Partial wave analysis for elastic scattering

- first consider the expansion of plane waves $e^{i\vec{k}.\vec{r}}$ in terms of spherical harmonics Y_{lm}. from chapter 6, we found that any plane wave can be expressed as

$$e^{i\vec{k}.\vec{r}} = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} C_{lm}\, \underbrace{j_l(kr)}_{\text{spherical Bessel function}}\, Y_l^m(\theta,\phi)$$

(well behaved function at zero and infinity)

now choosing the $\vec{k}$ in the z-direction, the wave function $e^{i\vec{k}.\vec{r}}$ is rotationally symmetric about this axis. i.e it does not depend on ϕ $\Rightarrow m=0 \Rightarrow Y_l^0 \rightarrow \sqrt{\frac{2l+1}{4\pi}}\, P_l(\cos\theta)$

$$\Rightarrow e^{i\vec{k}.\vec{r}} = \sum_{l=0}^{\infty} a_l\, j_l(kr)\, P_l(\cos\theta) \quad ; \quad a_l = (2l+1)\, i^l$$

$$= \sum_{l=0}^{\infty} (2l+1)\, i^l\, j_l(kr)\, \underbrace{P_l(\cos\theta)}_{\text{legender polynomilas } (m=0)}$$

let us try to decompose this solution into incoming and outgoing sherical waves.

as $r \rightarrow \infty$ $\quad j_l(kr) \approx \frac{\sin(kr - l\pi/2)}{kr} \approx \frac{1}{kr}\left[\frac{e^{i(kr-l\pi/2)} - e^{-i(kr-l\pi/2)}}{2i}\right]$

$$\Rightarrow e^{i\vec{k}.\vec{r}} = e^{ikr\cos\theta} = \sum_l (2l+1)\, i^l\, \frac{1}{kr}\left[\frac{e^{i(kr-l\pi/2)} - e^{-i(kr-l\pi/2)}}{2i}\right] P_l(\cos\theta)$$

$$= \frac{i}{2kr} \sum_l (2l+1)\, i^l \left[e^{-i(kr-l\pi/2)} - e^{i(kr-l\pi/2)}\right] P_l(\cos\theta)$$

$$e^{ikr\cos\theta} = \frac{i}{2kr}\sum_l (2l+1)\, i^l e^{-il\pi/2}\left[e^{il\pi/2} e^{-i(kr - l\pi/2)} - e^{ikr}\right] P_l(\cos\theta)$$

where $e^{-il\pi/2} = \left(e^{-i\pi/2}\right)^l = (-i)^l = \left(\frac{1}{i}\right)^l = \frac{1}{i^l}$

$$\Rightarrow e^{ikr\cos\theta} = \frac{i}{2kr}\sum_l (2l+1)\, P_l(\cos\theta)\left[\underbrace{(-1)^l e^{-ikr}}_{\text{incoming}} - \underbrace{e^{ikr}}_{\text{outgoing}}\right]; \text{ where } \boxed{e^{il\pi} = (-1)^l}$$

Now in the presence of a radial potential $V(r)$, only the phase of the outgoing wave will be modified. This is from flux conservation.

$$\Rightarrow e^{i\vec{k}\cdot\vec{r}} = e^{ikr\cos\theta} = \frac{i}{2kr}\sum_l (2l+1)\, P_l(\cos\theta)\left[(-1)^l e^{-ikr} - S_l(k)\, e^{ikr}\right] \quad (1)$$

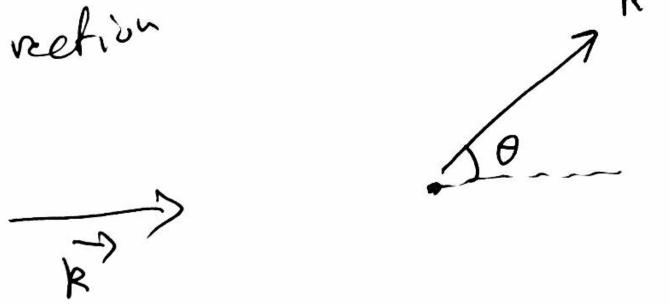
where the standard form of $S_l(k)$ is $e^{2i\delta_l(k)}$

δ_l : phase shift

let us call the last eq^n as eq^n # (1) as I will refere to it later.

- <u>scattering amplitude and phase shift</u>:

consider an incident wave $e^{i\vec{k}\cdot\vec{r}}$ that is being scattered by a central potential $V(r)$. let us choose again the $\vec{k}$ in the z-direction



after the scattering has taken place, the wave function at large r is given by

$$\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + f(\vec{k},\vec{k}')\frac{e^{ikr}}{r} \quad ; \quad f(\vec{k},\vec{k}') = f(\theta,\phi)$$

~~the~~ again both the incident wave and the scattered wave are rotationally symmetric about the z-axis $\Rightarrow$ the scattering amplitude does not depend on ϕ

$$\Rightarrow f(\theta,\phi) = f(\theta) \qquad \text{Azimuthal symmetry}$$

$f(\theta)$ can be expanded into a series of Legendre Polynomials

$$f(\theta) = \sum_{l=0}^{\infty} f_l \,(2l+1)\, P_l(\cos\theta) \quad ; \quad f_l : l^{th} \text{ partial wave amplitude}$$

lot of Physics in this quantity ?!!

$$\therefore \psi(\vec{r}) = \sum_{l=0}^{\infty} (2l+1)\, i^l j_l(kr)\, P_l(\cos\theta) + \frac{e^{ikr}}{r}\sum_{l=0}^{\infty} f_l\,(2l+1)\,P_l(\cos\theta)$$

$$= \sum_{l=0}^{\infty} (2l+1)\,P_l(\cos\theta)\left[i^l j_l(kr) + f_l\frac{e^{ikr}}{r}\right]$$

for large r, $j_l(kr) \approx \dfrac{\sin(kr - l\pi/2)}{kr}$

$$i^l j_l(kr) \approx i^l\frac{\sin(kr - l\pi/2)}{kr} = \frac{i^l}{kr}\,\frac{e^{i(kr-l\pi/2)} - e^{-i(kr-l\pi/2)}}{2i}$$

$$= \frac{i^l}{2i}\underbrace{e^{-il\pi/2}}_{\frac{1}{(i)^l}}\left[e^{ikr} - \underbrace{e^{il\pi}}_{(-1)^l} e^{-ikr}\right]\frac{1}{kr}$$

$$i^l j_l(kr) = \frac{1}{2ikr}\left[e^{ikr} - (-1)^l e^{-ikr}\right]$$

$$= \frac{i}{2kr}\left[(-1)^l e^{-ikr} - e^{ikr}\right]$$

$$\Rightarrow \Psi(\vec{r}) = \sum_{l=0}^{\infty} (2l+1) P_l(\cos\theta)\left[\frac{i}{2kr}\left((-1)^l e^{-ikr} - e^{ikr}\right) + f_l \frac{e^{ikr}}{r}\right]$$

$$= \frac{i}{2kr}\sum_{l=0}^{\infty} (2l+1) P_l(\cos\theta)\left[(-1)^l e^{-ikr} - e^{ikr} - 2ikf_l e^{ikr}\right]$$

$$= \frac{i}{2kr}\sum_{l=0}^{\infty} (2l+1) P_l(\cos\theta)\left[\underbrace{(-1)^l e^{-ikr}}_{\text{incoming}} - \underbrace{(1+2ikf_l)e^{ikr}}_{\text{outgoing}}\right]$$

comparing this eq^n with eq^n (1), both solution must have the same scattering amplitude where

$$\Rightarrow S_l(k) = e^{2i\delta_l} = 1 + 2ikf_l \;;$$

δ_l : phase shift which is the phase difference between incident and scattered waves

subject to $|S_l| = 1$

Notice that $\delta_l = 0$, when the potential is absent.

$$\Rightarrow e^{2i\delta_l} = 1 + 2ikf_l \Rightarrow f_l = \frac{e^{2i\delta_l} - 1}{2ik} = e^{i\delta_l}\frac{(e^{i\delta_l} - e^{-i\delta_l})}{2ik}$$

$$= \frac{1}{k} e^{i\delta_l} \sin\delta_l$$

$$\Rightarrow f(\theta) = \sum_l (2l+1)\frac{e^{i\delta_l}\sin\delta_l}{k} P_l(\cos\theta)$$

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = ff^*$$

$$\frac{d\sigma}{d\Omega} = \sum_{l,l'} (2l+1)(2l'+1)\, P_l(\cos\theta)\, P_{l'}(\cos\theta)\, f_l f_{l'}^*$$

$$\sigma = \int \frac{d\sigma}{d\Omega}\, d\Omega = \sum_{l,l'} (2l+1)(2l'+1)\, f_l f_{l'}^* \underbrace{\int d\Omega\, P_l(\cos\theta)\, P_{l'}(\cos\theta)}$$

$$2\pi \int \sin\theta\, d\theta\, P_l P_{l'}$$

let $x = \cos\theta$

$dx = -\sin\theta\, d\theta$

$$-2\pi \int_1^{-1} dx\, P_l P_{l'}$$

$$2\pi \int_{-1}^{1} dx\, P_l P_{l'}$$

$$2\pi \; \frac{2}{2l+1}\, \delta_{ll'}$$

$$= 4\pi \sum_l (2l+1)^2 \frac{|f|^2}{(2l+1)}$$

$$= 4\pi \sum_l (2l+1) |f_l|^2$$

$$= \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2\delta_l \quad ; \quad \sin\delta_l \leq 1$$

$\Rightarrow$ Notice that σ_{max} occurs when $\delta_l = \pi/2$ for l^{th} partial wave

$$\sigma_l^{max} = \frac{4\pi}{k^2}(2l+1) \quad \text{called resonance scattering}$$

- for forward scattering $(\theta \approx 0)$; $P_l(0) = 1$

$\{ P_0(x) = 1 \,;\, P_1(x) = x$
$P_2(x) = \frac{1}{2}(3x^2 - 1), \ldots$

$$f(\theta \to 0) = \sum_l (2l+1)\, \frac{e^{i\delta_l} \sin\delta_l}{k}$$

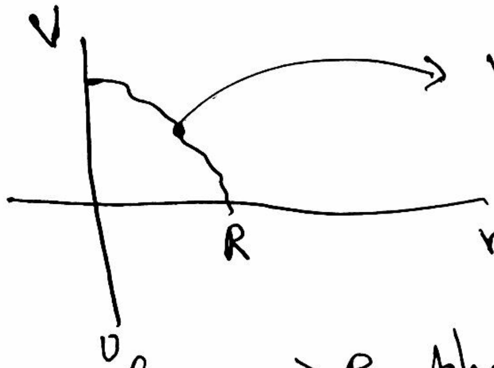
$$\operatorname{Im} f(\theta \to 0) = \frac{1}{k} \sum_l (2l+1) \sin^2\delta_l \geq 0 \quad \text{always}$$

compare with σ

$$\sigma = \frac{4\pi}{k} \operatorname{Im} f(0) \quad \text{called optical theory}$$

We see that the whole theory of scattering is reduced to the problem of calculating the phase shift δ_ℓ. once δ_ℓ is found, the scattering amplitude and the cross section can be calculated.

- to demonstrate the idea of calculating phase shift, consider the scattering of a wave from a finite range potential $\underline{\underline{R}}$, such that for $r>R$, we have free motion



need to match the log derivatives at the boundary $r=R$

now for $r>R$, the radial wave function $R_\ell(r)$ is a linear combination of $j_\ell(kr)$ and $n_\ell(kr)$

$$R_\ell(r) = A_\ell\, j_\ell(kr) + B_\ell\, n_\ell(r) \quad \text{------} \quad (*)$$

as $r \to \infty \Rightarrow R_\ell(r) \simeq A_\ell \dfrac{\sin(kr - \ell\pi/2)}{kr} - B_\ell \dfrac{\cos(kr - \ell\pi/2)}{kr}$

this however can be written as

$$R_\ell(r) \approx \frac{\sin(kr - \ell\pi/2 + \delta)}{kr} \quad ; \quad \delta: \text{ phase shift}$$

proof: $R_\ell(r) \approx \dfrac{1}{kr}\left[\sin(kr - \ell\pi/2)\cos\delta_\ell + \sin\delta_\ell \cos(kr - \ell\pi/2)\right]$

$$\approx \cos\delta_\ell \frac{\sin(kr - \ell\pi/2)}{kr} + \sin\delta_\ell \frac{\cos(kr - \ell\pi/2)}{kr}$$

$$\approx \cos\delta_\ell\, j_\ell(kr) - \sin\delta_\ell\, n_\ell(kr)$$

Comparing this with eq^n (*) we found $A_\ell = \cos\delta_\ell$
$B_\ell = -\sin\delta_\ell$

$\therefore\ R_\ell(r) = \cos\delta_\ell\, j_\ell - \sin\delta_\ell\, n_\ell$; δ_ℓ : phase shif

notice that in the absence of $V(r)$ (i.e $V(r)=0$), $\delta_\ell = 0$

the $R_\ell(r) = j_\ell(kr)$ which is finite at $r=0,\infty$

so it sounds that δ_ℓ measures the degree to which $R_n(r)$

differs from $j_\ell(kr)$ at $r \to \infty$.

so outside the potential range $r > R$, we have

$$R_\ell(r) = \cos\delta_\ell\, j_\ell - \sin\delta_\ell\, n_\ell \quad \text{---} \quad (**)$$

Now matching the Log derivatives at $r=R$, gives

$$\left(\frac{R_\ell'}{R_\ell}\right)_{out} = \underbrace{\left(\frac{R_\ell'}{R_\ell}\right)_{inside}}_{\lambda_\ell} \Rightarrow \left(\frac{R_\ell'}{R_\ell}\right)_{out} = \lambda_\ell$$

take the regular solution only

Now using $\frac{d}{dr} j_\ell(kr) = k j_\ell'$ and $\frac{d}{dr}(n_\ell(kr)) = k n_\ell'$

$$\Rightarrow k \left.\frac{(\cos\delta_\ell\, j_\ell' - \sin\delta_\ell\, n_\ell')}{(\cos\delta_\ell\, j_\ell - \sin\delta_\ell\, n_\ell)}\right|_{r=R} = \lambda_\ell$$

$$k\,\frac{(j_\ell' - \tan\delta_\ell\, n_\ell')}{j_\ell - \tan\delta_\ell\, n_\ell} = \lambda_\ell$$

solving for $\tan\delta_\ell \Rightarrow$ $$\tan\delta_\ell = \frac{k j_\ell' - \lambda_\ell j_\ell}{k n_\ell' - \lambda_\ell n_\ell} \quad \ldots (***)$$

to check the last result, take the case of $V(r) = 0$

$\Rightarrow R_\ell(\text{inside}) = j_\ell(kr)$

$\Rightarrow \lambda_\ell = k \dfrac{j_\ell'}{j_\ell}$ $\Rightarrow$ subsitute this into (xxx)

$$\Rightarrow \tan\delta_\ell = \frac{k j_\ell' - k \frac{j_\ell'}{\cancel{j_\ell}} \cancel{j_\ell}}{k n_\ell' - k \frac{j_\ell'}{j_\ell} n_\ell} = \frac{k j_\ell' - k j_\ell'}{k n_\ell' - \frac{j_\ell'}{j_\ell} n_\ell} = 0$$

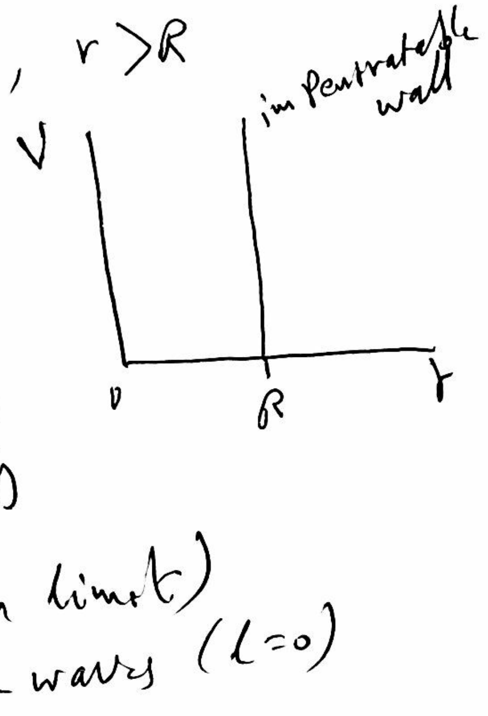
$\Rightarrow \delta_\ell = 0 \Rightarrow$ No Potential.

(No phase) $\Rightarrow$ No potential present

<u>Example 1</u> consider the scattering of a particle of mass m from a hard sphere potential

$$V(r) = \begin{cases} \infty, & r < R \\ 0, & r > R \end{cases}$$

$R(\text{inside}) = 0$



$$\Rightarrow \lambda_\ell = \left(\frac{R'}{R}\right)_{\text{inside}} = \frac{\overset{\text{not zero}}{R'}}{0} \longrightarrow \infty$$

$$\Rightarrow \tan\delta_\ell \approx \left.\frac{j_\ell(kr)}{n_\ell(kr)}\right|_{r=R} = \frac{j_\ell(kR)}{n_\ell(kR)}$$

c) Low energy limit (long wave length limit)

here scattering is dominated by s-waves ($\ell = 0$)

$$\tan\delta_0 = \frac{j_0(kR)}{n_0(kR)} = \frac{\sin(kR)/kR}{-\cos(kR)/kR} = -\tan(kR)$$

$\Rightarrow \delta_0 = -kR$ this is the lowest value of the phase shift. it is negative as it should be for repulsive potential the scattering amplitude is

$$f(\theta) = f_l = f_0 = \frac{1}{k} e^{i\delta_0} \sin\delta_0 = -\frac{1}{k} e^{-ikR} \sin(kR)$$

$$\frac{d\sigma}{d\Omega} = |f_0|^2 = \frac{\sin^2(kR)}{k^2} \Rightarrow \sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \frac{4\pi}{k^2} \sin^2(kR)$$

for low energies $kR \ll 1 \Rightarrow \sigma = \frac{4\pi}{\cancel{k^2}} \cancel{k^2} R^2 = 4\pi R^2$

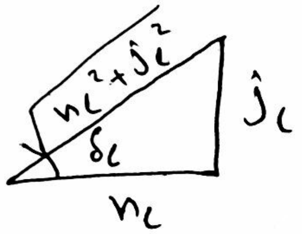
recall that for classical hard sphere $\sigma = \pi R^2$

long wavelength waves encloses the spherical potential from all sides.

c(i) high energy limit (short wave length limit)

now we have $\tan\delta_l = \frac{j_l(kR)}{n_l(kR)}$

we also know $\sigma = \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2\delta_l$



$$= \frac{4\pi}{k^2} \sum_l (2l+1) \frac{j_l^2(kR)}{j_l^2(kR) + n_l^2(kR)}$$

for $kR \gg 1 \Rightarrow j_l \sim \frac{\sin(kR - l\pi/2)}{kR}$.

$$n_l \sim -\frac{\cos(kR - l\pi/2)}{kR}$$

$$\Rightarrow \sigma \approx \frac{4\pi}{k^2} \sum_{l=0}^{l_{max}} (2l+1) \underbrace{\sin^2(kR - l\pi/2)}_{\text{oscillating fast}}$$

so take its average $= 1/2$

what is l_{max} ? $\Rightarrow$ Recall that $mvR = l\hbar$

$$l_{max} = \frac{mvR}{\hbar} = \frac{p}{\hbar} R = kR$$

$$\Rightarrow \sigma \approx \frac{4\pi}{k^2}\frac{1}{2}\sum_{l=0}^{kR}(2l+1) \underset{\text{for large } l}{\approx} \frac{4\pi}{k^2}\frac{1}{2}\sum 2l$$

$$\approx \frac{2\pi}{k^2}\int_0^{kR} dl\,(2l) = \frac{2\pi}{k^2}(kR)^2 = 2\pi R^2$$

twice the classical result

meaning that short wave lengths scatter from one half (face) of the sphere.

Notice that a typical wave functions for the hard sphere problem can be written as $u(r) = rR(r)$

where $u(r) = \begin{cases} 0, & r<R \\ A\sin(kr+\delta_0), & r>R \end{cases}$, one find

so from the contineouty of u at $r=R$,

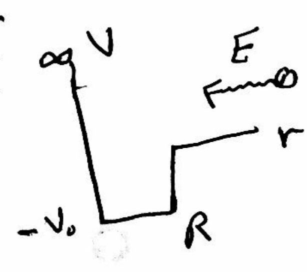
$\sin(kR+\delta_0) = 0 \Rightarrow kR+\delta_0 = 0 \Rightarrow \boxed{\delta_0 = -kR}$ as expected.

Example 2: consider the low-energy scattering by a spherical potential well $V(r) = \begin{cases} -V_0, & r<R \\ 0, & r>R \end{cases}$

the radial eq^n reads

for $r>R$,

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



for low energy, the s-waves scattering dominate ($l=0$)

$$\Rightarrow \frac{d^2 U_l}{dr^2} + k^2 U_l = 0 \Rightarrow \quad U_0 = A\sin(kr + \delta_0)$$

Recall that this is a combination of $\sin kr$ and $\cos kr$

$U_0 \sim A\{\sin kr \cos\delta_0 + \cos kr \sin\delta_0\}$

now for $r < R$

$$\frac{d^2 U_l}{dr^2} + \left[k'^2 - \frac{l(l+1)}{r^2}\right] U_l = 0, \quad k'^2 = \frac{2m}{\hbar^2}(E - (-V_0))$$

$$= \frac{2m}{\hbar^2}(E + V_0) \;;\; E > 0$$

$$\frac{d^2 U_l}{dr^2} + k'^2 U_l = 0$$

for $l = 0$, $\frac{d^2 U_0}{dr^2} + k'^2 U_0 = 0, \Rightarrow$

$\Rightarrow U_0(r) = B\sin k'r + C\cos k'r$, when $U_0(0)$ must vanish $\Rightarrow C = 0$

$= B\sin k'r$

matching the log derivative at $r = R$

$$\left. k\frac{\cos(kr + \delta_0)}{\sin(kr + \delta_0)}\right|_{r=R} = \left. k'\frac{\cos k'r}{\sin k'r}\right|_{r=R}$$

$$\Rightarrow \frac{1}{k}\tan(kR + \delta_0) = \frac{1}{k'}\tan(k'R)$$

at low energy $\tan(kR + \delta_0) \approx kR + \delta_0$

and $\tan(k'R) = k'R + \frac{1}{3}k'^3R^3$, where $\tan x = x + \frac{1}{3}x^3 + \ldots$

$$\Rightarrow \cancel{kR} + \delta_0 = \frac{k}{k'}\left(k'R + \frac{1}{3}k'^3R^3\right)$$

$$= \cancel{kR} + \frac{1}{3}kk'^2R^3$$

$\Rightarrow \delta = \frac{1}{3}kk'^2R^3$ which is Positive as expected for negative attractive potential

$$\sigma_T = \frac{4\pi}{k^2}\sin^2\delta_0 \approx \frac{4\pi}{k^2}\delta_0^2$$

$$\approx \frac{4\pi}{\cancel{k^2}}\frac{1}{9}\cancel{k^2}k'^4R^6 = \frac{4\pi}{9}k'^4R^6$$

$$\approx \frac{4\pi}{9}\frac{4m^2}{\hbar^4}(E+V_0)^2R^6 \quad ; \quad E \ll V_0$$

$$\approx \frac{16\pi}{9}\frac{m^2V_0^2}{\hbar^4}R^6$$

now for very deep well $V_0 \to \infty$, we have

$$\frac{1}{k}\tan(kR+\delta_0) = \frac{1}{k'}\tan(k'R)$$

$$\frac{1}{k}(kR+\delta_0) = \frac{1}{k'}\left(-i\left(\frac{e^{ik'R}-e^{-ik'R}}{e^{ik'R}-e^{-ik'R}}\right)\right) \approx -i$$

for deep well using $\tan x = -i\dfrac{e^{ix}-e^{-ix}}{e^{ix}-e^{-ix}}$

now

$$(k'R)^2 = \frac{2m}{\hbar^2}(E+V_0)R^2 \longrightarrow \infty$$

$$\Rightarrow e^{-ik'R} \longrightarrow 0$$

$$\Rightarrow \frac{1}{k}(kR+\delta_0) = \frac{-i}{k'} \Rightarrow kR+\delta_0 = \frac{k}{k'}(-i)$$

but $k' \gg k$ for deep well $\Rightarrow \dfrac{k}{k'} \to 0$

$$\Rightarrow kR+\delta_0 = 0 \Rightarrow \delta_0 = -kR$$

this result is similar to hard sphere scattering with $\sigma = 4\pi R^2$