lambda^2-y^2}$

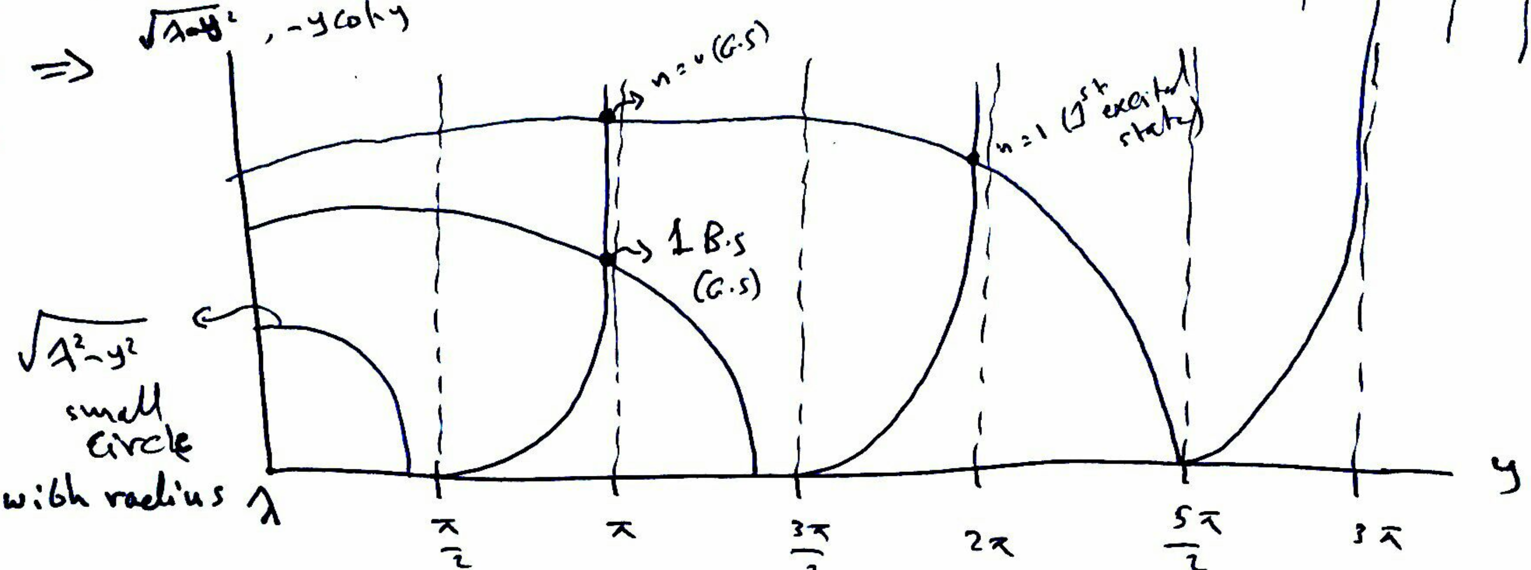
$\Rightarrow \boxed{\sqrt{\lambda^2-y^2} = -y\cot y}$

solve Graphically





$\Rightarrow$



Notice that $-y\cot y$ has two branches $(+,-)$. here we take only the $(+)$ branch as $y \geq 0$ or $\beta a \geq 0$ or $\beta \geq 0$

so if $\lambda < \frac{\pi}{2}$ or $\lambda^2 < \frac{\pi^2}{4}$ $\left(\frac{2ma^2V_0}{\hbar^2} < \frac{\pi^2}{4}\right)$ No B.S

$$V_0 < \frac{\pi^2\hbar^2}{8ma^2}$$

- if $\frac{\pi}{2} < \lambda < \frac{3\pi}{2}$ one ~~two~~ B.S (G.S)

$$\frac{\pi^2\hbar^2}{8ma^2} < V_0 < \frac{9\pi^2\hbar^2}{8ma^2}$$

- if $\frac{3\pi}{2} < \lambda < \frac{5\pi}{2}$ two B.S

$$\frac{9\pi^2\hbar^2}{8ma^2} < V_0 < \frac{25\pi^2\hbar^2}{8ma^2}$$ and so on