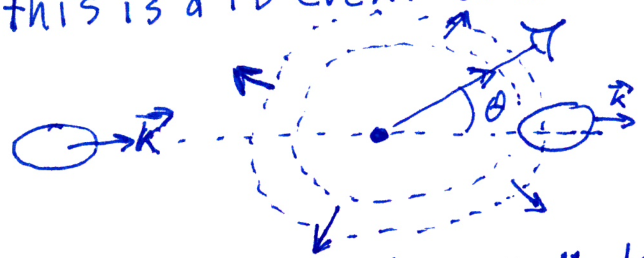
Quantum scattering in 3D: scattering of a single spinless particle in a central field $V(\vec{r}) = V(r)$

- this is a TD event so we're sending wavepackets towards the target



$$\psi(\vec{r},t) = \int d^3k\, \underbrace{\phi(\vec{k})}_{\text{sharply peaked around some } \vec{k}_0} \psi^{(+)}_{\vec{k}}(\vec{r}) \cdot e^{-iE_k t}$$

- more on scattering of wavepackets next time

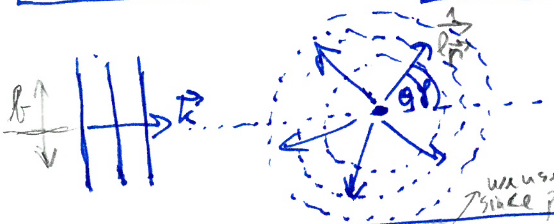
- since the wp. has a well-defined momentum we only focus on $\psi^{(+)}_{\vec{k}}(\vec{r})$:

$$\boxed{H\psi^{(+)}_{\vec{k}} = E_k \psi^{(+)}_{\vec{k}} + \text{b.c.}}$$

- by analogy with the 1D case the physical sol. is defined:

$$\boxed{\psi_{\vec{k}} \underset{r\to\infty}{\sim} \underbrace{e^{i\vec{k}\cdot\vec{r}}}_{\text{incoming wave}} + \underbrace{f(\theta,\varphi)}_{\text{scattering ampl.}} \cdot \underbrace{\frac{e^{ikr}}{r}}_{\text{outgoing sph. wave}}}$$

scattering ampl. → dimension of length



- the incoming plane-wave represents all impact parameters, so we can define:

we use flux since particle number is meaningless for plane wave

$$\boxed{\frac{d\sigma}{d\Omega} = \frac{\text{scattered flux / unit solid angle}}{\text{incident flux / unit area}}}$$

we only want the radial outgoing current

" $\rho(\vec{r})\cdot\vec{v}$ " classically (velocity)

- flux is given by current density: $\vec{j}(\vec{r}) = \mathrm{Re}\left[\psi^*(\vec{r})\frac{\vec{p}}{m}\psi(\vec{r})\right] = \frac{\hbar}{2im}\psi^*(\vec{r})\nabla\psi(\vec{r}) + \text{c.c.}$

$$\vec{j}_{inc} = \frac{\hbar\vec{k}}{m}, \quad \vec{j}_{out}(\vec{r}) = \frac{\hbar}{2im} f^*(\theta,\varphi)\frac{e^{-ikr}}{r}\cdot\nabla_{\vec{r}}\left[f(\theta,\varphi)\cdot\frac{e^{ikr}}{r}\right] + \text{c.c} =$$

$$= \frac{\hbar}{2im}|f(\theta,\varphi)|^2 \cdot \frac{e^{-ikr}}{r^2}\cdot\underbrace{\nabla_{\vec{r}}\left[e^{ikr}\right]}_{= ik e^{ikr}\hat{e}_r} + \underbrace{\mathcal{O}\left(\frac{1}{r^3}\right)}_{+\text{c.c.}} = \frac{\hbar k}{m}|f(\theta,\varphi)|^2\frac{\hat{e}_r}{r^2} + \mathcal{O}\left(\frac{1}{r^3}\right)$$

- we need scattered flux at a large distance from the potential going ~~through~~ into the solid angle $d\Omega$:

$$\text{scattered flux} = \lim_{r\to\infty} \vec{j}_{out}(\vec{r})\cdot d\vec{s} = \lim_{r\to\infty}\vec{j}_{out}(\vec{r})\cdot\hat{e}_r r^2 d\Omega = \frac{\hbar k}{m}|f(\theta,\varphi)|^2\cdot d\Omega$$

$\frac{d\sigma}{d\Omega}$ as per definition

$$\rightarrow \boxed{\frac{d\sigma}{d\Omega} = \frac{(\hbar k/m)\cdot|f(\theta,\varphi)|^2}{|\vec{j}_{inc}|} = |f(\theta,\varphi)|^2}$$

- We need to find $\psi^{(+)}_{\vec{k}}(\vec{r})$ fulfilling the b.c. above.
- We will do it first by the method of p.w. expansion.

$$\vec{\nabla} = \frac{\partial}{\partial r}\vec{e}_r + \frac{1}{r}\frac{\partial}{\partial\theta}\vec{e}_\theta + \frac{1}{r\sin(\theta)}\cdot\frac{\partial}{\partial\phi}\vec{e}_\phi$$

(optical theorem: the full flux is: $\vec{j} = \vec{j}_{inc} + \vec{j}_{interference} + \vec{j}_{out} \quad \Big| \oint d\vec{s}, \ r\to\infty$

$$\underbrace{0}_{\text{particle conservation}} = \oint \vec{j}\cdot d\vec{s} = \underbrace{\oint \vec{j}_{inc}\cdot d\vec{s}}_{=0} + \underbrace{\vec{j}_{intert} + \vec{j}_{out}}_{\oint d\vec{s} = 0 \text{ must be}}$$

optical theorem: $\sigma = \frac{4\pi}{k}\mathrm{Im}\left[f(\theta=0)\right]$

Partial wave method:

- analogue of the method ~~m~~ used in 1D
- we seek a basis which we can use to expand the $\psi_{\vec{k}}$ fulfilling the b.c.
- we assume: $V(\vec{r}) = V(r)$ (i.e. radially symmetric)

$\lim_{r\to\infty} r^2 V(\vec{r}) = 0$ (i.e. falls off faster than $1/r^2$)

less singular than r^{-2}

I. $V(r) = \mathcal{O}(r^{-3-\varepsilon})$ $r\to\infty$
II $V(r) = \mathcal{O}(r^{-2+\varepsilon})$ $r\to 0$
III $V(r)$ is continuous, except perhaps at a finite number of discontinuities

- let's use the symmetries of the problem:

$$\left.\begin{array}{l}[\hat{H}, \hat{L}^2] = 0 \\ [\hat{H}, \hat{L}_3] = 0\end{array}\right\} \Rightarrow$$ there exists a basis which simultaneously diagonalizes $\hat{H}, \hat{L}^2, \hat{L}_3$: $H|\phi_{lm}\rangle = E|\phi_{lm}\rangle$, $L^2|\phi_{lm}\rangle = l(l+1)\hbar^2|\phi_{lm}\rangle$, $L_3|\phi_{lm}\rangle = \ldots|\phi_{lm}\rangle$

spherical harmonics: $L^2 Y_{lm}(\Omega) = l(l+1)\hbar^2 Y_{lm}(\Omega)$

$L_3 Y_{lm}(\Omega) = m\hbar \cdot Y_{lm}(\Omega)$

$$\phi_{lm}(\vec{r}) = \frac{u_{lm}(r)}{r}\cdot Y_{lm}(\Omega)$$

all angular momenta contribute (in principle)

$$\boxed{\psi^{(+)}_{\vec{k}}(\vec{r}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} a^{(+)}_{lm}(\vec{k})\cdot\frac{u_l(r)}{r}\cdot Y_{lm}(\Omega)},$$ (i.e. analogue of: $\psi(x) = c_+u_+(x) + c_-u_-(x)$),

where $a^{(+)}_{lm}(\vec{k})$ have to be determined so that: $\psi_{\vec{k}}(\vec{r}) \to e^{i\vec{k}\cdot\vec{r}} + f(\theta,\varphi)\frac{e^{ikr}}{r}$

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + V(r) = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\cdot\frac{\partial}{\partial r}\right) + \frac{\hat{L}^2}{2mr^2} + V(r)$$

- the equation satisfied by $u_l(r)$ is found from the Sch. eq. for $\psi_{\vec{k}}(\vec{r})$: insert the expansion for $\psi_k(\vec{r})$

$\hat{H}\psi_{\vec{k}}(\vec{r}) = E_k\psi_{\vec{k}}(\vec{r})$;

$$\sum_{l'=0}^{\infty}\sum_{m'=-l'}^{l'} a^{(+)}_{l'm'}(\vec{k})\cdot\hat{H}\left[\frac{u_{l'm'}(r)}{r}Y_{l'm'}(\Omega)\right] = E_k\cdot\sum_{l''=0}^{\infty}\sum_{m''=-l''}^{l''} a^{(+)}_{l''m''}(\vec{k})\cdot\frac{u_{l''m''}(r)}{r}Y_{l''m''}(\Omega)$$

- now project the equation on sph. harm. $Y_{lm}(\Omega)$:

$$\sum_{l'=0}^{\infty}\sum_{m'=-l'}^{l'} a^{(+)}_{l'm'}(\vec{k})\cdot\left\langle Y_{lm}\left|\hat{H}\right|\frac{u_{l'm'}}{r}Y_{l'm'}\right\rangle = E_k\cdot a^{(+)}_{lm}(\vec{k})$$

$\hookrightarrow Y_{lm}$ diagonalizes $\hat{L}^2$ ~~H~~: $\hat{L}^2 Y_{lm} = l(l+1)\cdot\hbar^2\cdot Y_{lm}(\Omega)$ and

$$\int d\Omega\, Y^*_{lm} Y_{l'm'} = \delta_{ll'}\delta_{mm'}$$

depends only on l (not m) as expected

-

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{l(l+1)\hbar^2}{2mr^2} + V(r)\right]\frac{u_l(r)}{r} = E_k\frac{u_l(r)}{r}$$

$$\boxed{\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \underbrace{\frac{l(l+1)\hbar^2}{2mr^2} + V(r)}_{V_{eff}(r)}\right]u_l(r) = E_k u_l(r)}$$

$$V_{eff}(r) = V(r) + \frac{l(l+1)\cdot\hbar^2}{2mr^2}$$ (effective potential like in the classical case)

- expansion into spherical harmonics can be used also for non-spherical problems

- rewrite the last eq. mult. by $\left(-\frac{2m}{\hbar^2}\right)$:

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

- let's assume (as before) that $U(r)$ is negligible wrt $\frac{l(l+1)}{r^2}$ for $r>r_0$:

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

- solutions are Riccati-Bessel functions:

$$\hat{j}_l(kr)=kr\,j_l(kr)\longrightarrow\begin{cases} r\to 0: r^{l+1}+\mathcal{O}(r^{l+2}) & \text{regular sol.}\\ r\to+\infty: \sin\left(kr-\frac{l\pi}{2}\right)\end{cases}$$

spherical Bessel and Neumann fns.

$$\hat{n}_l(kr)=-kr\,n_l(kr)\longrightarrow\begin{cases} r\to 0: r^{-l}+\mathcal{O}(r^{-l+1}) & \text{irregular sol.}\\ r\to\infty: \cos\left(kr-\frac{l\pi}{2}\right)\end{cases}$$

real number that can always be expressed as some tan

- at $r>r_0$:

$$u_l(r)=A\,\hat{j}_l(kr)+B\cdot\hat{n}_l(kr)=A\Big[\hat{j}_l(kr)+\underbrace{\frac{B}{A}}_{\equiv\tan[\delta_l]}\hat{n}_l(kr)\Big]=$$

$$=\frac{A}{\cos[\delta_l]}\left[\hat{j}_l(kr)\cos[\delta_l]+\sin[\delta_l]\cdot\hat{n}_l(kr)\right]\sim\hat{j}_l(kr)\cos[\delta_l]+\sin[\delta_l]\hat{n}_l(kr)$$

- asymptotically $(r\to\infty)$: $\hat{j}_l(kr)\to\sin\left(kr-\frac{l\pi}{2}\right)$; $\hat{n}_l(kr)\to\cos\left(kr-\frac{l\pi}{2}\right)$

$$\boxed{u_l(r)\cong\sin\left[kr-\frac{l\pi}{2}+\delta_l\right]}\to\boxed{\text{asymptotic phase-shift}}$$

→ discuss the attractive/repulsive case as in 1D a chain!

Expansion of the physical solution:

$$\psi^{(+)}_{\vec{k}}(\vec{r})=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}a^{(+)}_{lm}(\vec{k})\cdot\frac{u_l(r)}{r}Y_{lm}(\hat{r})$$

we have $u_l(r)\xrightarrow[r\to\infty]{}\sin\left(kr-\frac{l\pi}{2}+\delta_l\right)=\frac{1}{2i}\left[e^{i(kr-\frac{l\pi}{2}+\delta_l)}-e^{-i(kr-\frac{l\pi}{2}+\delta_l)}\right]$

we want $\psi^{(+)}_{\vec{k}}(\vec{r})\xrightarrow{r\to\infty}e^{ikr}+f(\theta,\varphi)\frac{e^{ikr}}{r}$

- task is to find $a^{(+)}_{lm}(\vec{k})$

$$\frac{e^{ix}-e^{-ix}}{2i}$$

$$e^{i\vec{k}\cdot\vec{r}}=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}i^l j_l(kr)\cdot Y^*_{lm}(\hat{k})\cdot Y_{lm}(\hat{r})\xrightarrow{r\to\infty}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}i^l\frac{\sin\left(kr-\frac{l\pi}{2}\right)}{kr}Y^*_{lm}(\hat{k})Y_{lm}(\hat{r})$$

$$=\sum_l\sum_m\frac{i^l}{2ikr}\cdot\left[e^{i(kr-\frac{l\pi}{2})}-e^{-i(kr-\frac{l\pi}{2})}\right]Y^*_{lm}(\hat{k})Y_{lm}(\hat{r})$$

Last time:

- single particle scattering by a central field $V(\vec{r}) = V(r)$
- $H\psi^{(+)}_{\vec{k}}(\vec{r}) = E_k \psi^{(+)}_{\vec{k}}$ with b.c. $\psi^{(+)}_{\vec{k}} \underset{r\to\infty}{\sim} e^{i\vec{k}\cdot\vec{r}} + f(\theta,\varphi)\cdot \frac{e^{ikr}}{r}$

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

- We have found a standing-wave basis for expansion of the physical solution:

$$\psi^{(+)}_{\vec{k}}(\vec{r}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} a^{(+)}_{lm}(\vec{k})\cdot \frac{u_{lm}(kr)}{r} Y_{lm}(\hat{r}),$$ where $u_{lm}(kr)$ is a sol. of:

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

$$U(r) = \frac{2m}{\hbar^2}V(r), \quad k^2 = \frac{2mE}{\hbar^2}.$$

~~spherical symmetry~~

$u_l(kr) \underset{r\to\infty}{\sim} \sin\left[kr - \frac{l\pi}{2} + \delta_l(k)\right]$, $u_{lm}(kr) = u_l(kr)$ due to spherical symmetry.

$\delta_l(k)$: asymptotic phase-shift:

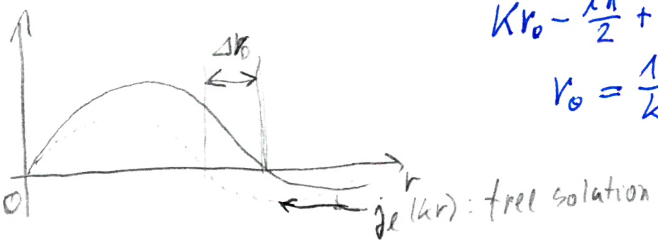
- sign of $\delta_l(k)$ is connected with attractive/repulsive character of the potential:

repulsive potential:

- we expect nodes of $\sin\left[kr - \frac{l\pi}{2} + \delta_l(k)\right]$ to be pushed out:

$$kr_0 - \frac{l\pi}{2} + \delta_l = n\cdot\pi \quad \text{(condition for the nodes)}$$

$$r_0 = \frac{1}{k}\left(n\cdot\pi + \frac{l\pi}{2}\right) - \underbrace{\frac{\delta_l}{k}}_{=\Delta r_0}$$

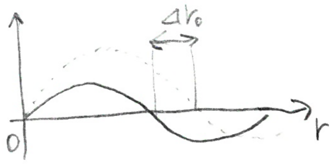


$$\Delta r_0 > 0 \iff -\frac{\delta_l}{k} > 0 \Rightarrow \boxed{\delta_l < 0}$$

attractive potential:

- nodes are pushed to lower r:

$$\Delta r_0 < 0 \iff -\frac{\delta_l}{k} < 0 \Rightarrow \boxed{\delta_l > 0}$$



- However, $\delta_l(k)$ is def. only up to a multiple of π so it seems that the connection is lost!
- We can turn the interaction smoothly on: $U(r) \to \lambda\cdot U(r)$, $\lambda: 0 \to 1$.
- works for all k except $k=0$ and $k=+\infty$.
- Alternatively we can count the number of nodes in the free solution $j_l(kr)$ and in $u_l(kr)$ occuring before the matching radius

Expansion of the physical solution: finding $f(\theta,\varphi)$

$$\psi^{(+)}_{\vec k}(\vec r) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} a^{(+)}_{lm}(\vec k)\cdot\frac{u_l(kr)}{r}\cdot Y_{lm}(\hat r) \underset{r\to\infty}{\sim} e^{i\vec k\cdot\vec r} + f(\theta,\varphi)\cdot\frac{e^{ikr}}{r}$$

~~we~~ task is to find $a^{(+)}_{lm}(\vec k)$: the only term dep. on r is $u_l(kr)$

We know: $u_l(r) \xrightarrow[r\to\infty]{} \sin[kr - \frac{l\pi}{2}+\delta_l(k)] = \frac{1}{2i}\left[e^{i(kr-\frac{l\pi}{2}+\delta_l)} - e^{-i(kr-\frac{l\pi}{2}+\delta_l)}\right]$ $\quad \frac{e^{ix}-e^{-ix}}{2i}$

$$e^{i\vec k\cdot\vec r} = 4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{l} i^l j_l(kr)\cdot Y^*_{lm}(\hat k)\cdot Y_{lm}(\hat r) \xrightarrow{r\to\infty} \sum_{l,m} 4\pi\, i^l\, \frac{\sin(kr-\frac{l\pi}{2})}{kr}\cdot Y^*_{lm}(\hat k)\cdot Y_{lm}(\hat r) =$$

TYPO! missing 4π!

I can choose which one of those to conjg. due to addi[illegible] th. of sph. harmonics: $\sum_m Y^*_{lm}(\hat k)Y_{lm}(\hat r) = (2l+1)P_l(\cos\theta)$

$$= 4\pi\sum_{l,m}\frac{i^l}{2ikr}\left[e^{i(kr-\frac{l\pi}{2})} - e^{-i(kr-\frac{l\pi}{2})}\right]\cdot Y^*_{lm}(\hat k)\cdot Y_{lm}(\hat r)$$

- we find $f(\theta,\varphi)$ by requiring that the difference between $\psi^{(+)}_{\vec k}(\vec r)$ and $e^{i\vec k\cdot\vec r}$ is a purely outgoing wave: $\boxed{\text{we set the incoming sph. wave to zero}}$

$$\psi^{(+)}_{\vec k}(\vec r) - e^{i\vec k\cdot\vec r} \underset{r\to\infty}{\sim} f(\theta,\varphi)\cdot\frac{e^{ikr}}{r}$$ → coefficient mult. the outgoing sph. wave

- incoming sph. wave contr. only:

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left[a^{(+)}_{lm}(\vec k)\cdot\frac{\cancel{u_l(kr)}}{r} + \frac{4\pi i^l}{2ikr}e^{-i(kr-\frac{l\pi}{2})}\cdot Y^*_{lm}(\hat k)\right]\cdot Y_{lm}(\hat r) = \sum_{l,m}\left[a^{(+)}_{lm}(\vec k)\cdot\frac{-e^{-i(kr-\frac{l\pi}{2})}\cdot e^{-i\delta_l}}{2ir} +$$
$$+ \frac{i^l\cdot 4\pi}{2ikr}e^{-i(kr-\frac{l\pi}{2})}\cdot Y^*_{lm}(\hat k)\right]\cdot Y_{lm}(\hat r) \equiv 0$$

$$\Rightarrow [\dots] = 0:\quad \frac{1}{2i}\left[\frac{i^l 4\pi}{k}\cancel{e^{-i(kr-\frac{l\pi}{2})}}\, Y^*_{lm}(\hat k) - a^{(+)}_{lm}(\vec k)\, e^{-i\delta_l}\,\cancel{e^{-i(kr-\frac{l\pi}{2})}}\right] = 0$$

$$\boxed{a^{(+)}_{lm}(\vec k) = \frac{4\pi i^l}{k}\cdot e^{i\delta_l}\, Y^*_{lm}(\hat k)}$$

- to determine $f(\theta,\varphi)$ we insert $a^{(+)}_{lm}(\vec k)$ into expansion of $\psi^{(+)}_{\vec k}(\vec r)$ and look at the asymptotics of the outgoing wave:

$$\left(\psi^{(+)}_{\vec k}(\vec r) - e^{i\vec k\cdot\vec r}\right)_{out} \underset{r\to\infty}{\sim} \sum_{l,m}\left[a^{(+)}_{lm}\,\frac{e^{i\delta_l}\cdot e^{i(kr-\frac{l\pi}{2})}}{2ir\cancel{k}} - \frac{i^l 4\pi}{2ikr}e^{i(kr-\frac{l\pi}{2})}\cdot Y^*_{lm}(\hat k)\right]\cdot Y_{lm}(\hat r) =$$

$$= \frac{e^{ikr}}{r}\cdot\sum_{l,m}\left[\frac{a^{(+)}_{lm}(\vec k)}{2i\cancel{k}}\cdot e^{i\delta_l}e^{-i\frac{l\pi}{2}} - \frac{i^l 4\pi}{2ik}\cdot e^{-i\frac{l\pi}{2}}\cdot Y^*_{lm}(\hat k)\right]\cdot Y_{lm}(\hat r) = \left|e^{-(i\frac{\pi}{2})\cdot l} = (+i)^{-l}\right| =$$

$$= \frac{e^{ikr}}{r}\sum_{l,m}\left[\frac{4\pi}{2i}\cdot\frac{\cancel{i^l}}{k}\cdot e^{i2\delta_l}\, Y^*_{lm}(\hat k)\cdot\cancel{(i)^{-l}} - \frac{4\pi}{2ik}\cdot\cancel{i^l}\cdot\cancel{(i)^{-l}}\, Y^*_{lm}(\hat k)\right]\cdot Y_{lm}(\hat r) =$$

TYPO! missing 4π

$$= \frac{e^{ikr}}{r}\cdot\sum_{l,m}\frac{4\pi}{2ik}\cdot\left[e^{i2\delta_l}\cdot Y^*_{lm}(\hat k) - Y^*_{lm}(\hat k)\right]Y_{lm}(\hat r) = \frac{e^{ikr}}{r}\,\frac{4\pi}{2ik}\sum_{l=0}^{\infty}\left(e^{i2\delta_l}-1\right)\underbrace{\sum_m Y^*_{lm}(\hat k)\,Y_{lm}(\hat r)}_{(2l+1)\cdot P_l(\cos\theta)}$$

angle between $\vec k$ and $\vec r$

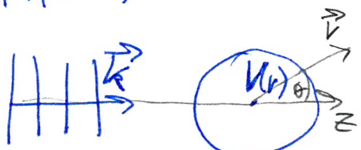
$$= \frac{e^{ikr}}{r}\cdot\frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left(e^{i2\delta_l}-1\right)\cdot P_l(\cos\theta) \Rightarrow f(\theta,\varphi) = \boxed{f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left(e^{i2\delta_l}-1\right)\cdot P_l(\cos\theta)} \quad (2)$$

- another way of writing $f(\theta,\varphi)$ is:

$$f(\theta) = \sum_{l=0}^{\infty} f_l \cdot P_l(\cos\theta), \quad f_l = \frac{1}{2ik}(2l+1)\cdot(e^{i2\delta_l}-1), \text{ where}$$

f_l is the partial wave scattering amplitude

- The form of $f(\theta,\varphi)$ is not surprising for spherical case: I can draw the coordinate axes any way I want so if I choose $\hat{z}\parallel\vec{k}$ I can write immediately



- the amplitude clearly dep. only on the angle between $\vec{k}$ and $\vec{r}$

$$e^{i\vec{k}\cdot\vec{r}} = e^{ikz} = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} i^l j_l(kr)\cdot Y^*_{lm}(\hat{\vec{k}}_z)\cdot Y_{lm}(\hat{\vec{r}}_z) = \sum_{l=0}^{\infty}(2l+1)\, i^l j_l(kr)\cdot P_l(\cos\theta)$$

and $$\psi^{(+)}_{\vec{k}}(\vec{r}) = \sum_{l=0}^{\infty}\frac{u_l(kr)}{r}\cdot P_l(\cos\theta)$$

$a_l^{(+)}(\vec{k})$

- then I'd proceed as before (homework): the usual textbook approach
- the point of the approach shown by me is that it is more general (expansion into spherical harmonics is applicable to non-spherical problems too)

$|\ldots|^2$ this form implies interference of pw amplitudes

Cross-sections:

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \left|\sum_{l=0}^{\infty} f_l\cdot P_l(\cos\theta)\right|^2$$

$$f_l = \frac{1}{2ik}(2l+1)(e^{i2\delta_l}-1)$$

Total cross-section:

$$\sigma(k) = \int d\Omega\left(\frac{d\sigma}{d\Omega}\right) = \int d\Omega\,|f(\theta)|^2 = 2\pi\int_0^{\pi} d\theta\sin\theta\cdot|f(\theta)|^2 = 2\pi\int_0^{\pi} d\theta\sin\theta\left|\sum_{l=0}^{\infty} f_l P_l(\cos\theta)\right|^2 =$$

$$= \frac{\pi}{2k^2}\cdot\sum_{l,l'}(2l+1)\cdot(2l'+1)\cdot\underbrace{(e^{i2\delta_l}-1)}_{e^{i\delta_l}(e^{i\delta_l}-e^{-i\delta_l})}\underbrace{(e^{-2i\delta_l}-1)}_{e^{-i\delta_l}(e^{-i\delta_l}-e^{i\delta_l})}\cdot\underbrace{\int_{-1}^{1}P_l(x)\cdot P_{l'}(x)\,dx}_{\frac{2}{2l+1}\cdot\delta_{l,l'}} = \boxed{\frac{4\pi}{k^2}\cdot\sum_{l=0}^{\infty}(2l+1)\cdot\sin^2(\delta_l)}$$

- unitarity limit since $\sin(\delta_l)\le 1$: $\sigma(k) = \sum_{l=0}^{\infty}\sigma_l(k)$, partial cross-section

$$\sigma_l(k) \le \frac{4\pi}{k^2}\cdot(2l+1)$$

Transformation between bases:

$\pm\pi \Rightarrow$ it only changes sign of $\sin(\cdot)$ $\Rightarrow$ physically irrelevant

we ~~ha~~ used $u_\ell(r) \rightarrow \sin\left[kr - \frac{\ell\pi}{2} + \delta_\ell\right] = \sin\left(kr - \frac{\ell\pi}{2}\right)\cos[\delta_\ell] +$

$+ \sin(\delta_\ell)\cdot\cos\left[kr - \frac{\ell\pi}{2}\right] = \underbrace{\cancel{\cos[\delta_\ell]}}_{\text{not important}}\cdot\left[\sin\left[kr - \frac{\ell\pi}{2}\right] + K_\ell \cdot \cos\left[kr - \frac{\ell\pi}{2}\right]\right]$

– this was the standing-wave basis

$$\boxed{K_\ell = \tan[\delta_\ell]}$$

"K-MATRIX"

– using the exponential form for $\sin(x)$ and $\cos(x)$

$$u_\ell(r) \xrightarrow[r\to\infty]{} \frac{e^{-i\delta_\ell}}{2i}\left[e^{-i\left(kr - \frac{\ell\pi}{2}\right)} - \underbrace{e^{2i\delta_\ell}}_{S_\ell} \cdot e^{i\left(kr - \frac{\ell\pi}{2}\right)}\right]$$

"S-MATRIX"

– this is the spherical wave basis

$$\boxed{S_\ell = \underbrace{T_\ell}_{\text{T-MATRIX}} + 1 = e^{2i\delta_\ell}}$$

– in absence of interaction $\delta_\ell = 0 \Rightarrow S_\ell = 1 \Rightarrow T_\ell = 0$

$\Rightarrow T_\ell$ ~~is~~ represents the actual scattering contribution to the amplitude S_ℓ of finding the particle in a given state after the collision

$$\boxed{S_\ell = \frac{1 + iK_\ell}{1 - iK_\ell}}$$

– "matrices"; in our case they are diagonal due to spherical sym.: $\begin{pmatrix} \ddots & & 0 \\ & \ddots & \\ 0 & & \ddots \end{pmatrix} = S_{\ell,\ell'}$

WHAT TEXT-BOOKS DON'T TELL YOU:

1) ORIENTATIONAL AVERAGING FOR NON-SPHERICAL POTENTIALS

2) INCOHERENT SUMMATION OF AMPLITUDES FOR DIFFERENT IMPACT PARAMETERS

Yesterday:

$$\psi^{(+)}_{\vec{k}} = \sum_{l,m} a^{(+)}_{lm}(\vec{k}) \frac{u_l(r)}{r} Y_{lm}(\Omega_{\vec{r}}) \,, \quad a^{(+)}_{lm}(\vec{k}) = \frac{4\pi i^l}{k} e^{i\delta_l} \cdot Y^*_{lm}(\vec{k})$$

we assumed $u_l(r) \xrightarrow[r\to\infty]{} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right)$

if we wrote $u_l(r) \xrightarrow[r\to\infty]{} A_l(k) \sin\left(kr - \frac{l\pi}{2} + \delta_l\right)$

and $\psi^{(+)}_{\vec{k}} \xrightarrow[r\to\infty]{} A(k)\left(\exp(i\vec{k}\cdot\vec{r}) + f(\theta,\varphi)\cdot\frac{e^{ikr}}{r}\right)$

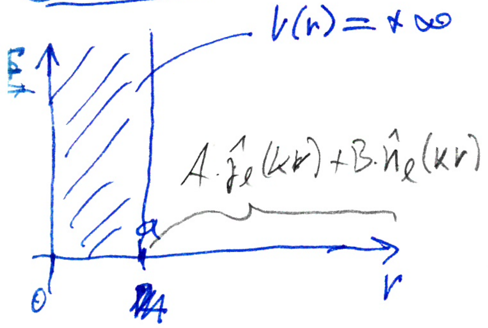
$$\Bigg\} \Rightarrow a^{(+)}_{lm}(\vec{k}) = \frac{A(k)}{A_l(k)} \cdot \frac{4\pi i^l}{k} e^{i\delta_l} \cdot Y^*_{lm}(\vec{k})$$

$$\Rightarrow \psi^{(+)}_{\vec{k}} = A(k) \sum_{l,m} \frac{4\pi i^l}{k} \cdot \frac{u_l(r)}{A_l(k)\, r} \cdot Y_{lm}(\Omega_{\vec{r}}) \xrightarrow[r\to\infty]{} \Big| u_l(r) \to A_l(k) \sin(\ldots) \Big| \Rightarrow$$

$\Rightarrow$ $\underline{A_l(k) \text{ cancel}}$ $\Rightarrow$ the result doesn't depend on normalization of $\underline{u_l(r)}$!

① Hard-sphere scattering: THIS DEMONSTRATES SEVERAL GENERAL PRINCIPLES OF QUANTUM SCATTERING

TUTORIAL 1



Task 1: find δ_ℓ

[- the b.c. $[\psi(r)=0]$ is pushed from $r=0$ to $r=a$ (at $r=a$ $\psi(r)=0$):]

$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + k^2\right]u_\ell(kr) = 0, \quad r>a, \quad k^2 = \frac{2mE}{\hbar^2}$$

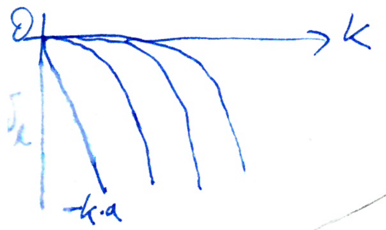
$$A\cdot\Big[\hat{j}_\ell(kr) + \frac{B}{A}\,\hat{n}_\ell(k\cdot r)\Big] \qquad \hat{j}_\ell \to \sin(kr - \tfrac{\ell\pi}{2}),\ \hat{n}_\ell \to \cos[kr - \tfrac{\ell\pi}{2}],\ \frac{B}{A} = \tan[\delta_\ell]$$

$u_\ell(r) = A\cdot\hat{j}_\ell(kr) + B\cdot\hat{n}_\ell(k\cdot r)$, $r>0 \Rightarrow$

- For $r=a$: $\boxed{u_\ell(ka)=0}$ $\iff$ $\displaystyle\frac{B}{A} = -\frac{\hat{j}_\ell(k\cdot a)}{\hat{n}_\ell(k\cdot a)} = \frac{-ka\, j_\ell(k\cdot a)}{-ka\cdot n_\ell(k\cdot a)} = \frac{j_\ell(ka)}{n_\ell(k\cdot a)}$ $\quad \hat{n}_\ell(k\cdot a) \xrightarrow{k\to\infty} \cos[ka - \tfrac{\ell\pi}{2}]$

$$\frac{B}{A} = \tan[\delta_\ell] \Rightarrow \boxed{\delta_\ell = \mathrm{ArcTan}\left[\frac{j_\ell(ka)}{n_\ell(ka)}\right]}$$

Task 2: Plot $\delta_\ell(k)$ for a well with radius $a=1$ and a range of k-values (e.g. $k=[0;\frac{10}{a}]$ and $L_{MAX}=5$) and angular momenta.

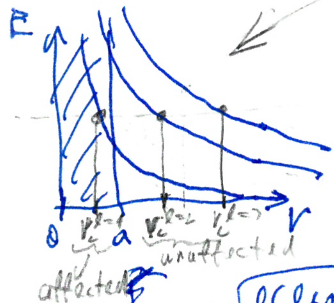


Q_1: What is going on with the phase-shifts at low energies?

A_1: Angular momentum barrier prevents the $u_\ell(r)$ from reaching the region of the hard sphere $(r<a)$: ~~un~~

Q_2: ~~What~~ How do we quantify this effect? (HINT: HOW WOULD WE DO IT CLASSICALLY?)

A_2: We use the classical turning point (below this radius the w.f. decreases exponentially) ↳ i.e. $u_\ell(r)$ behaves like the bound-state solution.



$\to$ determined by: $\boxed{\dfrac{\ell(\ell+1)}{r_c^2} = k^2}$

$$\Rightarrow r_c = \frac{\sqrt{\ell(\ell+1)}}{k} \sim \frac{\ell}{k}$$

$\Rightarrow$ if a is the range of the potential then pw for which $\boxed{ak<\ell}$ contribute significantly to the scattering (see case of $r_c^{\ell=1}$ above) amplitude $f(\theta)$.

~~Q_3: What partial wave~~ Q_3: What determines scattering at low energies $(k\to 0)$?

A_3: The s-wave scattering

Q_4: What is the s-wave phase-shift for hard sphere?

~~A_4: $\frac{B}{A} = \frac{j_\ell(ka)}{n_\ell(ka)} = \frac{ka\, j_\ell(ka)}{-(-ka\cdot n_\ell(ka))} = -\frac{\sin(ka-\frac{\ell\pi}{2})}{\cos(ka-\frac{\ell\pi}{2})} = -\tan(ka-\frac{\ell\pi}{2})$~~

A_4: for $\ell=0$: $\left[\frac{d^2}{dr^2}+k^2\right]u_0(kr)=0,\ r>a \Rightarrow u_0(kr) = A\cdot\underbrace{\sin(kr)}_{\hat{j}_0(kr)} + B\cdot\underbrace{\cos(kr)}_{\hat{n}_0(kr)}$ $\to$ repulsive potential $\Rightarrow \delta_0<0$

$\Rightarrow u_0(ka)=0 \Rightarrow \tan\left[-\frac{\sin(ka)}{\cos(ka)}\right] = \boxed{\delta_0 = -\mathrm{ArcTan}[\tan(ka)] = -ka}$

Q_5: What does the angular distribution look like? What is the cross-section?

A_5:
$$\frac{d\sigma}{d\Omega} = \left|\sum_{l=0}^{\infty} f_l(k)\cdot P_l(\cos\theta)\right|^2 \overset{k\to 0:\text{ only s-wave contr. survives}}{\sim} \left|f_0(k)\cdot \underbrace{P_0(\cos\theta)}_{\text{polyn. of order 0: } 1}\right|^2 = \left|\frac{1}{2ik}\left(\underset{l=0}{2l+1}\right)\left(e^{2i\delta_0}-1\right)\right|^2 =$$

$$= \left|\frac{e^{i\delta_0}\left(e^{i\delta_0} - e^{-i\delta_0}\right)}{2ik}\right|^2 = \frac{\sin^2(-ka)}{k^2} = \frac{\sin^2(ka)\,a^2}{a^2 k^2} \overset{k\to 0}{=} a^2 \Rightarrow \sigma = 4\pi a^2$$

$\left(\frac{\sin(ka)}{ka}\right)^2 a^2$; $\sin(\delta_0)$; can drop it

$\Rightarrow$ the angular distribution is isotropic and 4 times larger than the classical result $\left(\left(\frac{d\sigma}{d\Omega}\right)_{classical} = \frac{1}{4}a^2, \ (\sigma)_{classical} = \pi a^2\right)$

Q_6: Why do we see this difference at low energies?

A_6: The de Broglie wavelength is $\gg a \Rightarrow$ diffraction of the electron wave by a much smaller object.

Threshold behavior of the scattering phase-shifts:

- the s-wave behavior of the hard-sphere scattering is an example of a general principle valid for the short-range potentials ($r^2 V(r)\to 0,\ r\to\infty$), i.e. for potentials decaying faster than any power of r (Yukawa potential)
- we're going to need small-argument expansions of $\hat{j}_l(z)$ and $\hat{n}_l(z)$:

$$\hat{j}_l(z) = \frac{z^{l+1}}{(2l+1)!!} + O(z^{l+3}),\ z\to 0;\quad \hat{n}_l(z) = z^{-l}(2l-1)!! + O(z^{-l+2}),\ z\to 0.$$

- asymptotically (beyond the range) ~~for $r>a$, where a is the range~~ of the potential the radial wf. is the superposition of the free solutions:

$$u_l(kr) \overset{r>a}{\sim} \hat{j}_l(kr) + \tan(\delta_l)\cdot \hat{n}_l(kr)$$ (we need to reach the asymptotic region for finite r, not for $r\to\infty$)

- for low energies $k\to 0$ (and hence also $z=kr\to 0$)

$$u_l(kr) \overset{kr\to 0}{\sim} \frac{(kr)^{l+1}}{(2l+1)!!} + \tan(\delta_l)\cdot\frac{(2l-1)!!}{(kr)^l}.$$

- directly at threshold ($k=0$) the solution must become dependent only on r (up to a constant) ~~it must become proportional to the r-dependent solution~~

$$u_l(kr) \sim \frac{k^{l+1}}{(2l+1)!!}\left(r^{l+1} + \tan(\delta_l)\cdot\frac{(2l+1)!!}{k^{l+1}}\cdot\frac{(2l-1)!!}{k^l}\cdot\frac{1}{r^l}\right)$$ ← we have factorized the r-dependence

$\Rightarrow \tan(\delta_l)$ must compensate the k^{-2l-1} term $\Rightarrow$ $\boxed{\tan(\delta_l) \overset{k\to 0}{\sim} -\frac{(a_l k)^{2l+1}}{(2l+1)!!(2l-1)!!}}$ for convenience

$\Rightarrow$ $\boxed{\tan(\delta_l)\sim k^{2l+1}\ \text{Wigner's threshold law}}$ expresses the suppression of the wf. due to angular momentum barrier

- the proportionality const. a_l is called the partial-wave scattering length $\to [k]=\frac{1}{r} \Rightarrow [a]=r$

~~it has dimension of length only for l=0~~

Q: What is α_0 for hard-sphere?

A: $\tan[\delta_0] = -ka \Rightarrow \underbrace{\alpha_0 = a}_{\text{the radius of the sphere?}}$ (this explains the reason for the $\ominus$ sign in the def. of α_ℓ).

- With the scattering length defined we can write for the asymptotic behavior of the threshold solution: $u_\ell(kr) \sim \frac{(kr)^{\ell+1}}{(2\ell+1)!!} + \tan\delta_\ell \cdot \frac{(2\ell-1)!!}{(kr)^\ell}$

$$u_\ell(r) \overset{r\to\infty}{\sim} r^{\ell+1} - \frac{\alpha_\ell^{2\ell+1}}{r^\ell} \Rightarrow \alpha_\ell \text{ is the zero of the asymptotic behavior of the threshold solution}$$

$$0 = r^{\ell+1} - \frac{\alpha_\ell^{2\ell+1}}{r^\ell} \Rightarrow \boxed{r_0 = \alpha_\ell}$$

if $\alpha_\ell \to 0 \Rightarrow u_\ell(r) \xrightarrow{r\to\infty} r^{\ell+1}$ (i.e. like the regular solution in the absence of the potential: $\tan\delta_\ell \sim \alpha_\ell^{2\ell+1}$)

if $\alpha_\ell \to \infty \Rightarrow u_\ell(r) \overset{r\to\infty}{\Longrightarrow} r^{-\ell}$ (i.e. a normalizable state at $E=0$; i.e. bound state at threshold)

- for s-waves the terminology is not accurate for the case $\alpha_\ell \to \infty$ since:

$u_{\ell=0} \overset{r\to\infty}{\sim} r - a \sim 1 - \frac{r}{a} \Rightarrow a \to \infty \Leftrightarrow$ the solution becomes constant (and not normalizable) but we still call it b.s. at threshold (virtual state)

High energy behavior of hard sphere scattering:

$$\tan[\delta_\ell] = \frac{B}{A} = -\frac{\hat{j}_\ell(ka)}{\hat{n}_\ell(ka)} \xrightarrow{k\to\infty} -\frac{\sin(ka - \frac{\ell\pi}{2})}{\cos(ka - \frac{\ell\pi}{2})} = -\tan(ka - \frac{\ell\pi}{2})$$

$$\Rightarrow \boxed{\delta_\ell = -ka + \frac{\ell\pi}{2}}$$

What is the cross-section?

- we know that at momentum $\underline{k}$ only the PW with $\ell \leq ka$ contribute (i.e. $\underline{a}$ is equal to the classical turning point)

range of the potential

- therefore $\ell_{max} \cong ka$

$$\sigma = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\cdot\sin^2(\delta_\ell) \sim \frac{4\pi}{k^2}\cdot\sum_{\ell=0}^{\ell_{max}}(2\ell+1)\cdot\sin^2(-ka+\frac{\ell\pi}{2}) =$$

$$= \frac{4\pi}{k^2}\cdot\sum_{\ell=0}^{\ell_{max}}\left[\ell\cdot\sin^2(-ka+\frac{\ell\pi}{2}) + (\ell+1)\cdot\sin^2(-ka+\frac{\ell\pi}{2})\right] =$$

$$= \frac{4\pi}{k^2}\cdot\Big[\underbrace{\sin^2(-ka) + \overbrace{\sin^2(-ka+\tfrac{\pi}{2})}^{=\cos^2(-ka+\frac{\pi}{2})}}_{=1} + 2\cdot\left[\sin^2(-ka+\tfrac{\pi}{2}) + \sin^2(-ka+\pi)\right] + 3\cdot[\ldots]$$

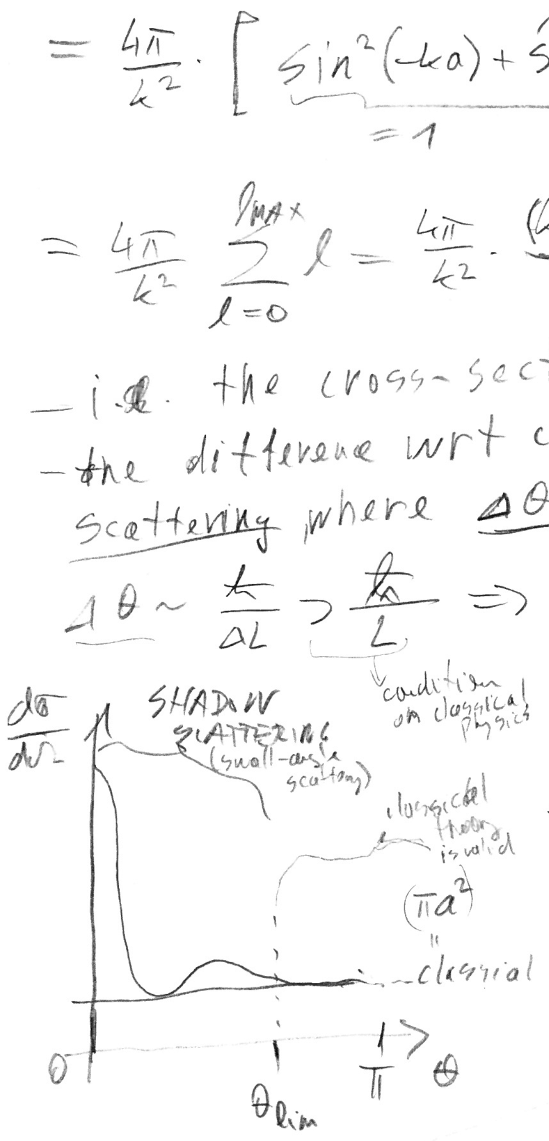
$\ell\cdot\sin^2(\ldots), \ell=1$ $\quad$ $(\ell+1)$, $\ell=1$ $\quad$ $\ell\cdot\sin^2(\ldots), \ell=2$

$$= \frac{4\pi}{k^2}\sum_{\ell=0}^{\ell_{max}}\ell = \frac{4\pi}{k^2}\cdot\frac{(ka+1)\cdot(ka+2)}{2} = \frac{2\pi}{k^2}\left[(ka)^2 + O(ka)\right] \xrightarrow{k\to\infty} \boxed{2\pi a^2}$$

- i.e. the cross-section is twice the classical result!
- the difference wrt classical result (i.e. quantum corrections) is due to small-angle scattering where $\Delta\theta \sim \theta \Rightarrow \boxed{\Delta\theta\Delta L \sim \hbar}$

$$\Delta\theta \sim \frac{\hbar}{\Delta L} > \frac{\hbar}{L} \Rightarrow \theta_{lim} \sim \frac{1}{L} = \frac{1}{mvb} = \frac{1}{k\cdot a} \Rightarrow$$ the peak becomes narrower (and larger)

condition on classical physics $\quad$ in a.u. $\quad$ estimate it as $b=a$ from the classical picture



$\Rightarrow$ hard-sphere scattering total cross section can never be explained classically (EVEN THOUGH $\lambda < a$)

$\Rightarrow$ hard-sphere scattering at high energies behaves unusually since the phase-shifts never go to zero (due to $V\to\infty$, $r<a$). (this is similar to dipolar scattering at all energies (long-range) due to the potential being longer-range than $\frac{1}{r^2}$)

$$\boxed{\Rightarrow \text{for short-range finite potentials } \delta_\ell \xrightarrow{k\to\infty} 0}$$

i.e. small-angle scattering dominates whenever PW-phase shifts for all ℓ are affected

T4

Q_{10}: Plot $\frac{d\sigma}{d\Omega}$ for intermediate k ($a = 1$; $k = 10 \Leftrightarrow$ Childs) and investigate convergence with ℓ ($l_{max} = 15$ is enough)

A_{10}: $L_{MAX} = 15$ is enough

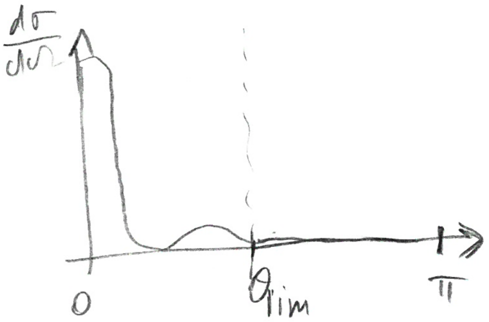
Q_{11}: What is the range of scattering angles for which the classical approximation is valid? What is $\frac{\lambda}{a}$?

A_{11}: It is $\Delta\theta \ll \theta \Rightarrow \boxed{\Delta\theta \cdot \Delta L \sim \hbar}$

$$\Delta\theta \sim \frac{\hbar}{\Delta L} > \frac{\hbar}{L} \Rightarrow \theta_{lim} \sim \frac{1}{L} = \frac{1}{mvb} = \frac{1}{k \cdot a}$$

in atomic units

$\Delta\theta \sim \theta$ is for forward scattering where $b \sim a$ (from classical picture)

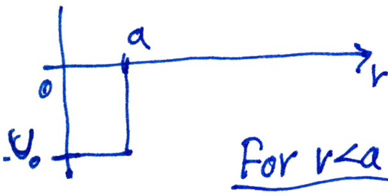


e.g. for ($a = 1$ and $k = \frac{1}{10}$) θ_{lim} is outside of the θ range (i.e. classical scattering is completely invalid)

– examples are low energy electron scattering from atoms and molecules ($\hookrightarrow (E \sim 10^2 eV)$) and ultracold chemistry.

(2) Square well:

$$U(r) = \begin{cases} -U_0 & (U_0 > 0), r < a, \\ 0 & r > a. \end{cases} \quad \left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - U(r) + k^2\right] u_\ell(kr) = 0$$



For $r < a$: $\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + \underbrace{U_0 + k^2}_{\equiv p^2}\right] u_\ell(pr) = 0 \Rightarrow u_\ell(pr) = C \cdot \hat{j}_\ell(pr)$ "$pr \cdot j_\ell(pr)$"

For $r > a$: $U_0 = 0 \Rightarrow u_\ell(kr) = N\left[\hat{j}_\ell(kr) + \tan[\delta_\ell] \cdot \hat{n}_\ell(kr)\right]$ where $\hat{j}_\ell(kr) = kr \cdot j_\ell(kr)$, $\hat{n}_\ell(kr) = -kr \cdot n_\ell(kr)$

match the full radial wf. $\frac{u_\ell}{r}$ to get rid of the $kr\, j_\ell(kr)$

Matching of log-der. at $r = a$: (normalization const. go away)

$$\gamma_\ell = \frac{j_\ell'(pa) \cdot p}{j_\ell(pa)} = \frac{[j_\ell'(ka) - \tan(\delta_\ell) \cdot n_\ell(ka)] \cdot k}{j_\ell(ka) - \tan(\delta_\ell) \cdot n_\ell(ka)}$$

– express $\tan(\delta_\ell)$ using γ_ℓ (the log.-der. at $r = a$):

$$\boxed{\tan(\delta_\ell) = \frac{k j_\ell'(ka) - \gamma_\ell \cdot j_\ell(ka)}{k \cdot n_\ell'(ka) - \gamma_\ell \cdot n_\ell(ka)}}$$

this is a general result even for potentials which are not strictly finite-range but can be "cutoff" at "neglected" $r = a$.

For $\ell = 0$: $j_0(x) = \frac{\sin(x)}{x}$; $n_0(x) = -\frac{\cos(x)}{x}$

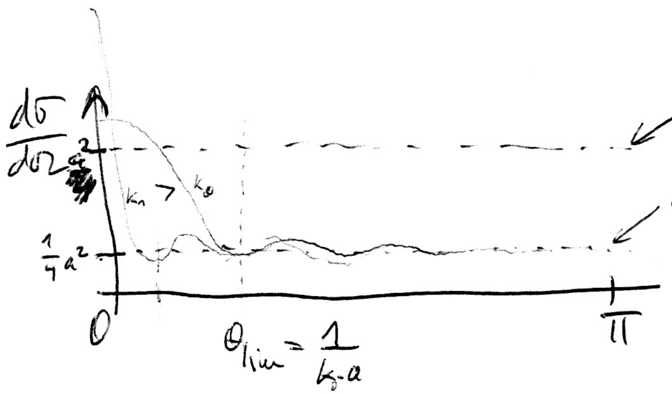
$$\tan\delta_0 = \frac{k \cdot \tan(pa) - p \cdot \tan(ka)}{p + k \cdot \tan(ka) \cdot \tan(pa)}$$

Verify numerically + compute partial cross-section (T5)

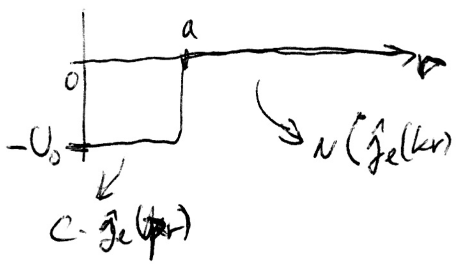
Last week:

examples of scattering: hard-sphere

- low energies $\overset{k \to 0}{}$ (non-classical), $\sigma = 4\pi a^2 = 4 \cdot \sigma_{classical}$
- high energies $\overset{k \to \infty}{}$ (classical for large scattering angles), $\sigma = 2\pi a^2 = 2 \cdot \sigma_{classic}$



today: square well



$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - U(r) + k^2\right] u_\ell(kr) = 0$$

$$U(r) = \begin{cases} -U_0 \ (U_0 > 0), & r \le a \\ 0, & r > a \end{cases}$$

$$\frac{\hat{j}_\ell'(pa)\cdot p}{\hat{j}_\ell(pa)} \equiv \gamma = \frac{\left[\hat{j}_\ell'(ka) + \tan\delta_\ell \cdot \hat{n}_\ell'(ka)\right]\cdot k}{\hat{j}_\ell(ka) + \tan\delta_\ell \, \hat{n}_\ell(ka)}$$

$$\gamma\left(\hat{j}_\ell(ka) + \tan\delta_\ell \, \hat{n}_\ell(ka)\right) = k \cdot \hat{j}_\ell'(ka) + \tan\delta_\ell \cdot k \, \hat{n}_\ell'(ka)$$

$$\tan\delta_\ell \left(+\hat{n}_\ell(ka)\cdot\gamma - k\,\hat{n}_\ell'(ka)\right) = k\,\hat{j}_\ell'(ka) - \gamma \cdot \hat{j}_\ell(ka)$$

$$\boxed{\tan\delta_\ell = \frac{-\gamma \cdot \hat{j}_\ell(ka) + k \cdot \hat{j}_\ell'(ka)}{\gamma \cdot \hat{n}_\ell(ka) - k \cdot \hat{n}_\ell'(ka)}}$$

general result for a short-range potential with radius "a" ... γ_ℓ is the log-derivative of the inner solution

$\ell = 0$: $\hat{j}_\ell = \sin$, $\hat{n}_\ell = \cos$

$$\tan\delta_0 = \frac{-\gamma \cdot \sin(ka) + k \cdot \cos(ka)}{\gamma \cdot \cos(ka) + k\sin(ka)} = \left| \gamma = \frac{\cos(pa)\cdot p}{\sin(pa)} \quad p = \sqrt{U_0 + k^2} \right| =$$

$$= \frac{-\frac{p\cdot\sin(ka)}{\tan(pa)} + k\cdot\cos(ka)}{\frac{\cos(ka)\cdot p}{\tan(pa)} + k\cdot\sin(ka)} = \frac{-p\cdot\tan(ka) + k\cdot\tan(pa)}{p + k\cdot\tan(pa)\cdot\tan(ka)}$$