Select/Special Topics *in*
'Theory of Atomic Collisions and Spectroscopy'

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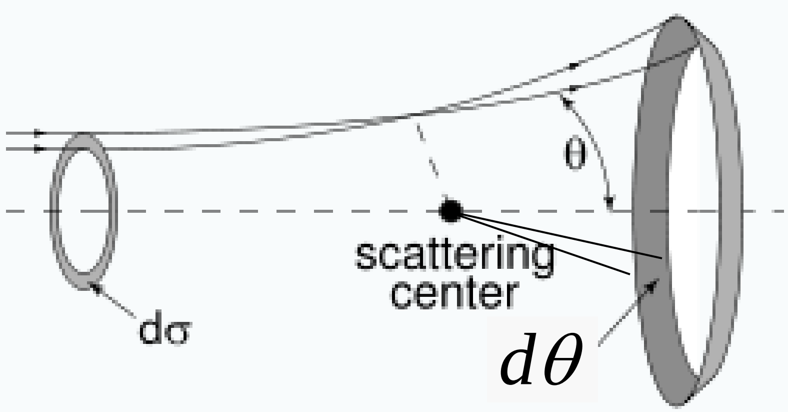
Lecture Number 02

Unit 1: Quantum Theory of Collisions



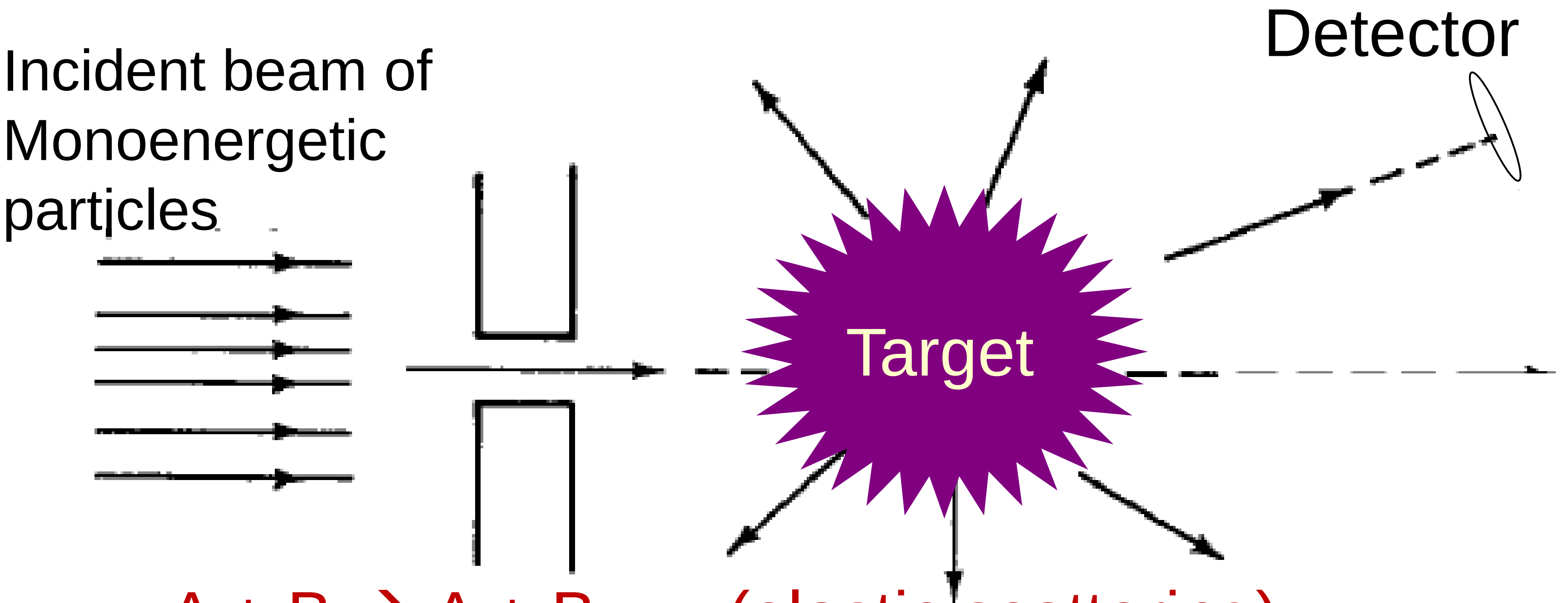
Primary Reference:

Quantum Theory of Collisions (Chapters-1,2,3,4)

by

Charles J Joachain

(North-Holland Publishing Co.)



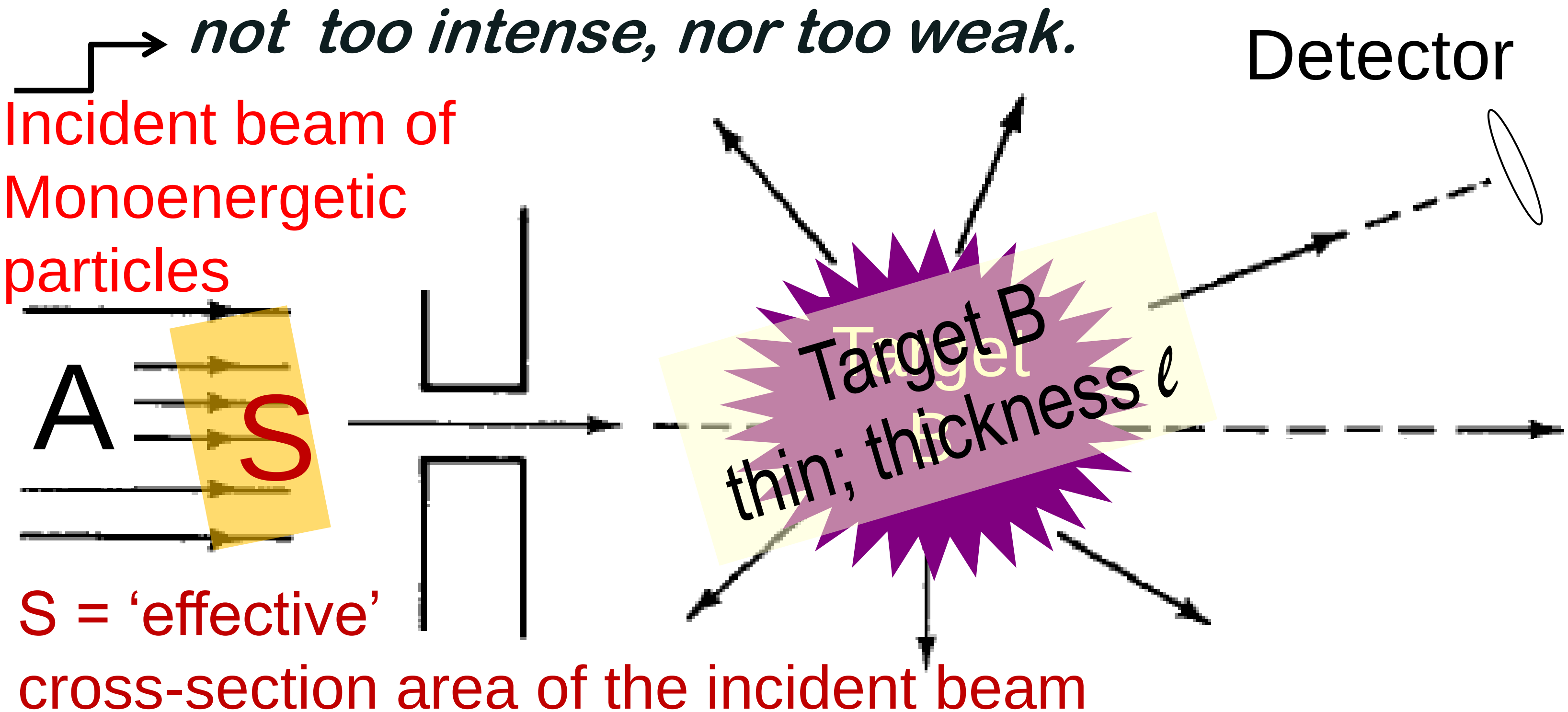
A + B → A + B (elastic scattering)

A + B → A* + B (inelastic scattering)

A + B → A* + B* * denotes new internal state

A + B → C + D ←reactive scattering - rearrangement when colliding particles are composite objects.

"channel" : possible mode of fragmentation pathway

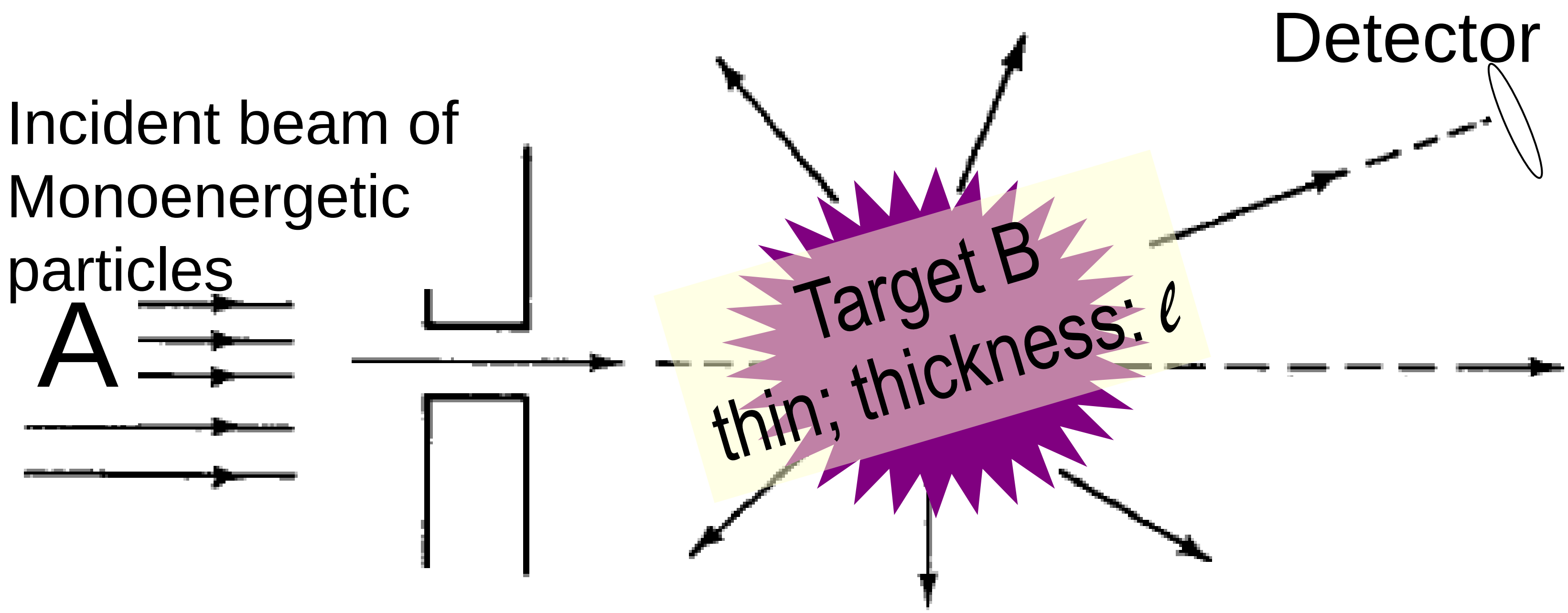


n_B : number of target particles B that intercept the incident beam

N_A : Number of particles A reaching the target per unit time

$\Phi_A =$ Flux of A w.r.t. target B

number of particles A x-ing per unit time per unit area normal to incident beam $(T^{-1})(L^{-2})$



N_A : Number of particles A reaching the target per unit time

N_{Int} : Number of particles A which interact with the target per unit time.

fraction of N_A

$$P \times N_A = N_{Int} \rightarrow T^{-1}$$

P : Probability that an incident particle interacts with the target and thereby gets removed from the incident flux by scattering

$P_{tot} \langle 1$, perhaps $\ll 1$, for thin target

$$N_{Int} = P \times N_A \rightarrow T^{-1}$$

$$\left(T^{-1}\right)\left(L^{-2}\right)$$

$$incident\ flux,\ \Phi_A = \frac{N_A}{S}$$

n_B : number of target particles B that intercept the incident beam

How is N_{Int} related to the target particles B?

$N_{Int} \ \alpha$ → n_B, → Φ_A

$$N_{Int} \ \alpha \ \Phi_A n_B$$

What should be the dimensions of the proportionality?

$$N_{Int} = \sigma_{tot} \times \Phi_A n_B$$

$\left(L^2\right)$

Scattering cross section

effective target area that interacts with the incident beam and scatters it

$$\sigma_{tot} = \frac{P \times N_A}{\Phi_A n_B}$$

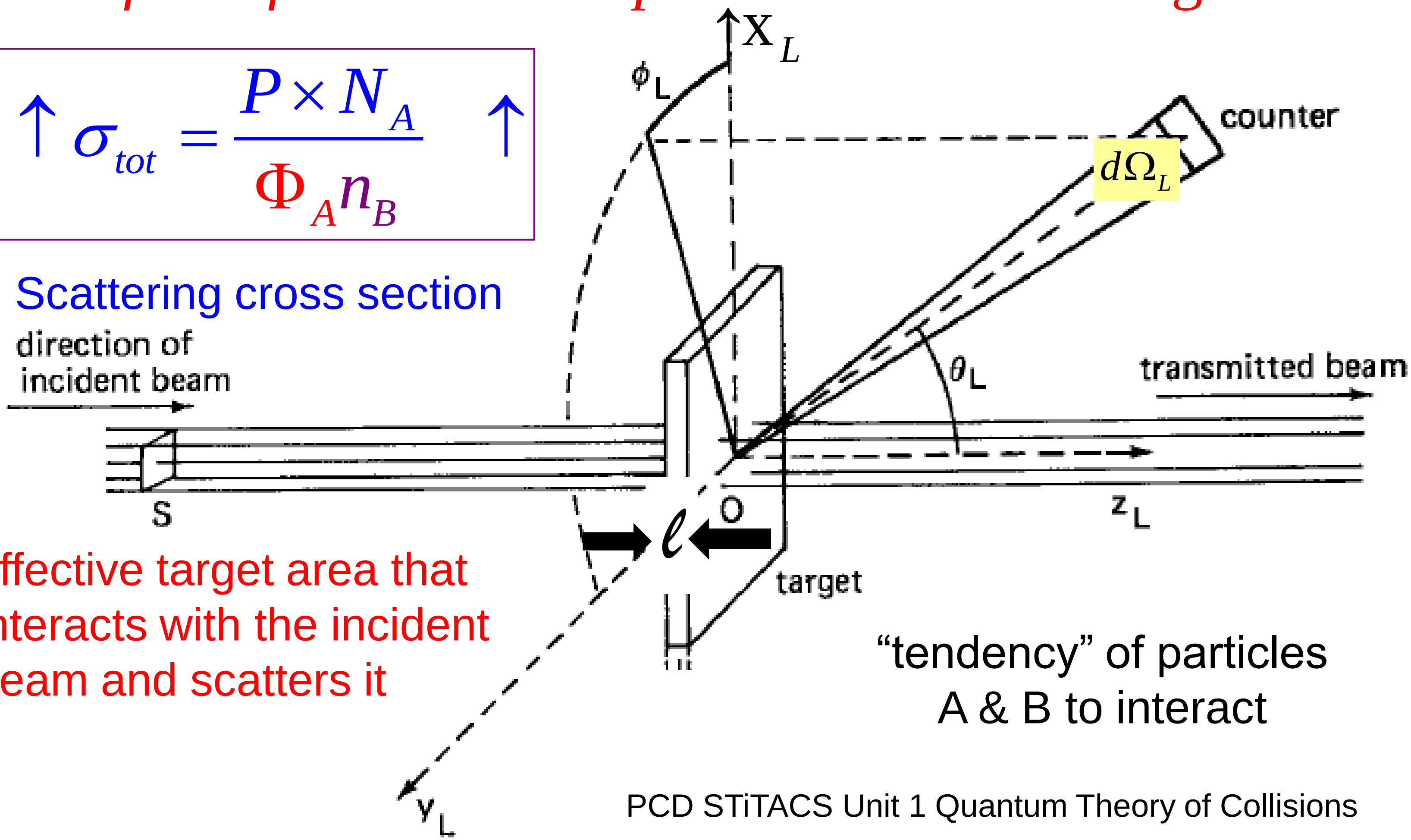
"tendency" of particles A & B to interact cross-section =

$$= \frac{\textit{number of events per unit time per unit scatterer}}{\textit{flux of the incident particles w.r.t. the target}}$$

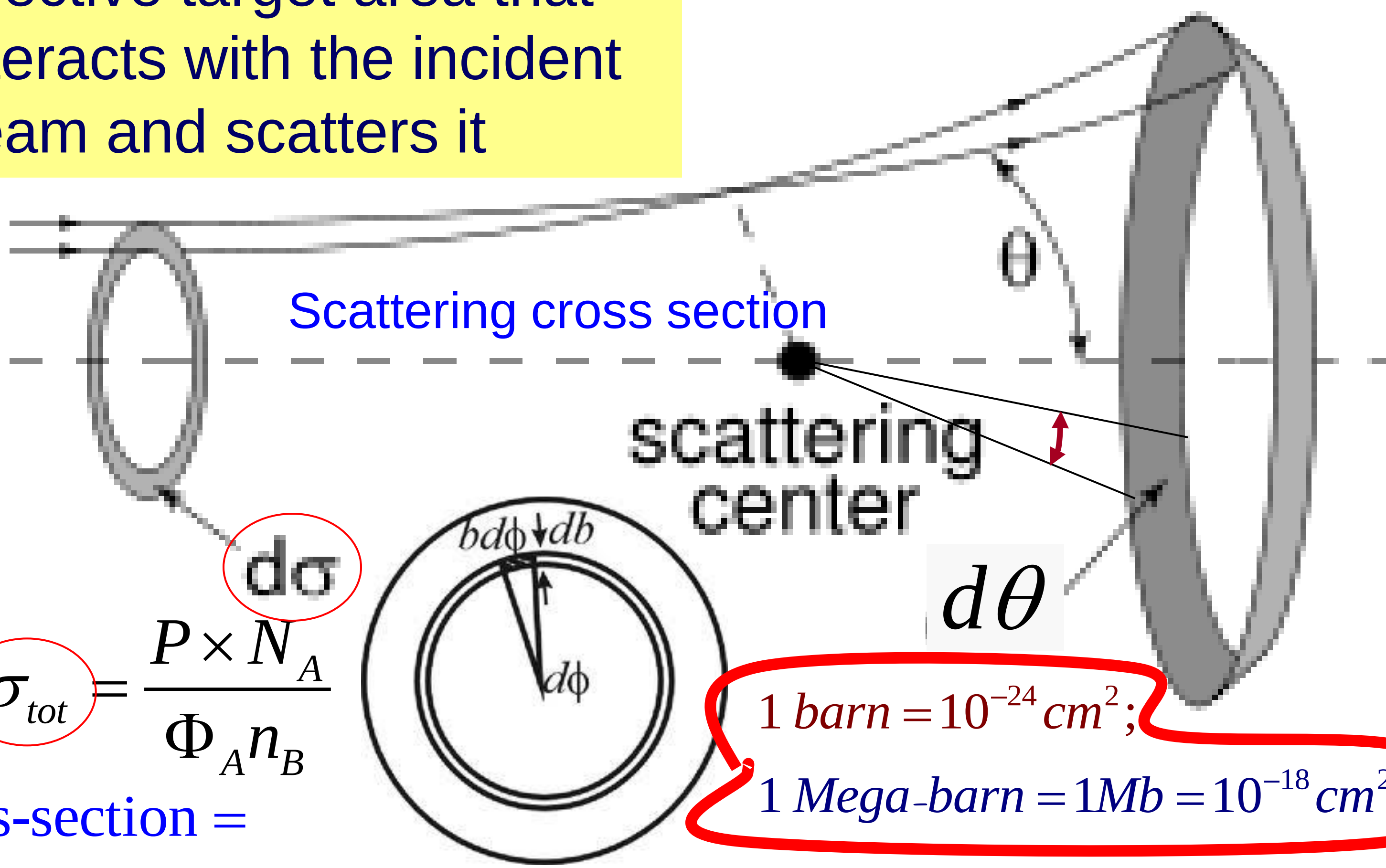
$$\uparrow \sigma_{tot} = \frac{P \times N_A}{\Phi_A n_B} \uparrow$$

Scattering cross section

effective target area that interacts with the incident beam and scatters it



"tendency" of particles A & B to interact effective target area that interacts with the incident beam and scatters it



$$\sigma_{tot} = \frac{P \times N_A}{\Phi_A n_B}$$

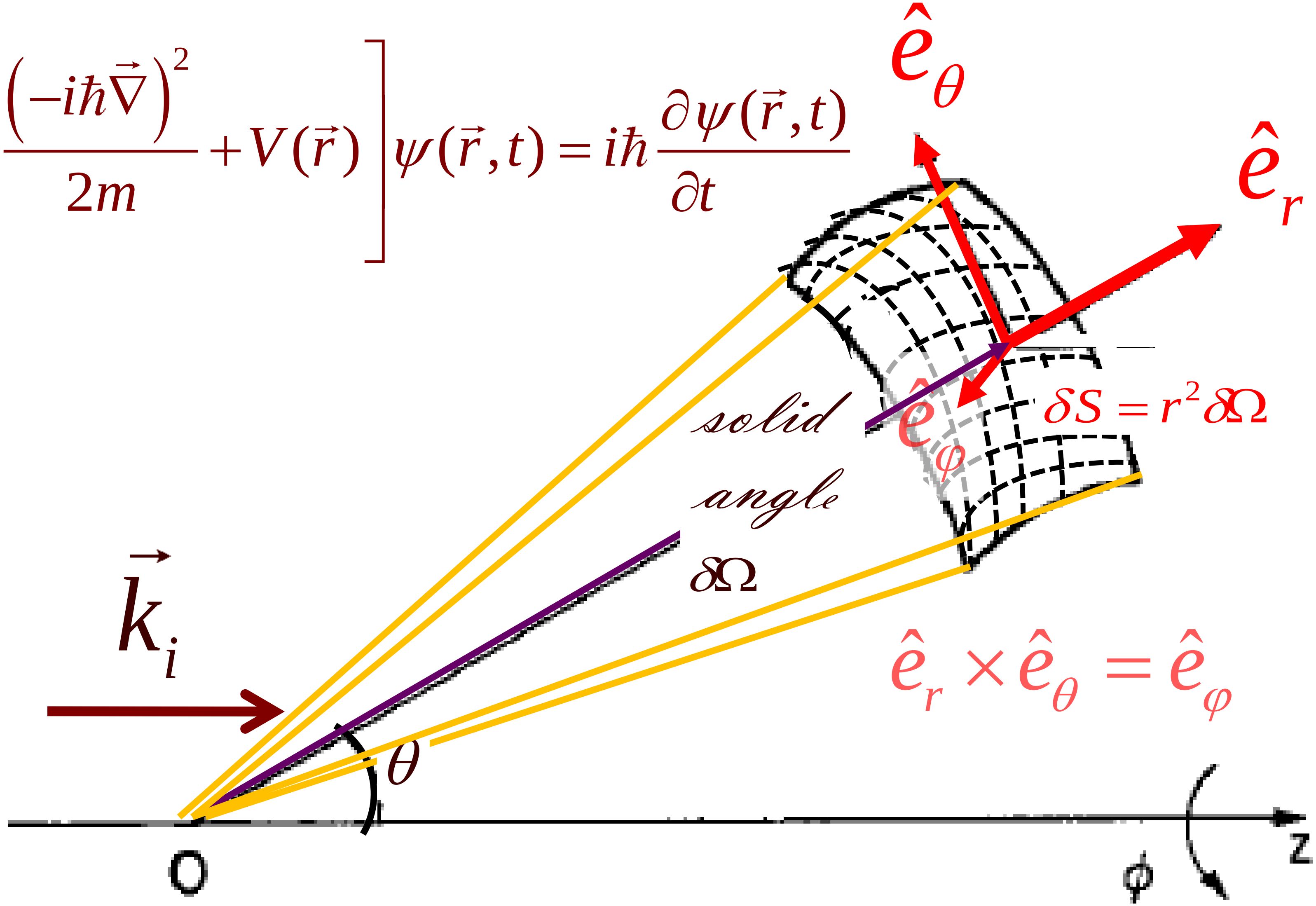
$1\ barn = 10^{-24}\ cm^2;$

$1\ Mega\text{-}barn = 1Mb = 10^{-18}\ cm^2$

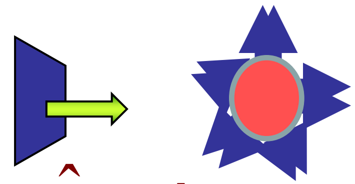
cross-section =

$$= \frac{number\ of\ events\ per\ unit\ time\ per\ unit\ scatterer}{flux\ of\ the\ incident\ particles\ w.r.t.\ the\ \text{target}}$$

$$\left[\frac{\left(-i\hbar\vec{\nabla}\right)^2}{2m}+V(\vec{r})\right]\psi(\vec{r},t)=i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}$$



$$\psi_{\vec{k}_i}(\vec{r}; r \to \infty) \to A\left[e^{i\vec{k}\bullet\vec{r}} + \frac{f(\hat{\Omega})}{r} e^{ikr} \right]$$



$$\hat{k} = \hat{e}_z$$

$$\psi_{inc}(\vec{r}) = e^{i\vec{k}\bullet\vec{r}} = e^{ikr\cos\theta} = e^{i\rho\mu}$$

$$\text{with } \rho = kr \ \& \ \mu = \cos\theta$$

$$e^{i\vec{k}\bullet\vec{r}} = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} c_{l,m} Y_l^m(\hat{r}) j_l(\rho) = \sum_{l=0}^{\infty} a_l P_l(\cos\theta) j_l(\rho)$$

$$e^{i\rho\mu} = \sum_{l=0}^{\infty} a_l P_l(\mu) j_l(\rho)$$

$$a_l = ?$$

$$e^{i\rho\mu} = \sum_{l=0}^{\infty} a_l P_l(\mu) j_l(\rho)$$

$$\int_{-1}^{+1} e^{i\rho\mu} P_{l'}(\mu)\, d\mu = \sum_{l=0}^{\infty} a_l \left[\int_{-1}^{+1} P_l(\mu) P_{l'}(\mu)\, d\mu \right] j_l(\rho)$$

$$= \sum_{l=0}^{\infty} a_l \left[\frac{2}{2l+1} \delta_{l'l} \right] j_l(\rho)$$

$$= a_{l'} \left[\frac{2}{2l'+1} \right] j_{l'}(\rho)$$

Orthogonality of the Legendre polynomials

Dropping the redundant 'prime'

$$\int_{-1}^{+1} e^{i\rho\mu} P_l(\mu)\, d\mu = a_l \left[\frac{2}{2l+1} \right] j_l(\rho)$$

$$\int_{-1}^{+1} e^{i\rho\mu} P_l(\mu)\, d\mu = a_l \left[\frac{2}{2l+1}\right] j_l(\rho)$$

1st 2nd function

$$P_l^{'}(\mu) = \frac{d}{d\mu} P_l(\mu)$$

$$\int_{-1}^{+1} e^{i\rho\mu} P_l(\mu)\, d\mu = \int_{-1}^{+1} P_l(\mu) e^{i\rho\mu} d\mu$$

Integral of a product of two functions

$$= \left[P_l(\mu)\frac{e^{i\rho\mu}}{i\rho}\right]_{-1}^{+1} - \int_{-1}^{+1} P_l^{'}(\mu)\frac{e^{i\rho\mu}}{i\rho} d\mu$$

$$\int_{-1}^{+1} e^{i\rho\mu} P_l(\mu)\, d\mu = \frac{P_l(\mu=1)e^{i\rho}}{i\rho} - \frac{P_l(\mu=-1)e^{-i\rho}}{i\rho}$$

$$-\frac{1}{i\rho}\int_{-1}^{+1} P_l^{'}(\mu) e^{i\rho\mu} d\mu$$

$$P_l(\mu=1) = 1$$

$$P_l(\mu=-1) = (-1)^l P_l(\mu=1) = (-1)^l$$

$$\int_{-1}^{+1} e^{i\rho\mu} P_l(\mu)\, d\mu = \frac{e^{i\rho} - (-1)^l e^{-i\rho}}{i\rho} - \frac{1}{i\rho}\int_{-1}^{+1} P_l^{'}(\mu) e^{i\rho\mu} d\mu$$

$$\int_{-1}^{+1} e^{i\rho\mu} P_l(\mu)\,d\mu = \frac{e^{i\rho} - (-1)^l e^{-i\rho}}{i\rho} - \underbrace{\frac{1}{i\rho}\int_{-1}^{+1} P_l'(\mu) e^{i\rho\mu}\,d\mu}_{O(\rho^2)}$$

ignorable as $\rho \to \infty$

$$\Rightarrow \int_{-1}^{+1} e^{i\rho\mu} P_l(\mu)\,d\mu = \frac{e^{i\rho} - (-1)^l e^{-i\rho}}{i\rho}$$

we had: $\int_{-1}^{+1} e^{i\rho\mu} P_l(\mu)\,d\mu = a_l \left[\frac{2}{2l+1}\right] j_l(\rho)$

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

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

$$a_l \left[\frac{2}{2l+1}\right] j_l(\rho) = \frac{e^{i\rho} - e^{il\pi} e^{-i\rho}}{i\rho}$$

$$a_l\left[\frac{2}{2l+1}\right]j_l(\rho)=\frac{e^{i\rho}-e^{il\pi}e^{-i\rho}}{i\rho}$$

$$a_l\left[\frac{2}{2l+1}\right]j_l(\rho)=\left[\frac{e^{i\rho}-e^{i\frac{l\pi}{2}}e^{i\frac{l\pi}{2}}e^{-i\rho}}{i\rho}\right]$$

$$a_l\left[\frac{2}{2l+1}\right]j_l(\rho)=e^{i\frac{l\pi}{2}}\left[\frac{e^{i\rho}e^{-i\frac{l\pi}{2}}-e^{i\frac{l\pi}{2}}e^{-i\rho}}{i\rho}\right]$$

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

$$=\left(i^2\right)^l=i^{2l}$$

$$e^{i\frac{l\pi}{2}}=\left(e^{i\frac{\pi}{2}}\right)^l=i^l$$

$$a_l\left[\frac{2}{2l+1}\right]j_l(\rho)=i^l\left[\frac{e^{i\left(\rho-\frac{l\pi}{2}\right)}-e^{-i\left(\rho-\frac{l\pi}{2}\right)}}{i\rho}\right]=i^l\left[\frac{2i\sin\left(\rho-\frac{l\pi}{2}\right)}{i\rho}\right]$$

$$a_l\left[\frac{2}{2l+1}\right]j_l(\rho)=i^l\left[\frac{e^{i\left(\rho-\frac{l\pi}{2}\right)}-e^{-i\left(\rho-\frac{l\pi}{2}\right)}}{i\rho}\right]$$

$$a_l\left[\frac{2}{2l+1}\right]j_l(\rho)=i^l\left[\frac{2i\sin\left(\rho-\frac{l\pi}{2}\right)}{i\rho}\right]$$

Now, $$j_l(\rho)\underset{\rho\to\infty}{=}\frac{\sin\left(\rho-\frac{l\pi}{2}\right)}{\rho}\qquad\Rightarrow a_l=i^l\left(2l+1\right)$$

$$e^{i\rho\mu}=\sum_{l=0}^{\infty}a_lP_l\left(\mu\right)j_l(\rho)$$

We got a_l from $\rho\to\infty$, but it is valid for all ρ since $a_l\neq fn(\rho)$.

$$\Rightarrow e^{i\rho\mu}=\sum_{l=0}^{\infty}i^l\left(2l+1\right)P_l\left(\mu\right)j_l(\rho)$$

i.e. $$e^{ikr\cos\theta}=\sum_{l=0}^{\infty}i^l\left(2l+1\right)P_l\left(\cos\theta\right)j_l(kr)$$

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos\theta) j_l(kr)$$

$$\theta = \angle\left(\hat{k}_i, \hat{r}\right)$$

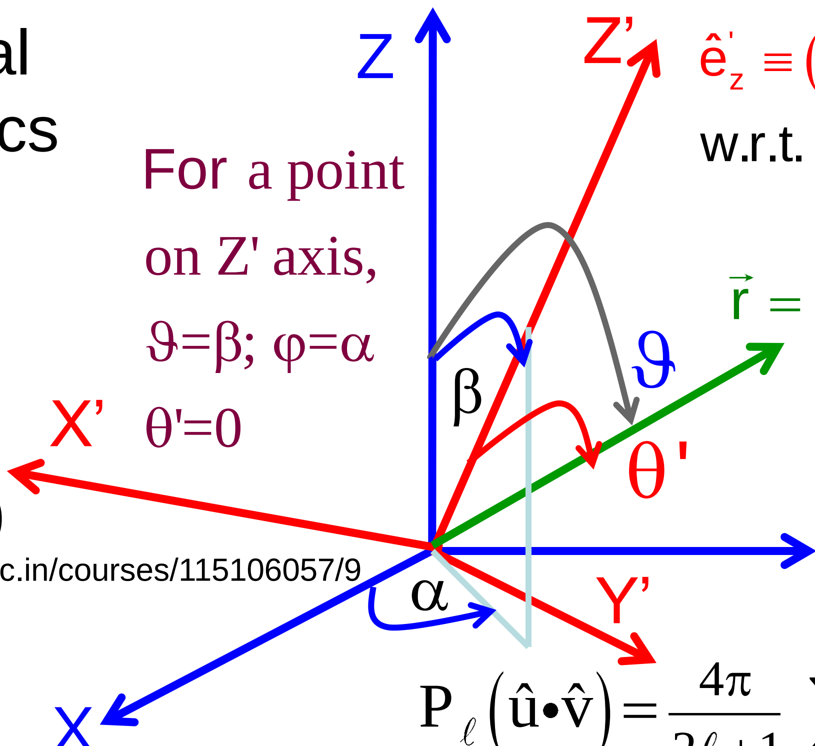
Spherical harmonics addition theorem (Unit 2, STiAP slide 94)

http://nptel.iitm.ac.in/courses/115106057/9

For a point on Z' axis,

$\vartheta=\beta;\ \varphi=\alpha$

$\theta'=0$



$\hat{e}_z^{'} \equiv (\beta,\alpha) \equiv \hat{u}$

w.r.t. (X,Y,Z)

$\hat{r} \equiv (\vartheta,\varphi) \equiv \hat{v}$

$\vec{r} = \vec{r}\,'$

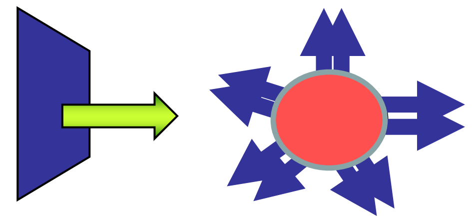
$\hat{r}\,' \equiv (\theta',\varphi') \equiv \hat{v}$

$$\vartheta = \angle\left(\hat{e}_z, \hat{r}\right)$$

$$P_\ell(\hat{u}\bullet\hat{v}) = \frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{\ell} Y^*_{\ell m}(\hat{v}) Y_{\ell m}(\hat{u})$$

$$e^{i\hat{k}_i\bullet\hat{r}} = 4\pi\sum_{l=0}^{\infty} i^l j_l(kr)\left[\sum_{m=-\ell}^{\ell} Y^*_{\ell m}\left(\hat{k}_i\right) Y_{\ell m}\left(\hat{e}_r\right)\right]$$

$$\psi_{\vec{k}_i}(\vec{r}; r \to \infty) \to A\left[e^{\vec{k}\bullet\vec{r}} + \frac{f(\hat{\Omega})}{r} e^{ikr} \right]$$



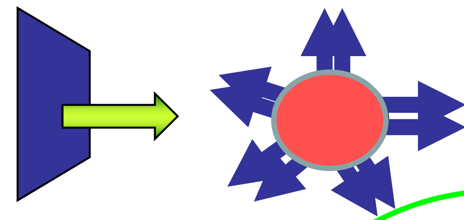
$$\psi_{inc}(\vec{r}; r \to \infty) \to \sum_l i^l \; (2l+1)\; P_l(\cos\theta) \; \frac{\sin(kr - \frac{l\pi}{2})}{kr}$$

$$\psi_{inc}(\vec{r}) \underset{r\to\infty}{\to} \sum_l i^l \; (2l+1)\; P_l(\cos\theta) \; \frac{e^{i\left(kr - \frac{l\pi}{2}\right)} - e^{-i\left(kr - \frac{l\pi}{2}\right)}}{2ikr}$$

$$e^{i\frac{l\pi}{2}} = \left(e^{i\frac{\pi}{2}} \right)^l = i^l$$

$$\psi_{inc}(\vec{r}) \underset{r\to\infty}{\to} \sum_l \; (2l+1)\; P_l(\cos\theta) \; \frac{e^{ikr} - e^{-ikr} e^{+i\frac{l\pi}{2}} e^{+i\frac{l\pi}{2}}}{2ikr}$$

$$\psi_{\vec{k}_i}(\vec{r}; r \to \infty) \to A\left[e^{\vec{k}\bullet\vec{r}} + \frac{f(\hat{\Omega})}{r} e^{ikr} \right]$$



$$\psi_{inc}(\vec{r}) \underset{r\to\infty}{\to} \sum_l (2l+1)\, P_l(\cos\theta)\, \frac{e^{ikr} - e^{-ikr} e^{+i\frac{l\pi}{2}} e^{+i\frac{l\pi}{2}}}{2ikr}$$

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

$$\psi_{inc}(\vec{r}) \underset{r\to\infty}{\to} \sum_l (2l+1)\, P_l(\cos\theta)\, \frac{e^{ikr} - e^{-ikr}(-1)^l}{2ikr}$$

$$\psi_{inc} \underset{r\to\infty}{\to} \frac{1}{2ikr} \sum_l (2l+1) \left[P_l(\cos\theta) e^{ikr} - P_l(\cos\theta)(-1)^l e^{-ikr} \right]$$

$$\psi_{inc} \underset{r\to\infty}{\to} \frac{1}{2ikr} \sum_l (2l+1) \left[P_l(\cos\theta) e^{ikr} - P_l(-\cos\theta) e^{-ikr} \right]$$

$$e^{ikz} \xrightarrow[r\to\infty]{} \frac{1}{2ikr}\sum_l (2l+1)\left[P_l(\cos\theta)e^{ikr} - P_l(-\cos\theta)e^{-ikr}\right]$$

What will be the result of scattering by a potential?

$$\psi_{Tot}(\vec{r}) \xrightarrow[r\to\infty]{}$$

$$\frac{1}{2ikr}\sum_l c_l(2l+1)\left[P_l(\cos\theta)e^{i(kr+\delta_l)} - P_l(-\cos\theta)e^{-i(kr+\delta_l)}\right]$$

δ_l : phase shift of the ℓ^{th} partial wave

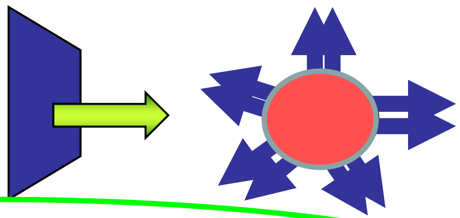
condition:

for potentials that fall

faster than the *Coulomb* potential, i.e. faster than $\frac{1}{r}$ as $r \to \infty$.

$$e^{ikz} \underset{r\to\infty}{\longrightarrow} \frac{1}{2ikr}\sum_l (2l+1)\left[P_l(\cos\theta)e^{ikr} - P_l(-\cos\theta)e^{-ikr}\right]$$

$$\psi_{\vec{k}_i}(\vec{r}; r\to\infty) \to A\left[e^{\vec{k}\cdot\vec{r}} + \frac{f(\hat{\Omega})}{r}e^{ikr}\right]$$



δ_l : phase shift of the ℓ^{th} partial wave

$$\psi_{Tot}(\vec{r}) \underset{r\to\infty}{\longrightarrow} \frac{1}{2ikr}\sum_l c_l(2l+1)\left[P_l(\cos\theta)e^{i(kr+\delta_l)} - P_l(-\cos\theta)e^{-i(kr+\delta_l)}\right]$$

Please refer to details from :

PCD STiAP Unit 6 Probing the Atom

Lecture link: http://nptel.iitm.ac.in/courses/115106057/27 & /28 & /29 & /30

$$\psi_{Tot}(\vec{r}) \xrightarrow[r\to\infty]{} \frac{1}{2ikr}\sum_l c_l (2l+1)\left[P_l(\cos\theta)e^{i(kr+\delta_l)} - P_l(-\cos\theta)e^{-i(kr+\delta_l)}\right]$$

choice of normalization

c_l depends on the boundary conditions

Please refer to details from :
PCD STiAP Unit 6 Probing the Atom

$$c_l = e^{\pm i\delta_l}$$

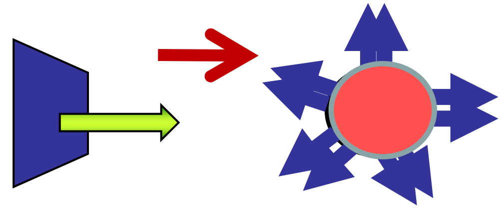
Lecture link: http://nptel.iitm.ac.in/courses/115106057/27 & /28 & /29 & /30

$\psi_{Tot}^{+}(\vec{r},t)\big] \rightarrow$ outgoing wave boundary conditions

$\psi_{Tot}^{-}(\vec{r},t)\big] \rightarrow$ ingoing wave boundary conditions

Outgoing wave boundary condition

$$\hat{k}_i = \hat{e}_z$$



$$\psi^{(+)}_{\vec{k}_i}(\vec{r}; r\to\infty) \underset{r\to\infty}{\longrightarrow} A(k)\left[e^{i\vec{k}_i\bullet\vec{r}} + \frac{f(\hat{\Omega})}{r}e^{ikr}\right]$$

$$f(\hat{\Omega}) = ? \quad [L]$$

scattering amplitude

$c_\ell = e^{i\delta_\ell}$ gives:

$$f(k,\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left[e^{2i\delta_l(k)} - 1\right]P_l(\cos\theta)$$

Faxen-Holtzmark's formalism

Each ℓ^{th} term gives the contribution of the ℓ^{th} **partial wave** to the scattering amplitude.

Reference: **Quantum Theory of Collisions** by Charles J Joachain
North-Holland Publishing Co. // Section 3.2 // see Eq.3.27, page 49

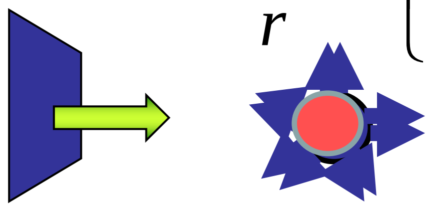
PCD STiTACS Unit 1 Quantum Theory of Collisions

$$\psi^{+}_{Tot}\left(\vec{r},t\right)\Big]_{r\to\infty} \longrightarrow$$

$C_l = e^{i\delta_l(k)}$

describes 'collisions'

$$e^{+i(kz-\omega t)} + \frac{e^{+i(kr-\omega t)}}{r}\left\{\frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left[e^{2i\delta_l(k)}-1\right]P_l(\cos\theta)\right\}$$



$C_l = e^{-i\delta_l(k)}$

describes 'photoionization'

$$\psi^{-}_{Tot}\left(\vec{r},t\right)\Big]_{r\to\infty} \longrightarrow$$

$$|\psi_f\rangle \to e^{ikz} - \frac{e^{-ikr}}{r}\sum_l (2l+1)\, P_l(-\cos\theta)\left(\frac{e^{-i2\delta_l}-1}{2ik}\right)$$

$$e^{+i(kz+\omega t)} + \frac{e^{+i(kr+\omega t)}}{r}\left\{\frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left[e^{2i\delta_l(k)}-1\right]P_l(\cos\theta)\right\}$$

Please refer to details from :

PCD STiAP Unit 6 Probing the Atom

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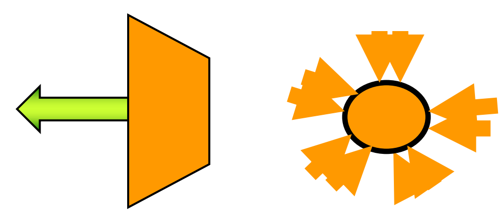
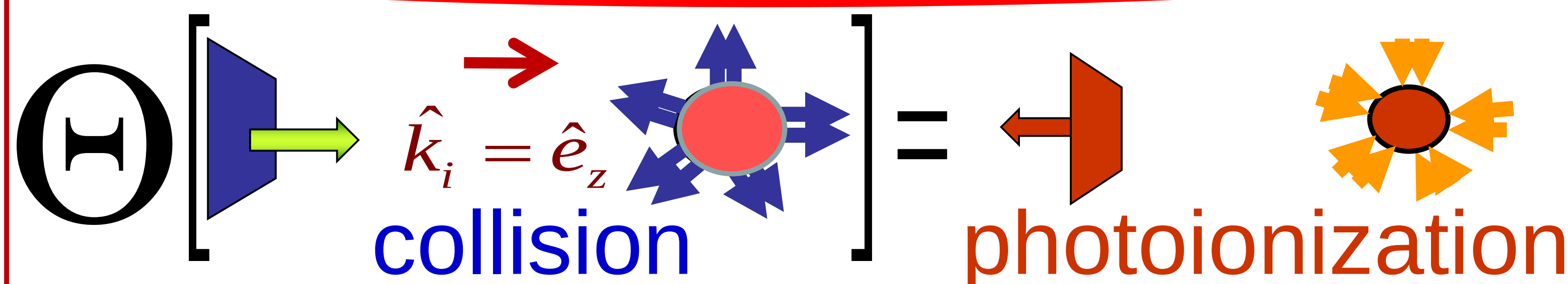


Θ : operator for

TIME REVERSAL SYMMETRY

$$\psi^{+}_{Tot}(\vec{r},t)\Big]_{r\to\infty} \longrightarrow e^{+i(kz-\omega t)} + \frac{e^{+i(kr-\omega t)}}{r}\left\{\frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left[e^{2i\delta_l(k)}-1\right]P_l(\cos\theta)\right\}$$



$$\psi^{-}_{Tot}(\vec{r},t)\Big]_{r\to\infty} \longrightarrow e^{+i(kz+\omega t)} + \frac{e^{+i(kr+\omega t)}}{r}\left\{\frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left[e^{2i\delta_l(k)}-1\right]P_l(\cos\theta)\right\}$$

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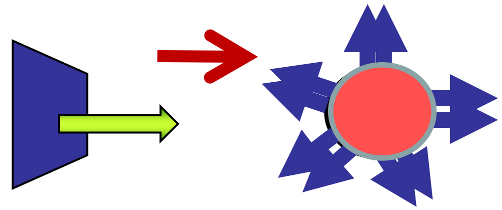
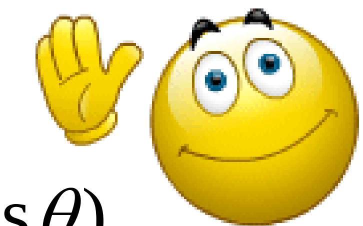
$C_l = e^{i\delta_l(k)}$

Outgoing wave boundary condition



'collisions'

$$\psi^{(+)}_{\vec{k}_i}(\vec{r}; r \to \infty) \xrightarrow[r\to\infty]{} A(k)\left[e^{i\vec{k}_i\cdot\vec{r}} + \frac{f(\hat{\Omega})}{r}e^{ikr}\right]$$



$$f(k,\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left[e^{2i\delta_l(k)} - 1\right]P_l(\cos\theta)$$

Contributions of the **partial waves** to the scattering amplitude.

Faxen-Holtzmark's formalism

QUESTIONS ?

Write to:

pcd@physics.iitm.ac.in

Next class:

OPTICAL THEOREM

Reference: **Quantum Theory of Collisions** by Charles J Joachain
North-Holland Publishing Co. // Section 3.2 // see Eq.3.27, page 49

PCD STiTACS Unit 1 Quantum Theory of Collisions

INTRODUCTORY lecture about this course on

Select/Special Topics from

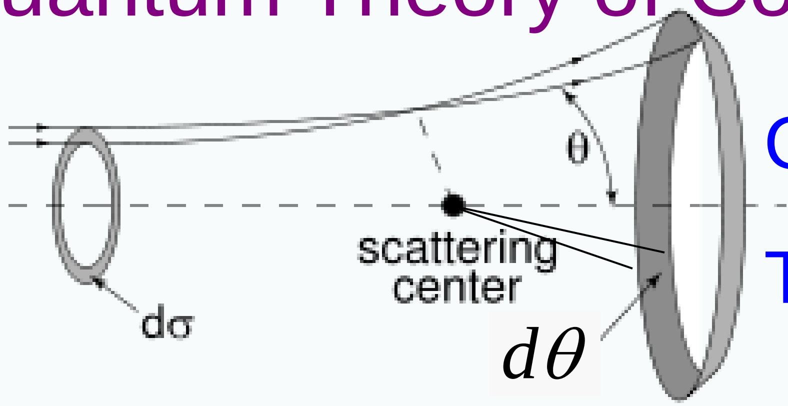
'Theory of Atomic Collisions and Spectroscopy'

P. C. Deshmukh

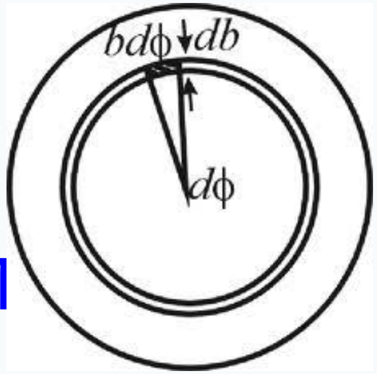
Department of Physics
Indian Institute of Technology Madras
Chennai 600036

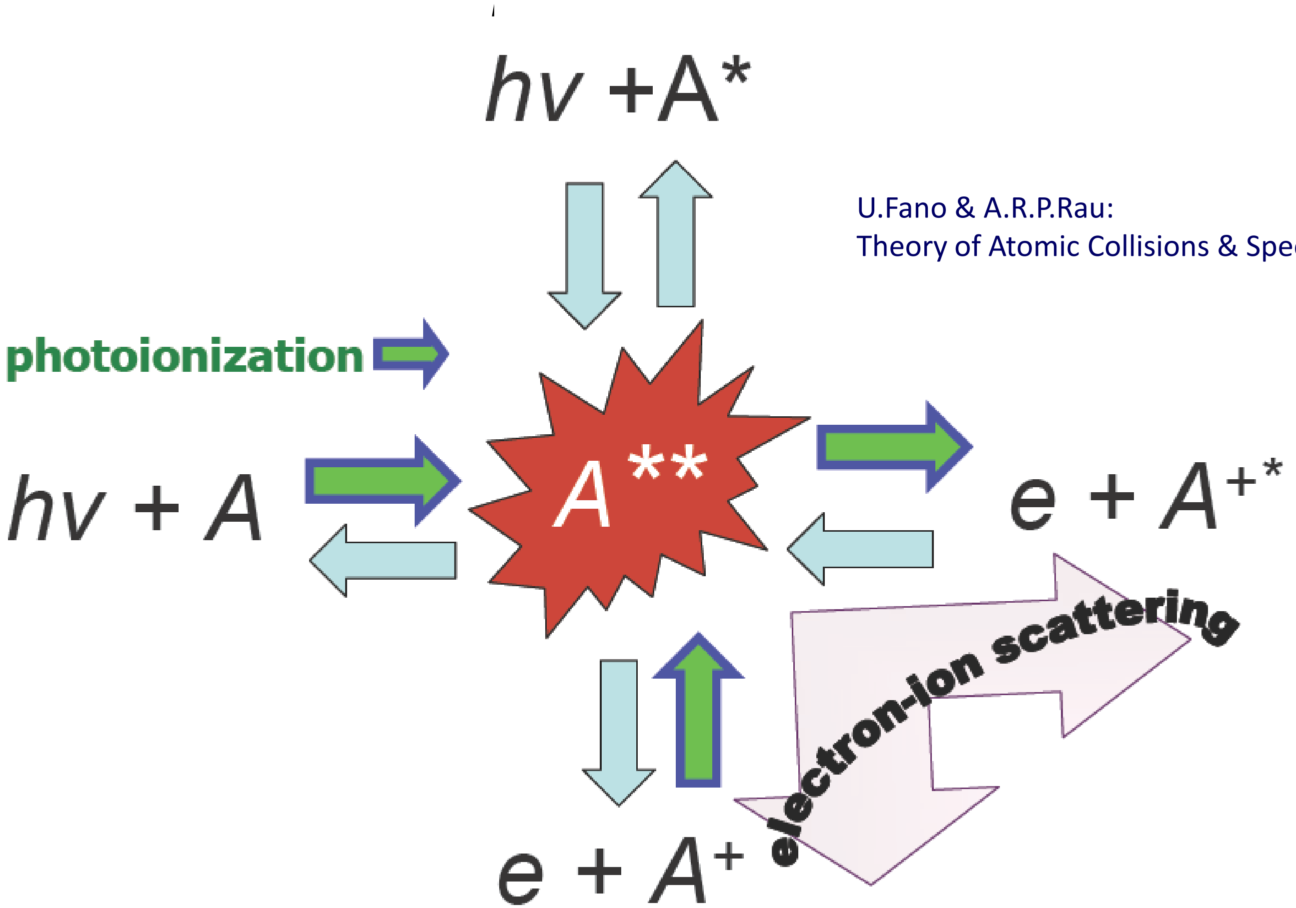
Unit 1 Lecture Number 03

Quantum Theory of Collisions



OPTICAL THEOREM





PHOTOIONIZATION & electron-ion scattering have same final state, but different initial states.

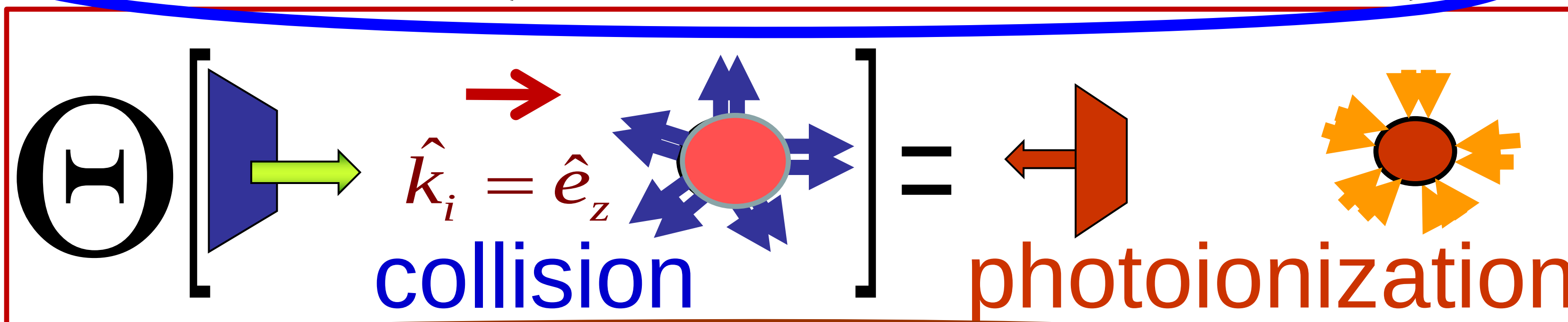
Please refer to details from :
PCD STiAP Unit 6 Probing the Atom

Lecture link: http://nptel.iitm.ac.in/courses/115106057/27 & /28 & /29 & /30

Θ : operator for

TIME REVERSAL SYMMETRY

$$\left.\psi^{+}_{Tot}(\vec{r},t)\right]_{r\to\infty} \longrightarrow e^{+i(kz-\omega t)} + \frac{e^{+i(kr-\omega t)}}{r}\left\{\frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left[e^{2i\delta_l(k)}-1\right]P_l(\cos\theta)\right\}$$



$$\left.\psi^{-}_{Tot}(\vec{r},t)\right]_{r\to\infty} \longrightarrow e^{+i(kz+\omega t)} + \frac{e^{+i(kr+\omega t)}}{r}\left\{\frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left[e^{2i\delta_l(k)}-1\right]P_l(\cos\theta)\right\}$$

Please refer to details from :
PCD STiAP Unit 6 Probing the Atom

Lecture link: http://nptel.iitm.ac.in/courses/115106057/27 & /28 & /29 & /30

$$\psi^{+}_{\vec{k}_i}(\vec{r}; r\to\infty) \xrightarrow[r\to\infty]{} A(k)\left[e^{i\vec{k}_i\bullet\vec{r}} + \frac{f(\hat{\Omega})}{r}e^{ikr}\right]$$

$$\left[f(\hat{\Omega})\right] \to L$$

scattering amplitude

$$\vec{j}(\vec{r}) = \frac{\hbar}{2mi}\left[\psi^*(\vec{r})\vec{\nabla}\psi(\vec{r}) - \psi(\vec{r})\vec{\nabla}\psi^*(\vec{r})\right]$$

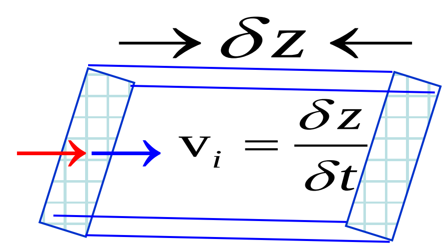
$$= \mathrm{Re}\left\{\frac{\hbar}{mi}\,\psi^*(\vec{r})\vec{\nabla}\psi(\vec{r})\right\}$$

Probability current density vector

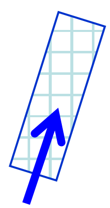
$$^{incident}\vec{j}(\vec{r}) = \mathrm{Re}\left\{\frac{\hbar}{mi}A(k)^* e^{-ik_i z}\times\left\{\hat{e}_x\frac{\partial}{\partial x} + \hat{e}_y\frac{\partial}{\partial y} + \hat{e}_z\frac{\partial}{\partial z}\right\}\left\{A(k)e^{ik_i z}\right\}\right\}$$

$$^{incident}\vec{j}(\vec{r}) = |A(k)|^2\frac{\hbar\vec{k}_i}{m} = |A(k)|^2\,\vec{v}_i$$

$$\to \hat{e}_z$$



$$\delta S\delta z = \delta V$$



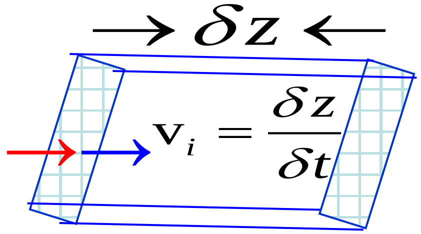
$$^{incident}\vec{j}(\vec{r})\cdot\overrightarrow{\delta S} = \vec{j}(\vec{r})\cdot\delta S\hat{e}_z = |A(k)|^2\,v_i\delta S = |A(k)|^2\frac{\delta z}{\delta t}\delta S = |A(k)|^2\frac{\delta V}{\delta t}$$

current through area δS

$$\psi^{+}_{\vec{k}_i}(\vec{r}; r\to\infty) \xrightarrow[r\to\infty]{} A(k)\left[e^{i\vec{k}_i\bullet\vec{r}} + \frac{f(\hat{\Omega})}{r} e^{ikr} \right]$$

$$^{incident}\vec{j}(\vec{r}) = |A(k)|^2 \frac{\hbar\vec{k}_i}{m} = |A(k)|^2\, \vec{\mathrm{v}}_i$$

$$\boxed{A(k)=1} \rightarrow \left[{}^{incident}\psi = e^{i\vec{k}_i\bullet\vec{r}} \right]$$



Probability density $\rightarrow \psi^*\psi = 1$

Current density: $^{incident}\vec{j}(\vec{r}) = \frac{\hbar\vec{k}_i}{m} = \vec{\mathrm{v}}_i$

$$^{incident}\delta\Phi_{\substack{through\\ area\ \delta S}} = {}^{incident}\vec{j}(\vec{r})\cdot\overrightarrow{\delta S} = \vec{j}(\vec{r})\cdot\delta S\hat{e}_z = \boxed{\mathrm{v}_i\delta S} = \frac{\delta z}{\delta t}\delta S = \frac{\delta V}{\delta t}$$

Density of particles: 1 particle per unit volume;

i.e. 1 particle x-sing unit area in unit time at velocity $\vec{\mathrm{v}}_i = \mathrm{v}_i\hat{e}_z$

$$\boxed{incident\ \text{flux per unit area: } {}^{i}\delta\Phi = \mathrm{v}_i}$$

$$\psi^{+}_{\vec{k}_i}(\vec{r}; r\to\infty) \underset{r\to\infty}{\longrightarrow} A(k)\left[e^{i\vec{k}_i\bullet\vec{r}} + \frac{f(\hat{\Omega})}{r} e^{ikr} \right]$$

scattered part

$$\psi^{+}_{\vec{k}_i}(\vec{r}; r\to\infty) \underset{r\to\infty}{\longrightarrow} A(k)\left[\frac{f(\hat{\Omega})}{r} e^{ikr} \right]$$

$$\vec{j}(\vec{r}) = \mathrm{Re}\left\{ \frac{\hbar}{mi} \psi^{*}(\vec{r})\vec{\nabla}\psi(\vec{r}) \right\}$$

scattered part

$$\vec{j}(\vec{r}) = \mathrm{Re}\left\{ |A(k)|^2 \frac{\hbar}{mi}\left[\frac{f^{*}(\hat{\Omega})}{r} e^{-ikr} \right]\left\{ \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\theta \frac{1}{r}\frac{\partial}{\partial\theta} + \hat{e}_\varphi \frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi} \right\}\left[\frac{f(\hat{\Omega})}{r} e^{ikr} \right]\right\}$$

$$\frac{1}{r}\frac{\partial}{\partial\theta}\left[\frac{f(\hat{\Omega})}{r} e^{ikr} \right] \to O\left(\frac{1}{r^2}\right)$$

$$\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}\left[\frac{f(\hat{\Omega})}{r} e^{ikr} \right] \to O\left(\frac{1}{r^2}\right)$$

$$O\left(\frac{1}{r^2}\right) \underset{r\to\infty}{\longrightarrow} \text{ignore w.r.t. } O\left(\frac{1}{r}\right)$$

scattered part

$$\vec{j}(\vec{r}) \approx \mathrm{Re}\left\{ |A(k)|^2 \frac{\hbar}{mi}\left[\frac{f^{*}(\hat{\Omega})}{r} e^{-ikr} \right] \hat{e}_r (ik) \left[\frac{f(\hat{\Omega})}{r} e^{ikr} \right]\right\}$$

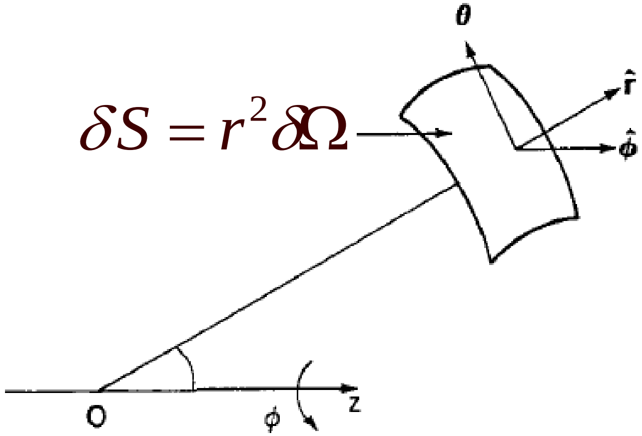
$$= |A(k)|^2 \frac{\hbar k}{m} \frac{\left|f(\hat{\Omega})\right|^2}{r^2} \hat{e}_r$$

incident flux

per unit area: ${}^{i}\delta\Phi = |A(k)|^2 \, \mathrm{v}_i$

scattered part $\vec{j}\left(\vec{r}\right) = |A(k)|^2 \dfrac{\hbar k}{m} \dfrac{|f(\hat{\Omega})|^2}{r^2} \hat{\mathrm{e}}_r$

$\delta S = r^2 \delta\Omega$



Scattered flux in the radial outward direction through elemental area $\delta S = r^2 \delta\Omega$

$${}^{s}\delta\Phi = \underset{\text{scattered part}}{\vec{j}\left(\vec{r}\right)} \cdot \delta S \hat{e}_r \approx |A(k)|^2 \frac{\hbar k}{m} \frac{|f(\hat{\Omega})|^2}{r^2} \hat{\mathrm{e}}_r \cdot \delta S \hat{e}_r$$

$\left[f(\hat{\Omega}) \right] \rightarrow L$

scattering amplitude

$|f(\hat{\Omega})|^2 \rightarrow L^2$

$$\psi^{+}_{\vec{k}_i}(\vec{r}; r \to \infty) \xrightarrow[r\to\infty]{} A(k)\left[e^{i\vec{k}_i \bullet \vec{r}} + \frac{f(\hat{\Omega})}{r} e^{ikr} \right]$$

$\left[f(\hat{\Omega}) \right] \to L$

scattering amplitude

incident flux per unit area: ${}^{i}\delta\Phi = |A(k)|^2 \mathrm{v}_i$

Scattered flux in the radial outward direction

$${}^{s}\delta\Phi = {}^{scattered}\vec{j}(\vec{r}) \cdot \delta S \hat{e}_r \approx |A(k)|^2 \frac{\hbar k}{m} \frac{|f(\hat{\Omega})|^2}{r^2} \hat{e}_r \cdot r^2 \delta\Omega \hat{e}_r$$

$$\frac{{}^{s}\delta\Phi}{{}^{i}\delta\Phi} = |f(\hat{\Omega})|^2 \delta\Omega$$

$|f(\hat{\Omega})|^2 : L^2$

$$\frac{d\sigma}{d\Omega} = \lim_{\delta\Omega \to 0} \frac{\delta\sigma}{\delta\Omega} = |f(\hat{\Omega})|^2$$

scattering x-sec per unit solid angle

differential x-sec

This definition is independent of the normalization

$$\psi^{+}_{\vec{k}_i}(\vec{r};r\to\infty)\xrightarrow[r\to\infty]{} A(k)\left[e^{i\vec{k}_i\bullet\vec{r}}+\frac{f(\hat{\Omega})}{r}e^{ikr}\right]$$

$\left[f(\hat{\Omega})\right]\to L$

scattering amplitude

Probability current density vector

$$\vec{j}(\vec{r})=\frac{\hbar}{2mi}\left[\psi^*(\vec{r})\vec{\nabla}\psi(\vec{r})-\psi(\vec{r})\vec{\nabla}\psi^*(\vec{r})\right]$$

$$=\mathrm{Re}\left\{\frac{\hbar}{mi}\;\psi^*(\vec{r})\vec{\nabla}\psi(\vec{r})\right\}$$

ψ : total wave function

Radial component of the probability current density vector

$$\vec{j}(\vec{r})\cdot\hat{e}_r=\mathrm{Re}\left\{\begin{array}{l}\frac{\hbar}{mi}A(k)^*\left[e^{-i\vec{k}_i\bullet\vec{r}}+\frac{f^*(\hat{\Omega})}{r}e^{-ikr}\right]\times\\ \left\{\hat{e}_r\frac{\partial}{\partial r}+\hat{e}_\theta\frac{1}{r}\frac{\partial}{\partial\theta}+\hat{e}_\varphi\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}\right\}\left\{A(k)\left[e^{i\vec{k}_i\bullet\vec{r}}+\frac{f(\hat{\Omega})}{r}e^{ikr}\right]\right\}\end{array}\right\}\cdot\hat{e}_r$$

$$\vec{j}(\vec{r})\cdot\hat{e}_r=\mathrm{Re}\left\{\frac{\hbar}{mi}\;|A(k)|^2\left(e^{-i\vec{k}_i\bullet\vec{r}}+\frac{f^*(\hat{\Omega})e^{-ikr}}{r}\right)\frac{\partial}{\partial r}\left(e^{i\vec{k}_i\bullet\vec{r}}+\frac{f(\hat{\Omega})e^{ikr}}{r}\right)\right\}$$

C.J.Joachain: Quantum Theory of Collisions Eq.3.34, p 51

$$\vec{j}(\vec{r})\cdot\hat{e}_r = \mathrm{Re}\left\{ \frac{\hbar}{mi} |A(k)|^2 \left(e^{-i\vec{k}_i\bullet\vec{r}} + \frac{f^*(\hat{\Omega})e^{-ikr}}{r} \right) \frac{\partial}{\partial r} \left(e^{i\vec{k}_i\bullet\vec{r}} + \frac{f(\hat{\Omega})e^{ikr}}{r} \right) \right\}$$

$$\vec{j}(\vec{r})\cdot\hat{e}_r \approx \left\{ \vec{j}_{\text{incident}}(\vec{r}) + \vec{j}_{\text{outgoing}}(\vec{r}) + \vec{j}_{\text{interference}}(\vec{r}) \right\}\cdot\hat{e}_r$$

$$O\left(\frac{1}{r^2}\right) \xrightarrow[r\to\infty]{} \text{ignored w.r.t. } O\left(\frac{1}{r}\right)$$

Radial component
of the probability current density vector

$$\vec{j}_{\text{interference}}(\vec{r})\cdot\hat{e}_r =$$

$$\mathrm{Re}\left\{ \frac{\hbar}{mi} |A(k)|^2 \left[e^{-i\vec{k}_i\bullet\vec{r}} \frac{\partial}{\partial r}\left(\frac{f(\hat{\Omega})e^{ikr}}{r} \right) + \frac{f^*(\hat{\Omega})e^{-ikr}}{r} \frac{\partial}{\partial r}\left(e^{i\vec{k}_i\bullet\vec{r}} \right) \right] \right\}$$

$$= \mathrm{Re}\left\{ \frac{\hbar}{mi} |A(k)|^2 \left[e^{-i\vec{k}_i\bullet\vec{r}} (ik) \frac{f(\hat{\Omega})e^{ikr}}{r} + \frac{f^*(\hat{\Omega})e^{-ikr}}{r} (ik\cos\theta) e^{i\vec{k}_i\bullet\vec{r}} \right] \right\}$$

$$\vec{j}_{\text{interference}}(\vec{r})\cdot\hat{e}_r =$$

Radial component
of the probability current density vector

$$\text{Re}\left\{ \frac{\hbar}{mi} |A(k)|^2 \left[e^{-i\vec{k}_i\bullet\vec{r}} \frac{\partial}{\partial r}\left(\frac{f(\hat{\Omega})e^{ikr}}{r}\right) + \frac{f^*(\hat{\Omega})e^{-ikr}}{r}\frac{\partial}{\partial r}\left(e^{i\vec{k}_i\bullet\vec{r}}\right)\right]\right\}$$

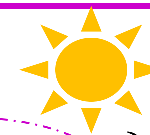
$$= \text{Re}\left\{ \frac{\hbar}{mi} |A(k)|^2 \left[e^{-i\vec{k}_i\bullet\vec{r}} (ik)\frac{f(\hat{\Omega})e^{ikr}}{r} + \frac{f^*(\hat{\Omega})e^{-ikr}}{r}(ik\cos\theta)e^{i\vec{k}_i\bullet\vec{r}}\right]\right\}$$

$$\text{O}\left(\frac{1}{r^2}\right)_{r\to\infty} \longrightarrow \text{ignored w.r.t. O}\left(\frac{1}{r}\right)$$

$$= \text{Re}\left\{ \frac{\hbar}{mi} |A(k)|^2 (ik) \left[\frac{f(\hat{\Omega})e^{ikr(1-\cos\theta)}}{r} + \cos\theta\frac{f^*(\hat{\Omega})e^{-ikr(1-\cos\theta)}}{r}\right]\right\}$$

C.J.Joachain: Quantum Theory of Collisions Eq.3.39, p 51

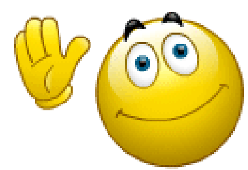
$\vec{j}_{\text{interference}}\left(\vec{r}\right)\cdot\hat{e}_r =$ Radial component of the probability current density vector



$$\mathrm{Re}\left\{ \frac{\hbar k}{m} \left|A(k)\right|^2 \left[\frac{f(\hat{\Omega})e^{ikr(1-\cos\theta)}}{r} + \cos\theta \frac{f^*(\hat{\Omega})e^{-ikr(1-\cos\theta)}}{r} \right] \right\}$$

Incident energy has some spread: → *spread in magnitude of the wave vector* k *to* $k+\Delta k$

$$\int_k^{k+\Delta k} e^{\pm ik'r(1-\cos\theta)}dk' = \left. \frac{e^{\pm ik'r(1-\cos\theta)}}{\pm ir\left(1-\cos\theta\right)} \right]_k^{k+\Delta k}$$



QUESTIONS ? Write to: pcd@physics.iitm.ac.in

$$\int_k^{k+\Delta k} e^{\pm ik'r(1-\cos\theta)}dk' = \frac{e^{\pm i\left(k+\Delta k\right)r(1-\cos\theta)} - e^{\pm ikr(1-\cos\theta)}}{\pm ir\left(1-\cos\theta\right)}$$

numerator $\rightarrow O(1)$

denominator: $r \rightarrow \infty$

Interference term is of importance only when $\cos\theta \approx 1$

$\theta \approx 0$

INTRODUCTORY lecture about this course on

Select/Special Topics from

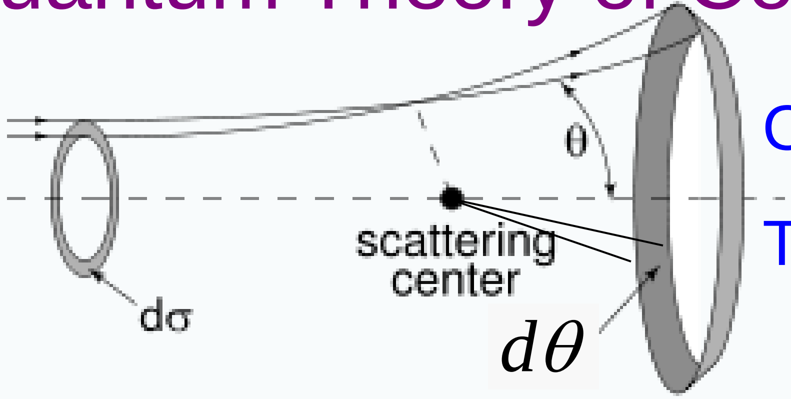
'Theory of Atomic Collisions and Spectroscopy'

P. C. Deshmukh

Department of Physics
Indian Institute of Technology Madras
Chennai 600036

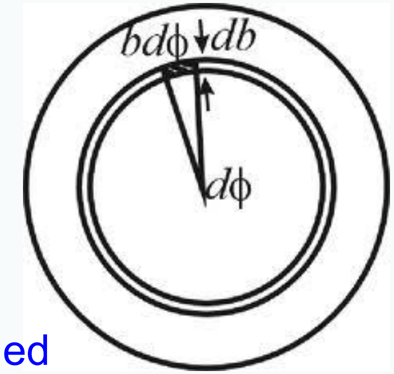
Unit 1 Lecture Number 04

Quantum Theory of Collisions



OPTICAL

THEOREM



…. continued

$$\vec{j}_{\text{interference}}(\vec{r})\cdot\hat{e}_r =$$

Radial component
of the probability current density vector

$$\mathrm{Re}\left\{ \frac{\hbar k}{m} \left|A(k)\right|^2 \left[\frac{f(\hat{\Omega})e^{ikr(1-\cos\theta)}}{r} + \cos\theta \frac{f^*(\hat{\Omega})e^{-ikr(1-\cos\theta)}}{r} \right] \right\}$$

Incident energy has some spread: → *spread in magnitude of the wave vector* k *to* $k+\Delta k$

$$\int_k^{k+\Delta k} e^{\pm ik'r(1-\cos\theta)}dk' = \left. \frac{e^{\pm ik'r(1-\cos\theta)}}{\pm ir(1-\cos\theta)} \right]_k^{k+\Delta k}$$

$$\int_k^{k+\Delta k} e^{\pm ik'r(1-\cos\theta)}dk' = \frac{e^{\pm i(k+\Delta k)r(1-\cos\theta)} - e^{\pm ikr(1-\cos\theta)}}{\pm ir(1-\cos\theta)}$$

numerator $\rightarrow O(1)$
denominator: $r \rightarrow \infty$

Interference term is of importance only when $\cos\theta \approx 1$
$\theta \approx 0$

$$\vec{j}_{\text{interference}}(\vec{r})\cdot\hat{e}_r =$$

$$\mathrm{Re}\left\{ \frac{\hbar k}{m} |A(k)|^2 \left[\frac{f(\hat{\Omega})e^{ikr(1-\cos\theta)}}{r} + \cos\theta \frac{f^*(\hat{\Omega})e^{-ikr(1-\cos\theta)}}{r} \right] \right\}$$

$$\int_k^{k+\Delta k} e^{\pm ik' r(1-\cos\theta)} dk' = \frac{e^{\pm i(k+\Delta k) r(1-\cos\theta)} - e^{\pm ikr(1-\cos\theta)}}{\pm ir(1-\cos\theta)}$$

numerator $\rightarrow O(1)$

denominator: $r \rightarrow \infty$

Interference term is of importance only when $\theta \approx 0$

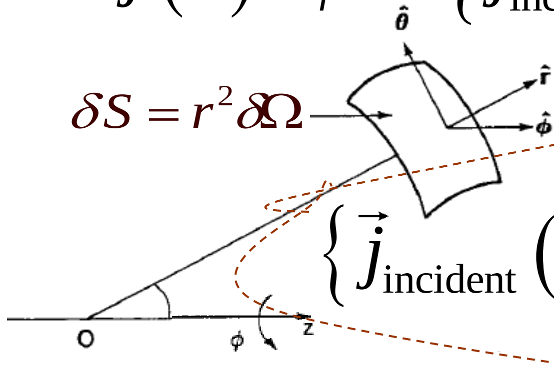
considering the spread in magnitude of the wave vector from k to $k+\Delta k \Rightarrow only\ \theta \approx 0$ is important with regard to 'INTERFERENCE TERM'

$$\int_k^{k+\Delta k} e^{\pm ik' r(1-\cos\theta)} dk' \underset{r\to\infty}{\lim} \rightarrow 0, \text{ except near } \theta \sim 0$$

'forward' scattering

$$\vec{j}(\vec{r})\cdot\hat{e}_r = \left\{\vec{j}_{\text{incident}}(\vec{r}) + \vec{j}_{\text{outgoing}}(\vec{r}) + \vec{j}_{\text{interference}}(\vec{r})\right\}\cdot\hat{e}_r$$

$$\delta S = r^2\delta\Omega$$



$$\vec{j}(\vec{r})\cdot r^2 d\Omega\hat{e}_r =$$

$$\left\{\vec{j}_{\text{incident}}(\vec{r}) + \vec{j}_{\text{outgoing}}(\vec{r}) + \vec{j}_{\text{interference}}(\vec{r})\right\}\cdot r^2 d\Omega\hat{e}_r$$

$$\theta \approx 0$$

$$\oiint \vec{j}(\vec{r})\cdot r^2 d\Omega\hat{e}_r =$$

$$= \oiint \left\{\vec{j}_{\text{incident}}(\vec{r}) + \vec{j}_{\text{outgoing}}(\vec{r}) + \vec{j}_{\text{interference}}(\vec{r})\right\}\cdot r^2 d\Omega\hat{e}_r$$

$$\oiint \vec{j}(\vec{r})\cdot\overrightarrow{dS} = \qquad \theta \approx 0$$

$$= \oiint \vec{j}_{incident}(\vec{r})\cdot\overrightarrow{dS} + \oiint \vec{j}_{outgoing}(\vec{r})\cdot\overrightarrow{dS} + \oiint \vec{j}_{\text{interference}}(\vec{r})\cdot\overrightarrow{dS}$$

$$= 0$$

$$\iiint dV\left\{\vec{\nabla}\bullet\vec{j}(\vec{r})\right\} = \oiint \vec{j}(\vec{r})\cdot\overrightarrow{dS} \quad ; \quad \vec{\nabla}\bullet\vec{j}(\vec{r}) = -\frac{\partial\rho}{\partial t}$$

$$0=\oiint \vec{j}_{incident}(\vec{r})\cdot\overrightarrow{dS}+\oiint \vec{j}_{outgoing}(\vec{r})\cdot\overrightarrow{dS}+\oiint \vec{j}_{\mathrm{interference}}(\vec{r})\cdot\overrightarrow{dS}$$

$$0=\oiint \vec{j}_{outgoing}(\vec{r})\cdot\overrightarrow{dS}+\oiint \vec{j}_{\mathrm{interference}}(\vec{r})\cdot\overrightarrow{dS}$$

$${}^{s}\delta\Phi={}^{scattered}_{outgoing}\ \vec{j}(\vec{r})\cdot\delta S\hat{e}_r\approx|A(k)|^2\frac{\hbar k}{m}\frac{\left|f(\hat{\Omega})\right|^2}{r^2}\hat{e}_r\cdot r^2\delta\Omega\hat{e}_r$$

$$\oiint \vec{j}_{outgoing}(\vec{r})\cdot\overrightarrow{dS}=\oiint\frac{\hbar k}{m}|A(k)|^2\frac{\left|f(\hat{\Omega})\right|^2}{r^2}\hat{e}_r\cdot r^2 d\Omega\hat{e}_r$$

$$\oiint \vec{j}_{outgoing}(\vec{r})\cdot\overrightarrow{dS}=\frac{\hbar k}{m}|A(k)|^2\oiint\left|f(\hat{\Omega})\right|^2 d\Omega=\frac{\hbar k}{m}|A(k)|^2\sigma_{total}$$

$$\frac{d\sigma}{d\Omega}=\left|f(\hat{\Omega})\right|^2$$

$$\oiint \vec{j}_{\mathrm{interference}}(\vec{r})\cdot\overrightarrow{dS}=\int_{\theta=0}^{\theta=0+\Delta\theta}\sin\theta d\theta\int_{\varphi=0}^{2\pi}d\varphi\,\vec{j}_{\mathrm{interference}}(\vec{r})\cdot\overrightarrow{dS}$$

$\theta\approx 0$

$\Delta\theta=?$

$small:\quad \Delta\theta\neq 0$

$$0 = \oiint \vec{j}_{outgoing}\left(\vec{r}\right)\cdot\overrightarrow{dS} + \oiint \vec{j}_{\text{interference}}\left(\vec{r}\right)\cdot\overrightarrow{dS}$$

small

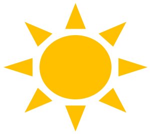
$\Delta\theta \neq 0$

$$= \frac{\hbar k}{m}\left|A(k)\right|^2 \sigma_{total} + \oiint \vec{j}_{\text{interference}}\left(\vec{r}\right)\cdot\hat{e}_r r^2 d\Omega$$

$$= \frac{\hbar k}{m}\left|A(k)\right|^2 \sigma_{total} + \int_{\theta=0}^{\theta=0+\Delta\theta} \sin\theta d\theta \int_{\varphi=0}^{2\pi} d\varphi \, \vec{j}_{\text{interference}}\left(\vec{r}\right)\cdot\hat{e}_r \, r^2$$

$$\vec{j}_{\text{interference}}\left(\vec{r}\right)\cdot\hat{e}_r =$$

$$\mathrm{Re}\left\{ \frac{\hbar k}{m} \left|A(k)\right|^2 \left[\frac{f(\hat{\Omega})e^{ikr(1-\cos\theta)}}{r} + \cos\theta \frac{f^*(\hat{\Omega})e^{-ikr(1-\cos\theta)}}{r} \right] \right\}$$



C.J.Joachain: Quantum Theory of Collisions Eq.3.39, p 51

$$0 = \frac{\hbar k}{m}\left|A(k)\right|^2 \sigma_{total} +$$

$NOTE : A(k)$ does not matter for subsequent analysis

$$2\pi \int_{\theta=0}^{\theta=0+\Delta\theta} \sin\theta d\theta \, \mathrm{Re}\left\{ \frac{\hbar k}{m} \left|A(k)\right|^2 \left[\frac{f(\hat{\Omega})e^{ikr(1-\cos\theta)}}{r} + \cos\theta \frac{f^*(\hat{\Omega})e^{-ikr(1-\cos\theta)}}{r} \right] \right\} r^2$$

$$0 = \sigma_{total} +$$

$$2\pi \int_{\theta=0}^{\theta=0+\Delta\theta} \sin\theta d\theta \operatorname{Re}\left\{ \left[\frac{f(\hat{\Omega})e^{ikr(1-\cos\theta)}}{r} + \cos\theta \frac{f^*(\hat{\Omega})e^{-ikr(1-\cos\theta)}}{r} \right] \right\} r^2$$

$$0 = \sigma_{total} + 2\pi \operatorname{Re} \left\{ \begin{array}{l} f(0)\ r\ e^{ikr} \int_{\theta=0}^{\theta=0+\Delta\theta} \sin\theta d\theta e^{-ikr\cos\theta} + \\ f^*(0)\ r\ e^{-ikr} \int_{\theta=0}^{\theta=0+\Delta\theta} \sin\theta d\theta e^{+ikr\cos\theta} \end{array} \right\}$$

$$\cos\theta = \mu$$

$$-\sin\theta d\theta = d\mu$$

$$0 = \sigma_{total} + 2\pi \operatorname{Re} \left\{ \begin{array}{l} f(0)\ r\ e^{ikr} \int_{\mu=\cos\Delta\theta}^{\mu=1} d\mu e^{-ikr\mu} + \\ f^*(0)\ r\ e^{-ikr} \int_{\mu=\cos\Delta\theta}^{\mu=1} d\mu e^{ikr\mu} \end{array} \right\}$$

$$0=\sigma_{total}+2\pi\,\mathrm{Re}\left\{f(0)\,r\,e^{ikr}\int_{\mu=\cos\Delta\theta}^{\mu=1}d\mu e^{-ikr\mu}+f^*(0)\,r\,e^{-ikr}\int_{\mu=\cos\Delta\theta}^{\mu=1}d\mu e^{ikr\mu}\right\}$$

$$0=\sigma_{total}+2\pi\,\mathrm{Re}\left\{f(0)\,r\,e^{ikr}\left[\frac{e^{-ikr\mu}}{-ikr}\right]_{\mu=\cos\Delta\theta}^{\mu=1}+f^*(0)\,r\,e^{-ikr}\left[\frac{e^{ikr\mu}}{ikr}\right]_{\mu=\cos\Delta\theta}^{\mu=1}\right\}$$

$$0=\sigma_{total}+2\pi\,\mathrm{Re}\left\{\begin{array}{l}f(0)\,r\,e^{ikr}\left[\dfrac{e^{-ikr}-e^{-ikr\cos\Delta\theta}}{-ikr}\right]+\\ f^*(0)\,r\,e^{-ikr}\left[\dfrac{e^{ikr}-e^{ikr\cos\Delta\theta}}{ikr}\right]\end{array}\right\}$$

$$0=\sigma_{total}+2\pi\,\mathrm{Re}\left\{\begin{array}{l}f(0)\left[\dfrac{1}{-ik}-\dfrac{e^{ikr(1-\cos\Delta\theta)}}{-ik}\right]+\\ f^*(0)\left[\dfrac{1}{ik}-\dfrac{e^{-ikr(1-\cos\Delta\theta)}}{ik}\right]\end{array}\right\}$$

$$0 = \sigma_{total} + 2\pi \,\mathrm{Re} \left\{ \begin{array}{l} f(0)\left[\dfrac{1}{-ik} - \dfrac{e^{ikr(1-\cos\Delta\theta)}}{-ik} \right] + \\ f^*(0)\left[\dfrac{1}{ik} - \dfrac{e^{-ikr(1-\cos\Delta\theta)}}{ik} \right] \end{array} \right\}$$

$$\int_k^{k+\Delta k} e^{\pm ik'r(1-\cos\Delta\theta)} dk' = \frac{e^{\pm i(k+\Delta k)r(1-\cos\Delta\theta)} - e^{\pm ikr(1-\cos\Delta\theta)}}{\pm ir(1-\cos\Delta\theta)}$$

$\Delta\theta \neq 0$ however small

$$0 = \sigma_{total} + 2\pi \,\mathrm{Re} \left\{ \begin{array}{l} f(0)\left[\dfrac{i}{k} + \underbrace{oscillatory\ terms}_{\to 0 \text{ as } r \to \infty} \right] + \\ f^*(0)\left[\dfrac{-i}{k} + oscillatory\ terms \right] \end{array} \right\}$$

$$0 = \sigma_{total} + 2\pi \,\mathrm{Re}\left\{ f(0) \left[\frac{i}{k}\right] + f^{*}(0) \left[\frac{-i}{k}\right] \right\}$$

$$0 = \sigma_{total} + 2\pi \,\mathrm{Re}\left\{ 2\,\mathrm{Re}\left(f(0) \left[\frac{i}{k}\right] \right) \right\}$$

The total scattering x-sec is equal to 4π/k times the imaginary part of the forward (complex) scattering amplitude

$$0 = \sigma_{total} + \frac{4\pi}{k} \mathrm{Re} \left\{ \mathrm{Re}\left(i \times f(0) \right) \right\}$$

$$f(0) = a + ib$$

$$i \times f(0) = ia - b$$

$$\mathrm{Re}\left[i \times f(0) \right] = -b$$

$$= -\mathrm{Im}\left[f(0) \right]$$

$(real$ number$)$

$$0 = \sigma_{total} + \frac{4\pi}{k} \left[-\mathrm{Im}\, f(0) \right]$$

$$\sigma_{total} = \frac{4\pi}{k} \left[\mathrm{Im}\, f(0) \right]$$

OPTICAL THEOREM

Bohr-Peierls-Placzek relation

$$\sigma_{total} = \frac{4\pi}{k}[\mathrm{Im}\, f(0)]$$

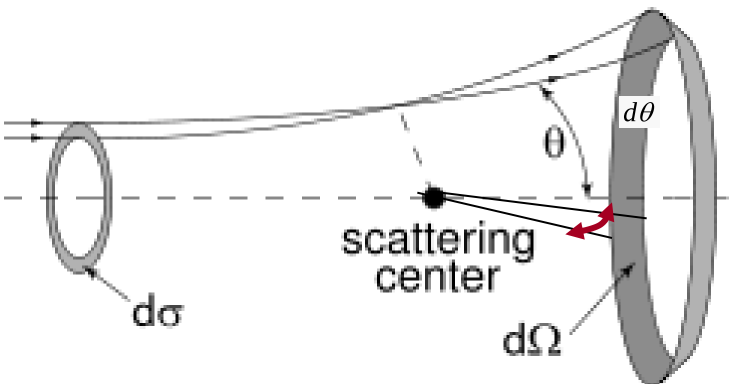
OPTICAL THEOREM

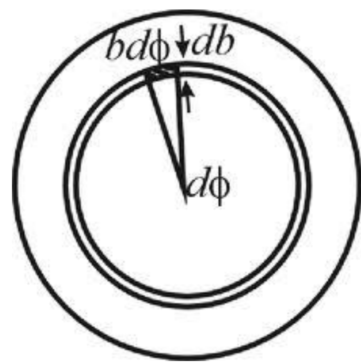
Bohr-Peierls-Placzek relation

ORIGINS:

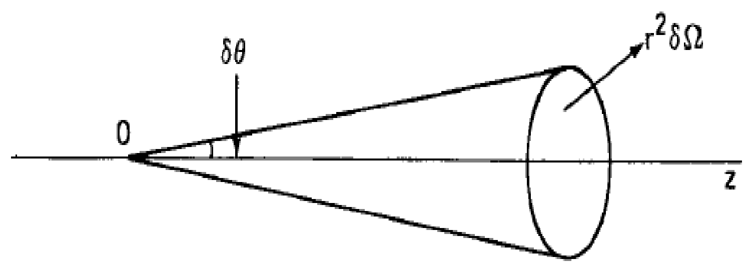
$$\iiint dV \left\{\vec{\nabla} \bullet \vec{j}(\vec{r})\right\} = \oiint \vec{j}(\vec{r}) \cdot \overrightarrow{dS} \quad ; \quad \vec{\nabla} \bullet \vec{j}(\vec{r}) = -\frac{\partial \rho}{\partial t}$$

independent of $A(k)$





"Shadow" of the target in the forward direction results from scattering of the incident beam by the target potential.



The angle $\delta\theta$ and area $r^2\,\delta\Omega$

C.J.Joachain: Quantum Theory of Collisions Fig. 3.3, p 53

Outgoing wave boundary condition $\psi^{(+)}_{\vec{k}_i}(\vec{r};r\to\infty)\underset{r\to\infty}{\longrightarrow} A(\vec{k}_i)\left[e^{i\vec{k}_i\bullet\vec{r}}+\frac{f(\hat{\Omega})}{r}e^{ikr}\right]$

$C_l = e^{i\delta_l(k)}$ describes 'collisions'

We have employed this boundary condition, inclusive of an ℓ-dependent normalization.

$A(\vec{k})$: energy dependent normalization of the incident wave that scales the scattered part as well.

OPTICAL THEOREM: independent of $A(\vec{k})$

scattering x-sec per unit solid angle
differential x-sec

$$\frac{d\sigma}{d\Omega}=\left|f(\hat{\Omega})\right|^2$$

This definition is independent of the normalization

$$\psi^{+}_{\vec{k}_i}(\vec{r};r\to\infty)\underset{r\to\infty}{\longrightarrow} A(\vec{k}_i)\left[e^{i\vec{k}_i\bullet\vec{r}}+\frac{f(\hat{\Omega})}{r}e^{ikr}\right]$$

scattering x-sec
per unit solid angle
differential x-sec

$$\frac{d\sigma}{d\Omega}=\left|f(\hat{\Omega})\right|^2$$

This definition is independent of the normalization

$$\psi^{+}_{Tot}(\vec{r},t)\Big]\underset{r\to\infty}{\longrightarrow}$$

$$\frac{1}{(2\pi)^{3/2}}A(\vec{k})\left[e^{+i(\vec{k}.\vec{r}-\omega t)}+\frac{e^{+i(kr-\omega t)}}{r}\left\{\frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left[e^{2i\delta_l(k)}-1\right]P_l(\cos\theta)\right\}\right]$$

We employed mono-energetic incident beam → idealization

$$\psi^{+}_{Tot}(\vec{r},t)\Big]_{r\to\infty} \longrightarrow$$

mono-energetic / idealization

$$\frac{1}{(2\pi)^{3/2}}A(\vec{k})\left[e^{+i\left(\vec{k}.\vec{r}-\omega t\right)}+\frac{e^{+i(kr-\omega t)}}{r}\left\{\frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left[e^{2i\delta_l(k)}-1\right]P_l(\cos\theta)\right\}\right]$$

$$\frac{d\sigma}{d\Omega}=\left|f(\vec{k}_i,\hat{\Omega})\right|^2$$ → monoenergetic idealization of incident beam properties

$$\Phi_{incident}(\vec{r},t)=\frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{+i\left(\vec{k}\cdot\vec{r}-\omega t\right)}\right]$$

$$=\frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{+i\left(\vec{k}\cdot\vec{r}-\omega(k)t\right)}\right]$$

Realistic incident wave packet

Does the expression for the differential scattering cross-section, *which is* $\frac{d\sigma}{d\Omega}=\left|f(\vec{k}_i,\hat{\Omega})\right|^2$ *hold good even to describe scattering of the wave packet?*

$$\Phi_{incident}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{+i\left(\vec{k}\cdot\vec{r}-\omega t\right)} \right]$$

$$= \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{+i\left(\vec{k}\cdot\vec{r}-\omega(k)t\right)} \right]$$

Realistic incident wave packet

$A(\vec{k})$ can be determined if the

wave-packet is known at t=0

$$\Phi_{incident}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{+i\left(\vec{k}\cdot\vec{r}-\omega t\right)} \right]$$

Realistic incident wave packet

$$= \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{+i\left(\vec{k}\cdot\vec{r}-\omega(k)t\right)} \right]$$

$$\omega(k) = \frac{E(k)}{\hbar} = \frac{\hbar^2 k^2}{2m}\frac{1}{\hbar} = \frac{\hbar k^2}{2m}$$

Group velocity

Particle velocity

$$\left[\frac{d\omega(k)}{dk}\right]_{k_i} = \frac{\hbar k_i}{m} = \mathrm{v}_i$$

$$\left[\vec{\nabla}_k \omega(\vec{k})\right]_{\vec{k}_i} = \vec{\mathrm{v}}_i$$

$$\Phi_{incident}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{+i\left(\vec{k}\cdot\vec{r} - \omega\left(\vec{k}\right)t\right)} \right]$$

Eq.3.57 / p55 / Joachain's Quantum Collision Theory

Realistic incident wave packet

$$\Phi_{incident}(\vec{r},0) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{+i\vec{k}\cdot\vec{r}} \right]$$

$A(\vec{k})$ can be determined if the wave-packet is known at t=0

$$A(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{r} \left[\Phi_{incident}(\vec{r},0) e^{-i\vec{k}\cdot\vec{r}} \right]$$

Eq.3.59 / p55 / Joachain's Quantum Collision Theory

wave-function in the momentum (rather, 'wave-vector') space known at t=0

Each individual wave $\frac{1}{(2\pi)^{3/2}} A(\vec{k}) e^{+i\left(\vec{k}\cdot\vec{r} - \omega(k)t\right)}$

travels at the phase velocity

$$v_\phi = \frac{\omega(k)}{k} = \frac{E(k)/\hbar}{k} = \frac{(\hbar k)^2/2m}{\hbar k} = \frac{\hbar k}{2m}$$

Eq.3.60 / p55 / Joachain's Quantum Collision Theory

Phase velocity is half the group velocity

$$\Phi_{incident}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{+i\left(\vec{k}\cdot\vec{r} - \omega\left(\vec{k}\right)t\right)} \right]$$

Realistic incident wave packet at t=0:

$$\Phi_{incident}(\vec{r},0) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{+i\vec{k}\cdot\vec{r}} \right]$$

narrow spread $\leftarrow \left|\overrightarrow{\Delta k}\right| \ll \left|\vec{k}_i\right|$

$$A(\vec{k}) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{r} \left[\Phi_{incident}(\vec{r},0) e^{-i\vec{k}\cdot\vec{r}} \right]$$

'spread/packed' in the region

$$\Delta r \simeq \frac{1}{\left|\overrightarrow{\Delta k}\right|}$$

Normalization:

$$\iiint d^3\vec{r} \left|\Phi_{incident}(\vec{r},0)\right|^2 = 1 = \iiint d^3\vec{k} \left|A(\vec{k})\right|^2$$

Let $A(\vec{k}) = \left|A(\vec{k})\right| e^{i\alpha\left(\vec{k}\right)}$

$$\Phi_{incident}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[\left|A(\vec{k})\right| e^{i\alpha\left(\vec{k}\right)} e^{+i\vec{k}\cdot\vec{r}} e^{-i\omega\left(\vec{k}\right)t} \right]$$

$$\Phi_{incident}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{+i\left(\vec{k}\cdot\vec{r} - \omega\left(\vec{k}\right)t\right)} \right]$$

Realistic incident wave packet at t=0:

Let $A(\vec{k}) = \left|A(\vec{k})\right| e^{i\alpha\left(\vec{k}\right)}$

$$\Phi_{incident}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[\left|A(\vec{k})\right| e^{i\alpha\left(\vec{k}\right)} e^{+i\vec{k}\cdot\vec{r}} e^{-i\omega\left(\vec{k}\right)t} \right]$$

$$\Phi_{incident}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left|A(\vec{k})\right| e^{i\beta\left(\vec{k}\right)}$$

$$\beta\left(\vec{k}\right) = \vec{k}\cdot\vec{r} - \omega(\vec{k})t + \alpha\left(\vec{k}\right)$$

Eq.3.65, 3.66 / p56 / Joachain's Quantum Collision Theory

$$\Phi_{incident}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[\left| A(\vec{k}) \right| e^{i\beta\left(\vec{k}\right)} \right] \quad \beta\left(\vec{k}\right) = \vec{k}\cdot\vec{r} - \omega(\vec{k})t + \alpha\left(\vec{k}\right)$$

Under what conditions is $\left|\Phi_{incident}(\vec{r},t)\right|$ the largest?

$e^{i\beta\left(\vec{k}\right)} \rightarrow$ oscillates in response to $\vec{k}$ since $\beta = \beta\left(\vec{k}\right)$

oscillating parts cancel each other's contributions to $\Phi_{incident}(\vec{r},t)$

For $\left|\Phi_{incident}(\vec{r},t)\right|$ to be large, these oscillations must not happen

β must not vary very much with respect to $\vec{k}$

The required condition is:

$$\left[\vec{\nabla}_k \beta(k)\right]_{\vec{k}=\vec{k}_i} = 0$$

condition for $\left|\Phi_{incident}(\vec{r},t)\right|$ to be the largest

$$\left[\vec{\nabla}_k \beta(k)\right]_{\vec{k}=\vec{k}_i} = 0$$

$$\beta\left(\vec{k}\right) = \vec{k}\cdot\vec{r} - \omega(\vec{k})t + \alpha\left(\vec{k}\right)$$
$$= kz - \omega(\vec{k})t + \alpha\left(\vec{k}\right)$$

Eq.3.65, 3.66 / p56 / Joachain's Quantum Collision Theory

1-dimensional case →

$$0 = \left.\frac{d\beta(k)}{dk}\right]_{k_i} = z - \left[\frac{d\omega(k)}{dk}\right]_{k_i} t + \left[\frac{d\alpha(k)}{dk}\right]_{k_i}$$

i.e. $z = \left[\frac{d\omega(k)}{dk}\right]_{k_i} t - \left[\frac{d\alpha(k)}{dk}\right]_{k_i}$

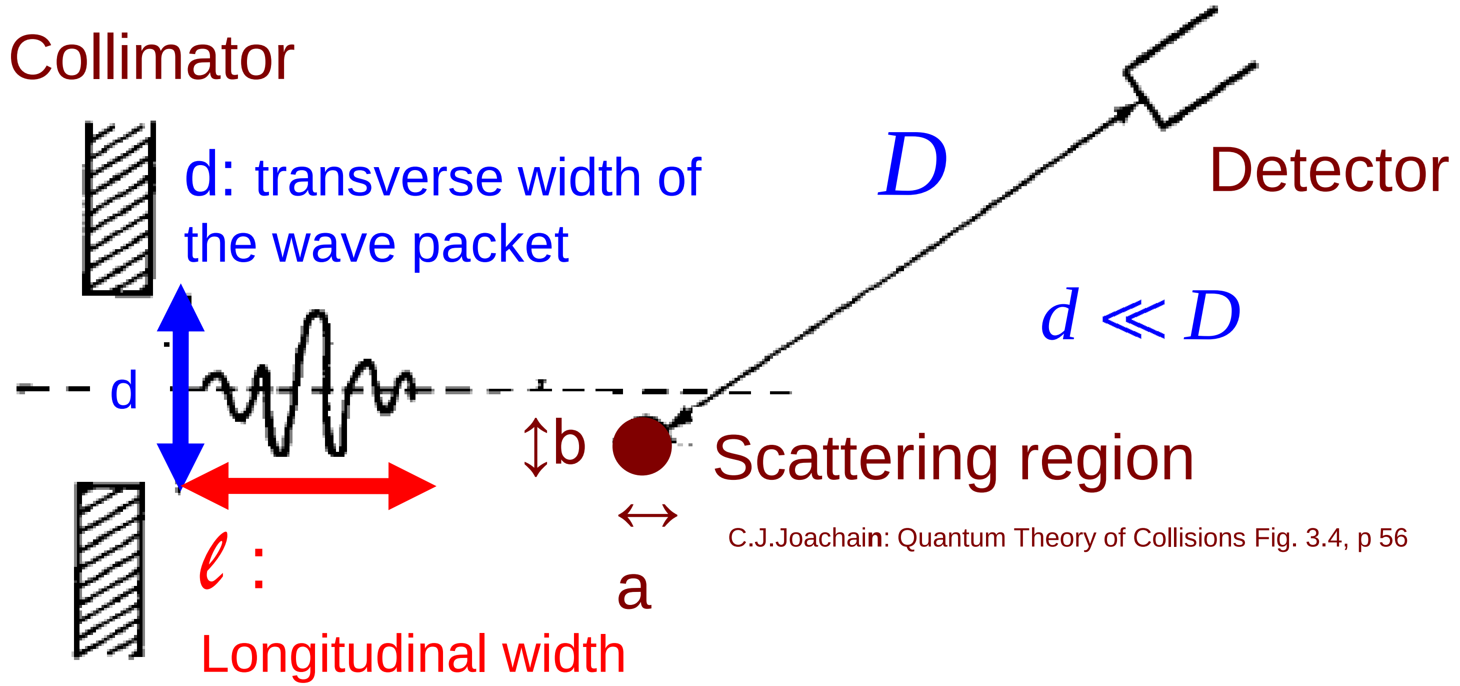
3-dimensional case →

$$\vec{r}(t) = \left[\vec{\nabla}_k \omega(\vec{k})\right]_{\vec{k}_i} t - \left[\vec{\nabla}_k \alpha(\vec{k})\right]_{\vec{k}_i}$$

Time origin: t_0 →

$$\vec{r}(t) = \vec{v}_i\left(t - t_0\right) + \vec{r}_0$$

since $\vec{v}_i = \left[\vec{\nabla}_k \omega(\vec{k})\right]_{\vec{k}_i}$ & $\vec{r}_0 = -\left[\vec{\nabla}_k \alpha(\vec{k})\right]_{\vec{k}_i}$



$$\ell \simeq \frac{1}{\Delta k}$$

$$d \simeq \ell \simeq \Delta r \simeq \frac{1}{\Delta k}$$

Schematic diagram of the characteristic lengths describing the scattering of a wave packet by a potential

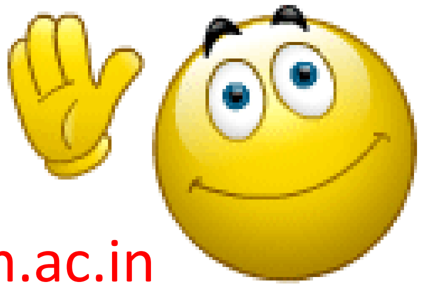
$$\Phi_{incident}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[\left| A(\vec{k}) \right| e^{i\beta\left(\vec{k}\right)} \right] \qquad \beta\left(\vec{k}\right) = \vec{k}\cdot\vec{r} - \omega(\vec{k})t + \alpha\left(\vec{k}\right)$$

$$\Phi_{incident}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[\left| A(\vec{k}) \right| e^{i\left\{\vec{k}\cdot\vec{r} - \omega(\vec{k})t + \alpha\left(\vec{k}\right)\right\}} \right]$$

$$\omega(\vec{k}) = \omega(\vec{k}_i) + \left[\vec{\nabla}_k \omega\left(\vec{k}\right) \right]_{\vec{k}_i} \cdot \left(\vec{k} - \vec{k}_i \right) + \ldots$$

$$= \omega(\vec{k}_i) + \vec{v}_i \cdot \left(\vec{k} - \vec{k}_i \right) + \ldots$$

$$= \omega(\vec{k}_i) + \vec{v}_i \cdot \vec{k} - \vec{v}_i \cdot \vec{k}_i + \ldots$$



QUESTIONS ? Write to: pcd@physics.iitm.ac.in

INTRODUCTORY lecture about this course on

Select/Special Topics from

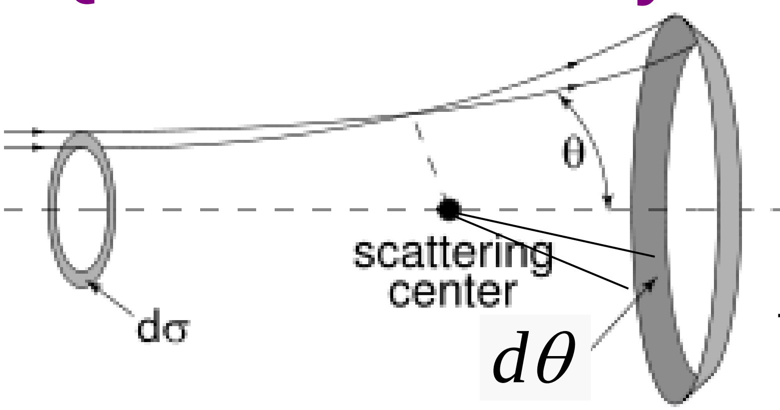
'Theory of Atomic Collisions and Spectroscopy'

P. C. Deshmukh

Department of Physics
Indian Institute of Technology Madras
Chennai 600036

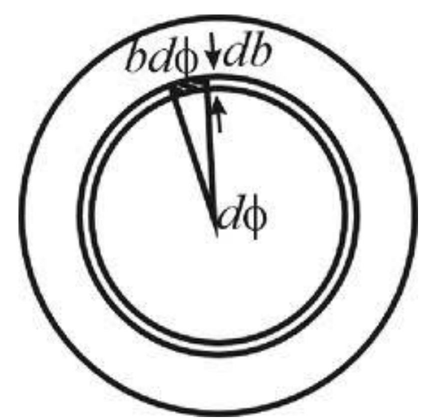
Unit 1 Lecture Number 05

Quantum Theory of Collisions



Differential scattering cross-section

$$\frac{d\sigma}{d\Omega} = \left| f(\vec{k}_i, \hat{\Omega}) \right|^2$$



$$\psi^{+}_{\vec{k}_i}(\vec{r}; r\to\infty) \underset{r\to\infty}{\longrightarrow} A(\vec{k}_i)\left[e^{i\vec{k}_i\bullet\vec{r}} + \frac{f(\hat{\Omega})}{r}e^{ikr}\right]$$

scattering x-sec
per unit solid angle
differential x-sec

$$\frac{d\sigma}{d\Omega} = \left|f(\hat{\Omega})\right|^2$$

$$\left.\psi^{+}_{Tot}(\vec{r},t)\right]_{r\to\infty}\longrightarrow$$

$$\frac{1}{(2\pi)^{3/2}}A(\vec{k})\left[e^{+i(\vec{k}.\vec{r}-\omega t)} + \frac{e^{+i(kr-\omega t)}}{r}\left\{\frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left[e^{2i\delta_l(k)}-1\right]P_l(\cos\theta)\right\}\right]$$

We employed mono-energetic incident beam → idealization

$$\psi^{+}_{Tot}(\vec{r},t)\Big]_{r\to\infty} \longrightarrow$$

mono-energetic / idealization

$$\frac{1}{(2\pi)^{3/2}} A(\vec{k})\left[e^{+i\left(\vec{k}.\vec{r}-\omega t\right)} + \frac{e^{+i(kr-\omega t)}}{r}\left\{ \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left[e^{2i\delta_l(k)}-1\right]P_l(\cos\theta)\right\}\right]$$

$$\frac{d\sigma}{d\Omega} = \left| f(\vec{k}_i,\hat{\Omega})\right|^2$$

$\rightarrow$ monoenergetic idealization of incident beam properties

$$\Phi_{incident}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{+i\left(\vec{k}\cdot\vec{r}-\omega t\right)}\right]$$

$$= \frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{+i\left(\vec{k}\cdot\vec{r}-\omega(k)t\right)}\right]$$

Realistic incident wave packet

Does the expression for the differential scattering cross-section,

which is

$$\frac{d\sigma}{d\Omega} = \left| f(\vec{k}_i,\hat{\Omega})\right|^2$$

hold good even to describe scattering of the wave packet?

$$\Phi_{incident}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{+i(\vec{k}\cdot\vec{r}-\omega(k)t)} \right]$$

$$A(\vec{k}) = \left|A(\vec{k})\right| e^{i\alpha(\vec{k})}$$

$$\Phi_{incident}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[\left|A(\vec{k})\right| e^{i\beta(\vec{k})} \right] \quad \beta(\vec{k}) = \vec{k}\cdot\vec{r} - \omega(\vec{k})t + \alpha(\vec{k})$$

Under what conditions is $\left|\Phi_{incident}(\vec{r},t)\right|$ the largest?

$e^{i\beta(\vec{k})} \rightarrow$ oscillates in response to $\vec{k}$ since $\beta = \beta(\vec{k})$

oscillating parts cancel each other's contributions to $\Phi_{incident}(\vec{r},t)$

For $\left|\Phi_{incident}(\vec{r},t)\right|$ to be large, these oscillations must not happen

β must not vary very much with respect to $\vec{k}$

The required condition is: $\left[\vec{\nabla}_k \beta(k)\right]_{\vec{k}=\vec{k}_i} = 0$

$$\left[\vec{\nabla}_k \beta(k)\right]_{\vec{k}=\vec{k}_i} = 0$$

condition for $\left|\Phi_{incident}(\vec{r},t)\right|$ to be the largest

$$\beta(\vec{k}) = \vec{k}\cdot\vec{r} - \omega(\vec{k})t + \alpha(\vec{k})$$
$$= kz - \omega(\vec{k})t + \alpha(\vec{k})$$

Eq.3.65, 3.66 / p56 / Joachain's Quantum Collision Theory

1-dimensional case →

$$0 = \left.\frac{d\beta(k)}{dk}\right]_{k_i} = z - \left[\frac{d\omega(k)}{dk}\right]_{k_i} t + \left[\frac{d\alpha(k)}{dk}\right]_{k_i}$$

i.e. $z = \left[\frac{d\omega(k)}{dk}\right]_{k_i} t - \left[\frac{d\alpha(k)}{dk}\right]_{k_i}$

3-dimensional case →

$$\vec{r}(t) = \left[\vec{\nabla}_k \omega(\vec{k})\right]_{\vec{k}_i} t - \left[\vec{\nabla}_k \alpha(\vec{k})\right]_{\vec{k}_i}$$

Time origin: t_0 →

$$\vec{r}(t) = \vec{v}_i\left(t - t_0\right) + \vec{r}_0$$

since $\vec{v}_i = \left[\vec{\nabla}_k \omega(\vec{k})\right]_{\vec{k}_i}$ & $\vec{r}_0 = -\left[\vec{\nabla}_k \alpha(\vec{k})\right]_{\vec{k}_i}$

$$\Phi_{incident}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[\left|A(\vec{k})\right| e^{i\beta(\vec{k})} \right] \qquad \beta(\vec{k}) = \vec{k}\cdot\vec{r} - \omega(\vec{k})t + \alpha(\vec{k})$$

$$\Phi_{incident}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[\left|A(\vec{k})\right| e^{i\left\{\vec{k}\cdot\vec{r} - \omega(\vec{k})t + \alpha(\vec{k})\right\}} \right]$$

$$\omega(\vec{k}) = \omega(\vec{k}_i) + \left[\vec{\nabla}_k \omega(\vec{k})\right]_{\vec{k}_i} \cdot (\vec{k} - \vec{k}_i) + \dots$$

$$= \omega(\vec{k}_i) + \vec{v}_i \cdot (\vec{k} - \vec{k}_i) + \dots$$

$$= \omega(\vec{k}_i) + \vec{v}_i \cdot \vec{k} - \vec{v}_i \cdot \vec{k}_i + \dots$$

Can we neglect higher order terms?

$$\vec{v}_i = \left[\vec{\nabla}_k \omega(\vec{k})\right]_{\vec{k}_i}$$

$$= \left[\vec{\nabla}_k \left(\frac{\hbar^2 k^2}{2m} \times \frac{1}{\hbar}\right)\right]_{\vec{k}_i}$$

$$= \frac{2\hbar^2 \vec{k}_i}{2m} \times \frac{1}{\hbar} = \frac{\hbar \vec{k}_i}{m}$$

$$\vec{v}_i \cdot \vec{k}_i = \frac{\hbar k_i^2}{m} = 2\omega(k_i)$$

since $\omega(k) = \frac{E(k)}{\hbar} = \frac{\hbar^2 k^2}{2m}\frac{1}{\hbar} = \frac{\hbar k^2}{2m}$

$$\omega(\vec{k}) = \omega(\vec{k}_i) + \vec{v}_i \cdot \vec{k} - 2\omega(\vec{k}_i) + \dots$$

$$\boxed{\omega(\vec{k}) = -\omega(\vec{k}_i) + \vec{v}_i \cdot \vec{k} + \dots}$$

$$\Phi_{incident}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[\left| A(\vec{k}) \right| e^{i\left\{\vec{k}\cdot\vec{r} - \omega(\vec{k})t + \alpha(\vec{k})\right\}} \right]$$

$$\omega(\vec{k}) \approx -\omega(\vec{k}_i) + \vec{\mathrm{v}}_i \cdot \vec{k}$$

$$\Phi_{incident}(\vec{r},t) =$$

$$\frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[\left| A(\vec{k}) \right| e^{i\left\{\vec{k}\cdot\vec{r} + \omega(\vec{k}_i)t - \vec{\mathrm{v}}_i\cdot\vec{k}t + \alpha(\vec{k})\right\}} \right]$$

$$\Phi_{incident}(\vec{r},t) =$$

$$\frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[\left| A(\vec{k}) \right| e^{i\left\{\vec{k}\cdot(\vec{r} - \vec{\mathrm{v}}_i t) + \omega(\vec{k}_i)t + \alpha(\vec{k})\right\}} \right]$$

$$\Phi_{incident}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[\left|A(\vec{k})\right| e^{i\left\{\vec{k}\cdot(\vec{r}-\vec{\mathrm{v}}_i t)+\omega(\vec{k}_i)t+\alpha(\vec{k})\right\}} \right]$$

$$\alpha(\vec{k}) = \alpha(\vec{k}_i) + \left[\vec{\nabla}_k \alpha(\vec{k})\right]_{\vec{k}_i} \cdot \left(\vec{k}-\vec{k}_i\right) + \ldots$$

$$\alpha(\vec{k}) = \alpha(\vec{k}_i) + \left[-\vec{r}_0\right] \cdot \left(\vec{k}-\vec{k}_i\right) + \ldots \quad \text{with } \left(-\vec{r}_0\right) = \left[\vec{\nabla}_k \alpha(\vec{k})\right]_{\vec{k}_i}$$

Can we neglect higher order terms?

$$\Phi_{incident}(\vec{r},t) =$$

$$\frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[\left|A(\vec{k})\right| e^{i\left\{\vec{k}\cdot(\vec{r}-\vec{\mathrm{v}}_i t)+\omega(\vec{k}_i)t+\alpha(\vec{k}_i)-\vec{r}_0\cdot\left(\vec{k}-\vec{k}_i\right)\right\}} \right]$$

$$= \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[\left|A(\vec{k})\right| e^{i\left\{\vec{k}\cdot(\vec{r}-\vec{\mathrm{v}}_i t)+\omega(\vec{k}_i)t+\alpha(\vec{k}_i)-\vec{r}_0\cdot\vec{k}+\vec{r}_0\cdot\vec{k}_i\right\}} \right]$$

$$\Phi_{incident}(\vec{r},t) =$$

$$= \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[\left| A(\vec{k}) \right| e^{i\left\{ \vec{k}\cdot(\vec{r}-\vec{\mathrm{v}}_i t) + \omega(\vec{k}_i)t + \alpha(\vec{k}_i) - \vec{r}_0\cdot\vec{k} + \vec{r}_0\cdot\vec{k}_i \right\}} \right]$$

$$\alpha(\vec{k}) = \alpha(\vec{k}_i) - \vec{r}_0\cdot\vec{k} + \vec{r}_0\cdot\vec{k}_i$$

$$\Phi_{incident}(\vec{r},t) =$$

$$= \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[\left| A(\vec{k}) \right| e^{i\left\{ \vec{k}\cdot(\vec{r}-\vec{\mathrm{v}}_i t) + \omega(\vec{k}_i)t + \alpha(\vec{k}) \right\}} \right]$$

$$\Phi_{incident}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{i\left\{ \vec{k}\cdot(\vec{r}-\vec{\mathrm{v}}_i t) + \omega(\vec{k}_i)t \right\}} \right]$$

since $A(\vec{k}) = \left| A(\vec{k}) \right| e^{i\alpha(\vec{k})}$

$$\Phi_{incident}(\vec{r},t)=\frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{i\left\{\vec{k}\cdot(\vec{r}-\vec{v}_i t)+\omega(\vec{k}_i)t\right\}}\right]$$

$$\Phi_{incident}(\vec{r},t)=$$
$$e^{i\omega(\vec{k}_i)(t-t_0)}\frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{i\vec{k}\cdot(\vec{r}-\vec{v}_i t)}e^{i\omega(\vec{k}_i)t_0}\right]$$

note

$$\Phi_{incident}(\vec{r},0)=\frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{+i\vec{k}\cdot\vec{r}}\right]$$

same form

$$\Rightarrow \Phi_{incident}(\vec{r},t)=e^{i\omega(\vec{k}_i)(t-t_0)}\Phi_{incident}\left(\vec{r}(t)-\vec{v}_i(t-t_0),t_0\right)$$

Eq.3.79 / p57 / Joachain's Quantum Collision Theory

$$\vec{r}(t)=\vec{r}_0+\vec{v}_i(t-t_0);\quad \text{i.e.}\quad \vec{r}(t)-\vec{v}_i(t-t_0)=\vec{r}_0$$

$$\Phi_{incident}(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{+i(\vec{k}\cdot\vec{r}-\omega(k)t)} \right]$$

Realistic incident wave packet

$$= e^{i\omega(\vec{k}_i)(t-t_0)} \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{i\vec{k}\cdot(\vec{r}-\vec{v}_i t)} e^{i\omega(\vec{k}_i)t_0} \right]$$

since $\Phi_{incident}(\vec{r},0) = \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{+i\vec{k}\cdot\vec{r}} \right]$

$$\Phi_{incident}(\vec{r},t) = e^{i\omega(\vec{k}_i)(t-t_0)} \Phi_{incident}\left(\vec{r}(t) - \vec{v}_i(t-t_0), t_0\right)$$

$$\vec{r}(t) = \vec{r}_0 + \vec{v}_i(t-t_0); \quad \text{i.e.} \quad \vec{r}(t) - \vec{v}_i(t-t_0) = \vec{r}_0$$

free wave packet centered around the point $\vec{r}_0$ at time t_0 will have same shape as a wave packet centered around the point $\vec{r}_0 + \vec{v}_i(t-t_0)$ at time t

$$\omega(\vec{k}) = \omega(\vec{k}_i) + \left[\vec{\nabla}_k \omega\left(\vec{k}\right)\right]_{\vec{k}_i} \cdot \left(\vec{k} - \vec{k}_i\right) + \ldots$$

$$= \omega(\vec{k}_i) + \vec{\mathrm{v}}_i \cdot \left(\vec{k} - \vec{k}_i\right) + \ldots$$

Higher order terms ignored

Can we neglect higher order terms?

$$\alpha(\vec{k}) = \alpha(\vec{k}_i) + \left[\vec{\nabla}_k \alpha(\vec{k})\right]_{\vec{k}_i} \cdot \left(\vec{k} - \vec{k}_i\right) + \ldots$$

$$\alpha(\vec{k}) = \alpha(\vec{k}_i) + \left[-\vec{r}_0\right] \cdot \left(\vec{k} - \vec{k}_i\right) + \ldots$$

Under what conditions can we ignore higher order terms?

$$\omega(k) = \omega(k_i) + \left[\frac{d\omega(\vec{k})}{dk}\right]_{k_i} \cdot (k - k_i) + \ldots$$

$$\omega(\vec{k}) = \omega(\vec{k}_i) + \vec{v}_i \cdot (\vec{k} - \vec{k}_i) + ..$$
$$= -\omega(\vec{k}_i) + \vec{v}_i \cdot \vec{k} + ..$$

condition to ignore higher order terms:

$$\left[\frac{d^2\omega(\vec{k})}{dk^2}\right]_{k_i} (k - k_i)^2 \rightarrow small$$

$$\omega(k) = \frac{E(k)}{\hbar} = \frac{\hbar^2 k^2}{2m}\frac{1}{\hbar} = \frac{\hbar k^2}{2m}$$

$$\frac{d\omega(k)}{dk} = \frac{2\hbar k}{2m} = \frac{\hbar k}{m}$$

$$\frac{d^2\omega(k)}{dk^2} = \frac{\hbar}{m}$$

$$\frac{\hbar}{m}(k - k_i)^2 t \lll 1$$

$$t \leq \left(2D \big/ v_i \right)$$

Phase velocity;
half the group velocity

$$\frac{\hbar}{m}(\Delta k)^2 \left(\frac{2D}{v_i}\right) \lll 1$$

$$\frac{\hbar}{m}(\Delta k)^2\left(\frac{2mD}{\hbar k_i}\right) \lll 1 \qquad \text{i.e.} \quad \frac{(\Delta k)^2}{k_i}2D \lll 1$$

$$recall: \quad (\Delta k)(\Delta r) \sim 1 \Rightarrow (\Delta k) \simeq (\Delta r)^{-1}$$

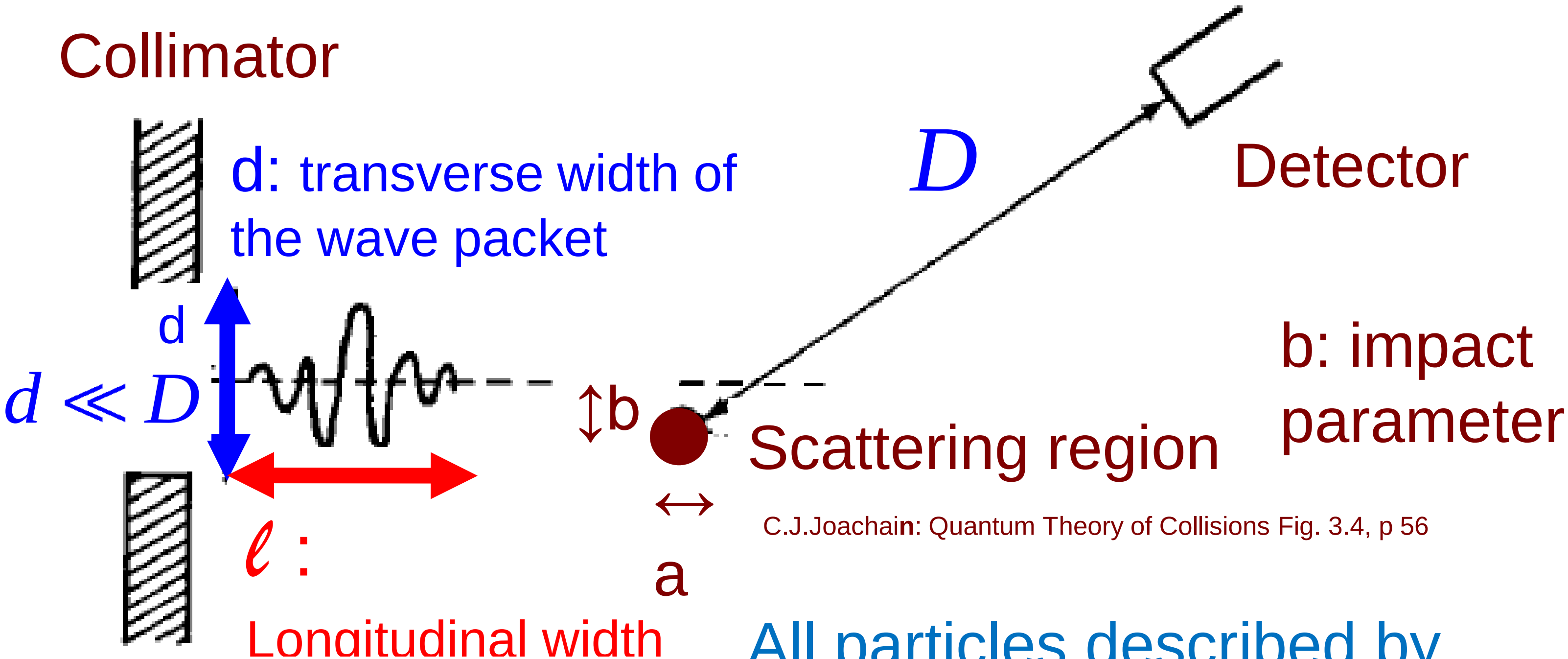
$$\therefore \quad \lambda_i 2D \lll (\Delta r)^2$$

$$\text{i.e.} \quad \sqrt{\lambda_i 2D} \lll (\Delta r)$$

In most experiments: $10^{-3} cm$ $\qquad$ $10^{-1} cm$

✓

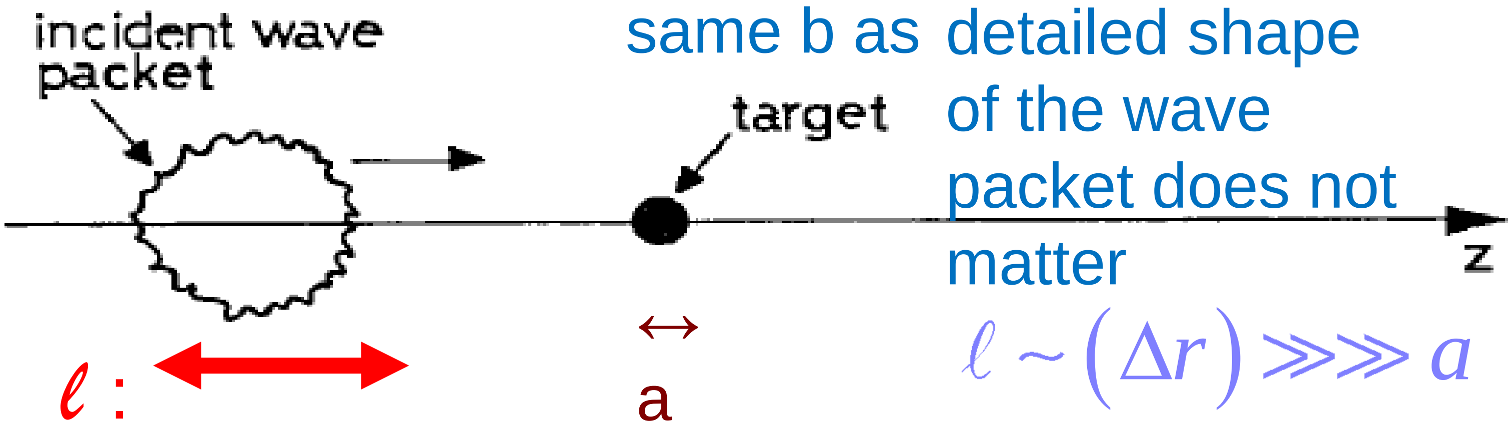
Hence we can indeed ignore higher order terms.



C.J.Joachain: Quantum Theory of Collisions Fig. 3.4, p 56

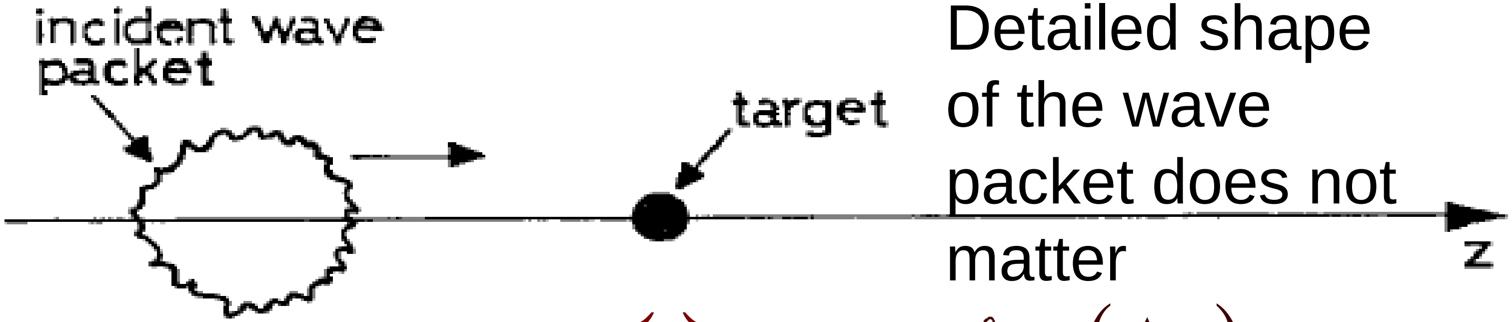
All particles described by same b as detailed shape of the wave packet does not matter

$$\ell \sim (\Delta r) \ggg a$$



Longitudinal width

C.J.Joachain: Quantum Theory of Collisions Fig. 3.5, p 58



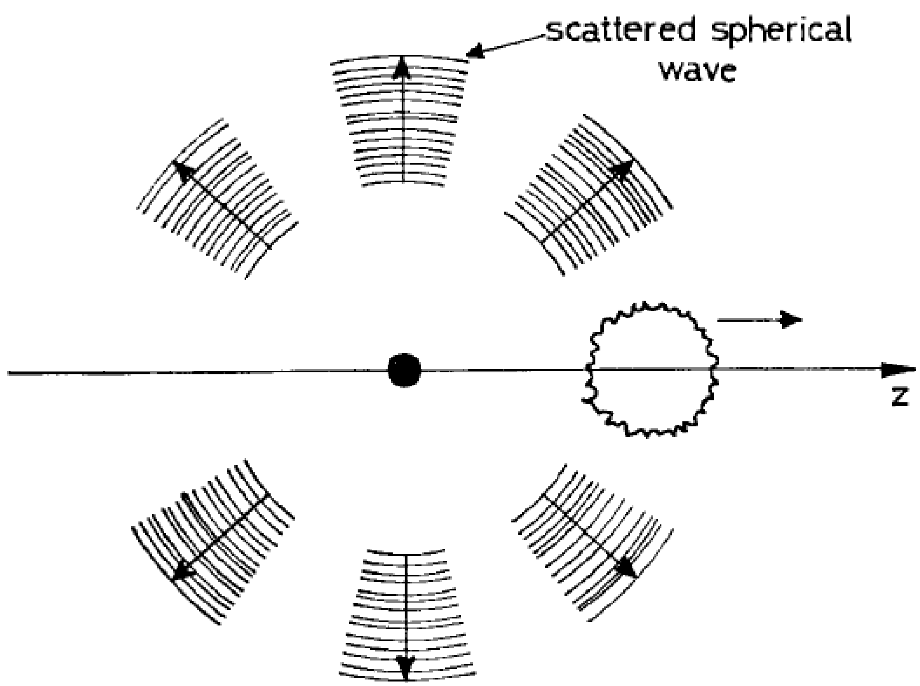
Detailed shape of the wave packet does not matter

$\ell \sim (\Delta r) \ggg a$

ℓ : ⟷ Longitudinal width

↔ a

C.J.Joachain: Quantum Theory of Collisions Fig. 3.5, p 58



Free particle wave packet

$$\Phi_{incident}(\vec{r},t)=\frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{+i\left(\vec{k}\cdot\vec{r}-\omega\left(\vec{k}\right)t\right)}\right]$$

$$\omega(\vec{k})=\omega(\vec{k}_i)+\vec{\mathrm{v}}_i\cdot\left(\vec{k}-\vec{k}_i\right)+..$$
$$=-\omega(\vec{k}_i)+\vec{\mathrm{v}}_i\cdot\vec{k}+..$$

$$\omega\left(k\right)=\frac{E\left(k\right)}{\hbar}=\frac{\hbar^2k^2}{2m}\frac{1}{\hbar}=\frac{\hbar k^2}{2m}$$

Free particle wave packet impacting at $\vec{b}: impact\ parameter$

$$\Phi_{\vec{b}}(\vec{r},t)=\frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{+i\left\{\vec{k}\cdot\left(\vec{r}-\vec{b}\right)-\omega\left(\vec{k}\right)t\right\}}\right]$$

C.J.Joachain: Quantum Theory of Collisions Eq. 3.86, p 58

$$\Phi_{\vec{b}}(\vec{r},t)=\frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{-i\vec{k}\cdot\vec{b}}\ e^{+i\vec{k}\cdot\vec{r}}\ e^{-i\omega\left(\vec{k}\right)t}\right]$$

$$\Phi_{\vec{b}}(\vec{r},t)=\frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{-i\vec{k}\cdot\vec{b}}\ e^{+i\vec{k}\cdot\vec{r}}\ e^{+i\omega\left(\vec{k}_i\right)t}\ e^{-i\vec{k}\cdot\vec{\mathrm{v}}_it}\right]$$

$$\Phi_{\vec{b}}(\vec{r},t)=\frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{-i\vec{k}\cdot\vec{b}}\ e^{+i\vec{k}\cdot\vec{r}}\ e^{+i\omega(\vec{k}_i)t}\ e^{-i\vec{k}\cdot\vec{\mathrm{v}}_i t}\right]$$

multiplying the integrand by:

$$\left\{e^{+i\vec{k}_i\cdot(\vec{r}-\vec{b})}e^{-i\vec{k}_i\cdot\vec{\mathrm{v}}_i t}\right\}\times\left\{e^{-i\vec{k}_i\cdot(\vec{r}-\vec{b})}e^{+i\vec{k}_i\cdot\vec{\mathrm{v}}_i t}\right\}=1$$

$$\Phi_{\vec{b}}(\vec{r},t)=\frac{1}{(2\pi)^{3/2}}e^{+i\omega(\vec{k}_i)t}e^{+i\vec{k}_i\cdot(\vec{r}-\vec{b})}e^{-i\vec{k}_i\cdot\vec{\mathrm{v}}_i t}\times$$

$$\iiint d^3\vec{k}\left[A(\vec{k})\ e^{+i(\vec{k}-\vec{k}_i)\cdot(\vec{r}-\vec{b})}\ e^{-i(\vec{k}-\vec{k}_i)\cdot\vec{\mathrm{v}}_i t}\right]$$

$$\Phi_{\vec{b}}(\vec{r},t)=\frac{1}{(2\pi)^{3/2}}e^{+i\omega(\vec{k}_i)t}e^{+i\vec{k}_i\cdot(\vec{r}-\vec{b})}e^{-i\vec{k}_i\cdot\vec{\mathrm{v}}_it}\times$$

$$\iiint d^3\vec{k}\left[A(\vec{k})\,e^{+i(\vec{k}-\vec{k}_i)\cdot(\vec{r}-\vec{b})}\;e^{-i(\vec{k}-\vec{k}_i)\cdot\vec{\mathrm{v}}_it}\right]$$

$$\Phi_{\vec{b}}(\vec{r},t)=\frac{1}{(2\pi)^{3/2}}e^{+i\omega(\vec{k}_i)t}e^{+i\vec{k}_i\cdot(\vec{r}-\vec{b}-\vec{\mathrm{v}}_it)}\times$$

$$\iiint d^3\vec{k}\left[A(\vec{k})\,e^{+i(\vec{k}-\vec{k}_i)\cdot(\vec{r}-\vec{b}-\vec{\mathrm{v}}_it)}\right]$$

$$\Phi_{\vec{b}}(\vec{r},t)=e^{+i\left\{\vec{k}_i\cdot(\vec{r}-\vec{b}-\vec{\mathrm{v}}_it)+\omega(\vec{k}_i)t\right\}}\chi\left(\vec{r}-\vec{b}-\vec{\mathrm{v}}_it\right)$$

$$\chi\left(\vec{r}-\vec{b}-\vec{\mathrm{v}}_it\right)=\frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})\,e^{+i(\vec{k}-\vec{k}_i)\cdot(\vec{r}-\vec{b}-\vec{\mathrm{v}}_it)}\right]$$

← determines the shape of the wave packet

Eq.3.88 / p.58 / Joachain's QCT

$$\Phi_{\vec{b}}(\vec{r},t) = e^{+i\left\{\vec{k}_i\cdot\left(\vec{r}-\vec{b}-\vec{\mathrm{v}}_i t\right)+\omega\left(\vec{k}_i\right)t\right\}}\chi\left(\vec{r}-\vec{b}-\vec{\mathrm{v}}_i t\right)$$

$$\chi\left(\vec{r}-\vec{b}-\vec{\mathrm{v}}_i t\right) = \frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})\, e^{+i\left(\vec{k}-\vec{k}_i\right)\cdot\left(\vec{r}-\vec{b}-\vec{\mathrm{v}}_i t\right)}\right]$$

←determines the shape of the wave packet

Recall that:

Normalization:

$$\iiint d^3\vec{r}\ \left|\Phi_{incident}(\vec{r},0)\right|^2 = 1 = \iiint d^3\vec{k}\ \left|A(\vec{k})\right|^2$$

$$\Rightarrow \iiint d^3\vec{s}\ \left|\chi(\vec{s})\right|^2 = 1$$

Free particle wave packet interacting with the scatterer at $\vec{b}$: *impact parameter*

$$\Phi_{\vec{b}}(\vec{r},t)=\frac{1}{(2\pi)^{3/2}}e^{+i\left\{\vec{k}_i\cdot\left(\vec{r}-\vec{b}-\vec{v}_i t\right)+\omega\left(\vec{k}_i\right)t\right\}}\chi\left(\vec{r}-\vec{b}-\vec{v}_i t\right)$$

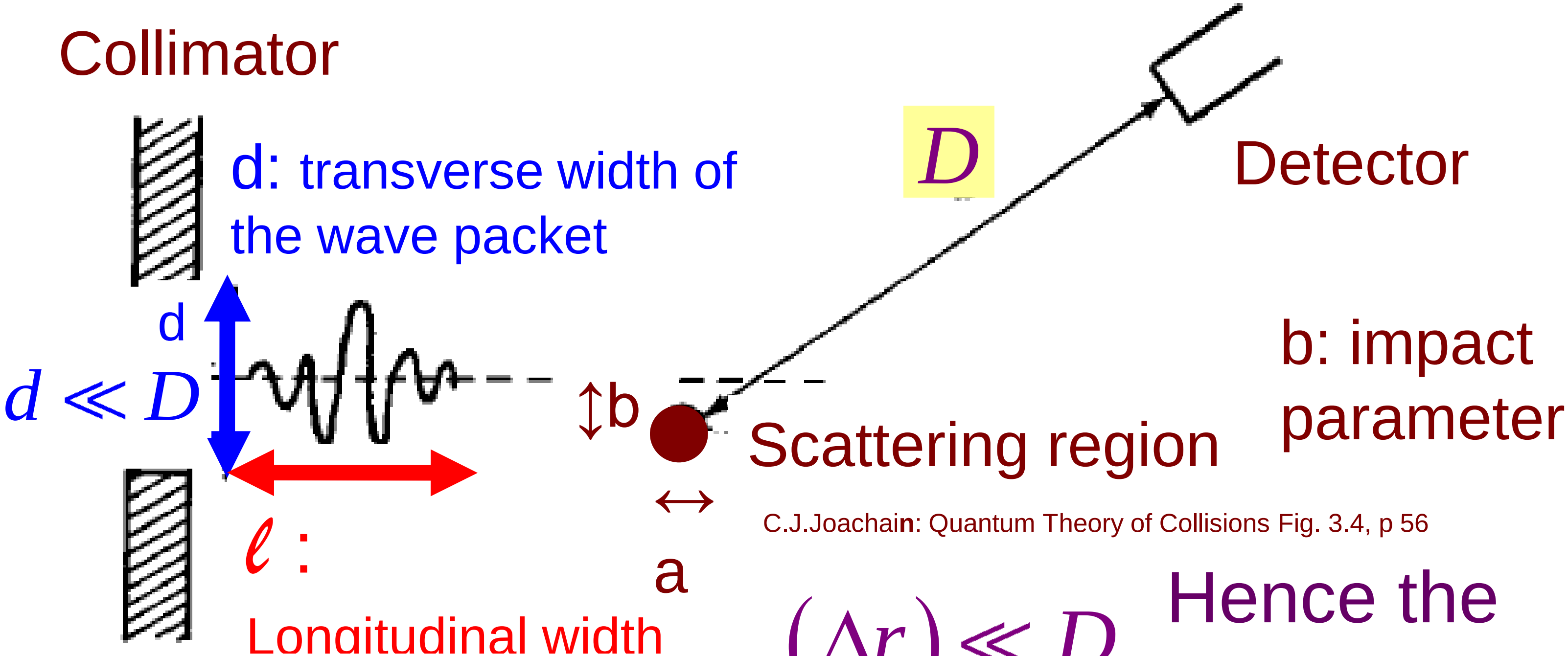
$$\Phi_{\vec{b}}(\vec{r},t)=\frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{+i\left\{\vec{k}\cdot\left(\vec{r}-\vec{b}\right)-\omega\left(\vec{k}\right)t\right\}}\right]$$

Free particle case

$$\Phi_{\vec{b}}(\vec{r},t)=\frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{-i\vec{k}\cdot\vec{b}}\,\boxed{e^{+i\vec{k}\cdot\vec{r}}}\;e^{-i\omega\left(\vec{k}\right)t}\right]$$

wave packet for the complete scattering problem

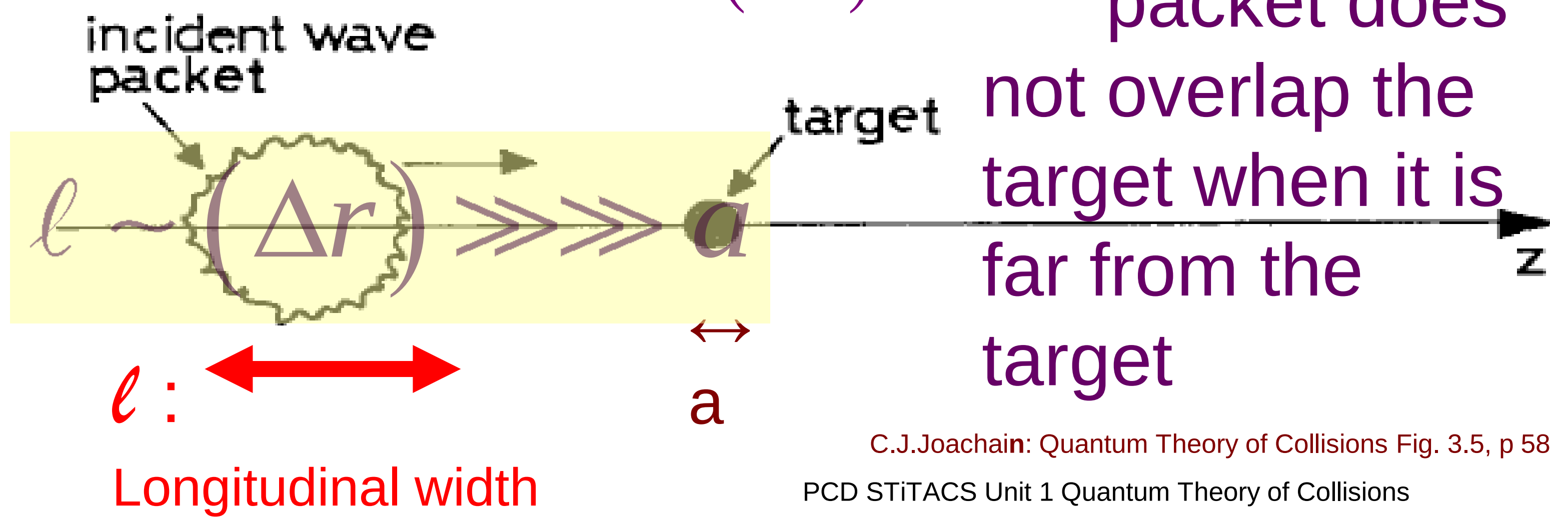
$$\Psi^{+}_{\vec{b}}(\vec{r},t)=\frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{-i\vec{k}\cdot\vec{b}}\,\boxed{\psi^{+}_{\vec{k}}(\vec{r})}\,e^{-i\omega\left(\vec{k}\right)t}\right]$$



C.J.Joachain: Quantum Theory of Collisions Fig. 3.4, p 56

$$(\Delta r) \ll D$$

Hence the packet does not overlap the target when it is far from the target

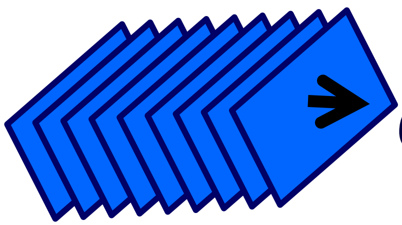


C.J.Joachain: Quantum Theory of Collisions Fig. 3.5, p 58

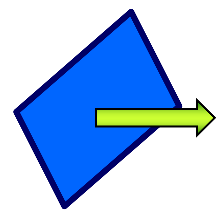
$$\psi^{+}_{\vec{k}_i}(\vec{r};r\to\infty)\xrightarrow[r\to\infty]{} A(k)\left[e^{i\vec{k}_i\bullet\vec{r}}+\frac{f(\hat{\Omega})}{r}e^{ikr}\right]$$

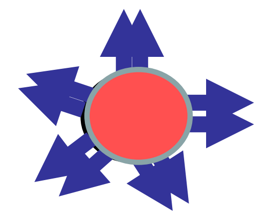
wave packet for the complete scattering problem

$$\Psi^{+}_{\vec{b}}(\vec{r},t)=\frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{-i\vec{k}\cdot\vec{b}}\ \ \psi^{+}_{\vec{k}}(\vec{r})\ e^{-i\omega(\vec{k})t}\right]$$



$$e^{+i(kz-\omega t)}\qquad \hat{k}_i=\hat{e}_z$$



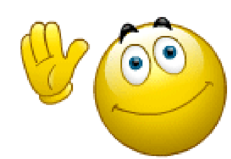


In the next class, we complete the proof that:

$$\frac{d\sigma}{d\Omega}=\left|f(\vec{k}_i,\hat{\Omega})\right|^2$$

is appropriate expression even to describe scattering of the wave packet.

QUESTIONS ? Write to: pcd@physics.iitm.ac.in



INTRODUCTORY lecture about this course on

Select/Special Topics from

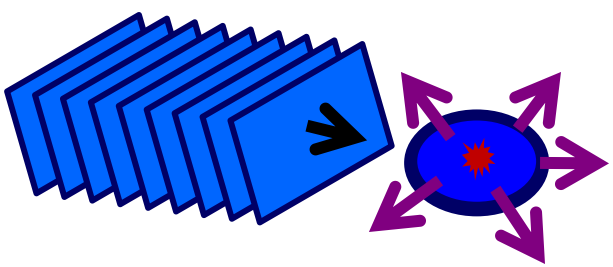
'Theory of Atomic Collisions and Spectroscopy'

P. C. Deshmukh

Department of Physics
Indian Institute of Technology Madras
Chennai 600036

Unit 1 Lecture Number 06

Quantum Theory of Collisions



i) Differential x-sec (wave-packets)

$$\frac{d\sigma}{d\Omega} = \left| f(\vec{k}_i, \hat{\Omega}) \right|^2$$

ii) Partial wave analysis

Reference:
Quantum Collision Theory
– C.J.Joachain Chapters 3 & 4

Free particle wave packet interacting with the scatterer at $\vec{b}$: *impact parameter*

$$\Phi_{\vec{b}}(\vec{r},t)=\frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{-i\vec{k}\cdot\vec{b}}\boxed{e^{+i\vec{k}\cdot\vec{r}}}\;e^{-i\omega(\vec{k})t}\right]$$

wave packet for the complete scattering problem

$$\Psi^{+}_{\vec{b}}(\vec{r},t)=\frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{-i\vec{k}\cdot\vec{b}}\boxed{\psi^{+}_{\vec{k}}(\vec{r})}\,e^{-i\omega(\vec{k})t}\right]$$

Since the packet does not overlap the target when it is far from the target, we may use the asymptotic form: $\psi^{+}_{\vec{k}_i}(\vec{r};r\to\infty)\underset{r\to\infty}{\longrightarrow}A(k)\left[e^{i\vec{k}_i\bullet\vec{r}}+\frac{f(\hat{\Omega})}{r}e^{ikr}\right]$

$$\Psi^{+}_{\vec{b}}(\vec{r},t)\underset{r\to\infty}{\longrightarrow}\boxed{\Phi_{\vec{b}}(\vec{r},t)}+\frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{-i\vec{k}\cdot\vec{b}}\boxed{\frac{f(\hat{\Omega})}{r}e^{ikr}}\;e^{-i\omega(\vec{k})t}\right]$$

incident wave packet *scattered wave packet*

$$\Phi_{\vec{b}}(\vec{r},t)=\frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{-i\vec{k}\cdot\vec{b}}\;\; e^{+i\vec{k}\cdot\vec{r}}\;\; e^{-i\omega(\vec{k})t}\right]$$

$$\Psi^+_{\vec{b}}(\vec{r},t)\underset{r\to\infty}{\to}\Phi_{\vec{b}}(\vec{r},t)+\frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{-i\vec{k}\cdot\vec{b}}\;\;\frac{f(\hat{\Omega})}{r}\underbrace{e^{ikr}\;\; e^{-i\omega(\vec{k})t}}\right]$$

incident wave packet *scattered wave packet*

$$\Psi^+_{\vec{b}}(\vec{r},t)\underset{r\to\infty}{\to}\Phi_{\vec{b}}(\vec{r},t)+\frac{1}{(2\pi)^{3/2}}\iiint d^3\vec{k}\left[A(\vec{k})e^{-i\vec{k}\cdot\vec{b}}\;\; f(\hat{\Omega})\frac{e^{i(kr-\omega(\vec{k})t)}}{r}\right]$$

$$\Psi^+_{\vec{b}}(\vec{r},t)\;\underset{r\to\infty}{\overset{t\to-\infty}{\longrightarrow}}\;\Phi_{\vec{b}}(\vec{r},t)$$

Eef van Beveren

←←← http://cft.fis.uc.pt/eef

C.J.Joachai**n**: Quantum Theory of Collisions Eq. 3.86, p 58

$$\Psi^+_{\vec{b}}(\vec{r},t)\;\underset{r\to\infty}{\overset{t\to+\infty}{\longrightarrow}}\;\;?$$

$$\Psi^{+}_{\vec{b}}(\vec{r},t) \underset{r\to\infty}{\longrightarrow} \Phi_{\vec{b}}(\vec{r},t) + \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{-i\vec{k}\cdot\vec{b}} \; f(\hat{\Omega}) \frac{e^{i\left(kr-\omega(\vec{k})t\right)}}{r} \right]$$

$$k \simeq k_i + \hat{k}_i \cdot (\vec{k} - \vec{k}_i)$$

$$\omega(\vec{k}) \simeq \omega(\vec{k}_i) + \vec{v}_i \cdot \left(\vec{k} - \vec{k}_i\right)$$

$$e^{i\left(kr-\omega(\vec{k})t\right)} = e^{ik_i r} e^{i\hat{k}_i\cdot\left(\vec{k}-\vec{k}_i\right)r} e^{-i\omega(\vec{k}_i)t} e^{-i\vec{v}_i\cdot\left(\vec{k}-\vec{k}_i\right)t}$$

$$\Psi^{+}_{\vec{b}}(\vec{r},t) \underset{r\to\infty}{\longrightarrow} \Phi_{\vec{b}}(\vec{r},t) + \frac{1}{(2\pi)^{3/2}} \iiint d^3\vec{k} \left[A(\vec{k}) e^{-i\vec{k}\cdot\vec{b}} \; f(\vec{k},\hat{\Omega}) \frac{e^{ik_i r} e^{i\hat{k}_i\cdot\left(\vec{k}-\vec{k}_i\right)r} e^{-i\omega(\vec{k}_i)t} e^{-i\vec{v}_i\cdot\left(\vec{k}-\vec{k}_i\right)t}}{r} \right]$$

$$f(\vec{k},\hat{\Omega}) = \left| f(\vec{k},\hat{\Omega}) \right| e^{i\Lambda(\vec{k},\hat{\Omega})} \simeq \left| f(\vec{k}_i,\hat{\Omega}) \right| e^{i\Lambda(\vec{k},\hat{\Omega})}$$

$$\Psi^{+}_{\vec{b}}(\vec{r},t) \underset{r\to\infty}{\longrightarrow} \Phi_{\vec{b}}(\vec{r},t) + \frac{1}{(2\pi)^{3/2}} \left| f(\vec{k}_i,\hat{\Omega}) \right| \frac{e^{ik_i r} e^{-i\omega(\vec{k}_i)t}}{r} \iiint d^3\vec{k} \left[A(\vec{k}) e^{-i\vec{k}\cdot\vec{b}} e^{i\hat{k}_i\cdot\left(\vec{k}-\vec{k}_i\right)r} e^{-i\vec{v}_i\cdot\left(\vec{k}-\vec{k}_i\right)t} e^{i\Lambda(\vec{k},\hat{\Omega})} \right]$$

$$\Psi^{+}_{\vec{b}}(\vec{r},t) \underset{r\to\infty}{\longrightarrow} \Phi_{\vec{b}}(\vec{r},t) +$$

$$+\frac{1}{(2\pi)^{3/2}}\left|f(\vec{k}_i,\hat{\Omega})\right|\frac{e^{ik_i r}e^{-i\omega(\vec{k}_i)t}}{r}\iiint d^3\vec{k}\left[A(\vec{k})e^{-i\vec{k}\cdot\vec{b}}e^{i\hat{k}_i\cdot(\vec{k}-\vec{k}_i)r}e^{-i\vec{v}_i\cdot(\vec{k}-\vec{k}_i)t}e^{i\Lambda(\vec{k},\hat{\Omega})}\right]$$

$$\Lambda(\vec{k},\hat{\Omega}) \simeq \Lambda(\vec{k}_i,\hat{\Omega}) + \left[\vec{\nabla}_k \Lambda(\vec{k}_i,\hat{\Omega})\right]_{\vec{k}=\vec{k}_i}\cdot\left(\vec{k}-\vec{k}_i\right)$$

$$= \Lambda(\vec{k}_i,\hat{\Omega}) + \vec{\rho}(\hat{\Omega})\cdot\left(\vec{k}-\vec{k}_i\right); \qquad \left|\vec{\rho}(\hat{\Omega})\right| \ll \Delta r = \ell$$

$$\vec{\rho}(\hat{\Omega}) = \left[\vec{\nabla}_k \Lambda(\vec{k}_i,\hat{\Omega})\right]_{\vec{k}=\vec{k}_i}$$

$$\Psi^{+}_{\vec{b}}(\vec{r},t) \underset{r\to\infty}{\longrightarrow} \Phi_{\vec{b}}(\vec{r},t) +$$

$$+\left[\frac{1}{(2\pi)^{3/2}}\left|f(\vec{k}_i,\hat{\Omega})\right|\frac{e^{ik_i r}e^{-i\omega(\vec{k}_i)t}}{r}\times \iiint d^3\vec{k}\left[A(\vec{k})e^{-i\vec{k}\cdot\vec{b}}e^{i\hat{k}_i\cdot(\vec{k}-\vec{k}_i)r}e^{-i\vec{v}_i\cdot(\vec{k}-\vec{k}_i)t}e^{i\Lambda(\vec{k}_i,\hat{\Omega})}e^{i\vec{\rho}(\hat{\Omega})\cdot(\vec{k}-\vec{k}_i)}\right]\right]$$

$$\Psi^{+}_{\vec{b}}(\vec{r},t) \underset{r\to\infty}{\rightarrow} \Phi_{\vec{b}}(\vec{r},t) + \left[\frac{1}{(2\pi)^{3/2}} \left| f(\vec{k}_i,\hat{\Omega}) \right| \frac{e^{ik_i r} e^{-i\omega(\vec{k}_i)t}}{r} \times \iiint d^3\vec{k} \left[A(\vec{k}) e^{-i\vec{k}\cdot\vec{b}} e^{i\hat{k}_i\cdot(\vec{k}-\vec{k}_i)r} e^{-i\vec{v}_i\cdot(\vec{k}-\vec{k}_i)t} e^{i\Lambda(\vec{k}_i,\hat{\Omega})} e^{i\vec{\rho}(\hat{\Omega})\cdot(\vec{k}-\vec{k}_i)} \right] \right]$$

$$\Psi^{+}_{\vec{b}}(\vec{r},t) \underset{r\to\infty}{\rightarrow} \Phi_{\vec{b}}(\vec{r},t) + \left[\frac{1}{(2\pi)^{3/2}} \left| f(\vec{k}_i,\hat{\Omega}) \right| \frac{e^{ik_i r} e^{-i\omega(\vec{k}_i)t}}{r} e^{i\Lambda(\vec{k}_i,\hat{\Omega})} e^{-i\vec{k}_i\cdot\vec{b}} \times \iiint d^3\vec{k} \left[A(\vec{k}) e^{-i(\vec{k}-\vec{k}_i)\cdot\vec{b}} e^{i\left[r\hat{k}_i - \vec{v}_i t + \vec{\rho}(\hat{\Omega})\right]\cdot(\vec{k}-\vec{k}_i)} \right] \right]$$

$$\Psi^{+}_{\vec{b}}(\vec{r},t) \underset{r\to\infty}{\longrightarrow} \Phi_{\vec{b}}(\vec{r},t) +$$

$$+\left[\begin{array}{l} \dfrac{1}{(2\pi)^{3/2}} \left| f(\vec{k}_i,\hat{\Omega}) \right| \dfrac{e^{ik_i r} e^{-i\omega(\vec{k}_i)t}}{r} e^{i\Lambda(\vec{k}_i,\hat{\Omega})} e^{-i\vec{k}_i\cdot\vec{b}} \times \\ \iiint d^3\vec{k} \left[A(\vec{k}) e^{-i\left(\vec{k}-\vec{k}_i\right)\cdot\vec{b}} e^{i\left[r\hat{k}_i - \vec{\mathrm{v}}_i t + \vec{\rho}(\hat{\Omega})\right]\cdot\left(\vec{k}-\vec{k}_i\right)} \right] \end{array}\right]$$

$$\Psi^{+}_{\vec{b}}(\vec{r},t) \underset{r\to\infty}{\longrightarrow} \Phi_{\vec{b}}(\vec{r},t) +$$

$f(\vec{k}_i,\hat{\Omega})$

$$+\left[\begin{array}{l} \dfrac{1}{(2\pi)^{3/2}} \left\{ \left| f(\vec{k}_i,\hat{\Omega}) \right| e^{i\Lambda(\vec{k}_i,\hat{\Omega})} \right\} \dfrac{e^{ik_i r} e^{-i\omega(\vec{k}_i)t}}{r} e^{-i\vec{k}_i\cdot\vec{b}} \times \\ \iiint d^3\vec{k} \left[A(\vec{k}) e^{-i\left(\vec{k}-\vec{k}_i\right)\cdot\vec{b}} e^{i\left[r\hat{k}_i - \vec{\mathrm{v}}_i t + \vec{\rho}(\hat{\Omega})\right]\cdot\left(\vec{k}-\vec{k}_i\right)} \right] \end{array}\right]$$

$$\Psi^{+}_{\vec{b}}(\vec{r},t) \underset{r\to\infty}{\longrightarrow} \Phi_{\vec{b}}(\vec{r},t) +$$

$$+\left[\frac{1}{(2\pi)^{3/2}} f(\vec{k}_i,\hat{\Omega}) \frac{e^{ik_i r} e^{-i\omega(\vec{k}_i)t}}{r} e^{-i\vec{k}_i\cdot\vec{b}} \times \iiint d^3\vec{k}\left[A(\vec{k}) e^{i\left[r\hat{k}_i - \vec{\mathrm{v}}_i t + \vec{\rho}(\hat{\Omega}) - \vec{b}\right]\cdot\left(\vec{k}-\vec{k}_i\right)}\right]\right]$$

↓shape of the
↓wave packet

we had: $$(2\pi)^{-3/2}\iiint d^3\vec{k}\left[A(\vec{k})\, e^{+i\left(\vec{k}-\vec{k}_i\right)\cdot\left(\vec{r}-\vec{b}-\vec{\mathrm{v}}_i t\right)}\right] = \chi\left(\vec{r}-\vec{b}-\vec{\mathrm{v}}_i t\right)$$

$$\Rightarrow (2\pi)^{-3/2}\iiint d^3\vec{k}\left[A(\vec{k}) e^{i\left[r\hat{k}_i - \vec{\mathrm{v}}_i t + \vec{\rho}(\hat{\Omega}) - \vec{b}\right]\cdot\left(\vec{k}-\vec{k}_i\right)}\right] = \chi\left(r\hat{k}_i - \vec{\mathrm{v}}_i t + \vec{\rho}(\hat{\Omega}) - \vec{b}\right)$$

$$\Psi^{+}_{\vec{b}}(\vec{r},t) \underset{r\to\infty}{\longrightarrow} \Phi_{\vec{b}}(\vec{r},t) +$$

$$+ f(\vec{k}_i,\hat{\Omega}) \frac{e^{i\left\{k_i r - \omega(\vec{k}_i)t\right\}}}{r} e^{-i\vec{k}_i\cdot\vec{b}} \chi\left(r\hat{k}_i - \vec{\mathrm{v}}_i t + \vec{\rho}(\hat{\Omega}) - \vec{b}\right)$$

$$\Psi^+_{\vec{b}}(\vec{r},t) \underset{r\to\infty}{\longrightarrow} \Phi_{\vec{b}}(\vec{r},t) +$$

$$+ f(\vec{k}_i,\hat{\Omega}) \frac{e^{i\{k_i r - \omega(\vec{k}_i)t\}}}{r} e^{-i\vec{k}_i\cdot\vec{b}} \chi\left(r\hat{k}_i - \vec{\mathrm{v}}_i t + \vec{\rho}(\hat{\Omega}) - \vec{b}\right)$$

$$\left|\Psi^{+\,\text{scattered part only}}_{\vec{b}}(\vec{r},t)\right|^2 = \left|f(\vec{k}_i,\hat{\Omega})\right|^2 \frac{1}{r^2}\left|\chi\left(\vec{\rho}(\hat{\Omega}) + \hat{k}_i r - \vec{\mathrm{v}}_i t - \vec{b}\right)\right|^2$$

Probability of scattering along the direction $\hat{\Omega}$

$$P_b(\hat{\Omega}) = \int_0^\infty r^2 dr \left|\Psi^{+\,\text{scattered}}_{\vec{b}}(\vec{r},t)\right|^2 = \left|f(\vec{k}_i,\hat{\Omega})\right|^2 \int_0^\infty r^2 dr \frac{1}{r^2}\left|\chi\left(\vec{\rho}(\hat{\Omega}) + \hat{k}_i r - \vec{\mathrm{v}}_i t - \vec{b}\right)\right|^2$$

$$= \left|f(\vec{k}_i,\hat{\Omega})\right|^2 \int_0^\infty dr \left|\chi\left(\vec{\rho}(\hat{\Omega}) + \hat{k}_i\left(r - \mathrm{v}_i t\right) - \vec{b}\right)\right|^2 \quad \text{since } \vec{\mathrm{v}}_i = \hat{k}_i \mathrm{v}_i$$

Probability of scattering along the direction $\hat{\Omega}$

$$P_{\vec{b}}(\hat{\Omega}) = \left| f(\vec{k}_i, \hat{\Omega}) \right|^2 \int_0^{\infty} dr \left| \chi\left(\vec{\rho}(\hat{\Omega}) + \hat{k}_i \left(r - \mathrm{v}_i t \right) - \vec{b} \right) \right|^2$$

$$P_{\vec{b}}(\hat{\Omega}) = \left| f(\vec{k}_i, \hat{\Omega}) \right|^2 \int_{-\infty}^{\infty} dz \left| \chi\left(\vec{\rho}(\hat{\Omega}) + \hat{k}_i z - \vec{b} \right) \right|^2 \qquad z = r - \mathrm{v}_i t$$

$$\frac{d\sigma}{d\Omega} = \iint d^2\vec{b} P_b(\hat{\Omega}) = \left| f(\vec{k}_i, \hat{\Omega}) \right|^2 \int_{-\infty}^{\infty} dz \iint d^2\vec{b} \left| \chi\left(\vec{\rho}(\hat{\Omega}) + \hat{k}_i z - \vec{b} \right) \right|^2$$

Whole space integral

$$\vec{s} = \vec{\rho}(\hat{\Omega}) + \hat{k}_i z - \vec{b} \qquad \iiint d^3\vec{s} \left| \chi(\vec{s}) \right|^2 = 1$$

$$\frac{d\sigma}{d\Omega} = \left| f(\vec{k}_i, \hat{\Omega}) \right|^2$$

← Appropriate expression even to describe scattering of the wave packet.

Having established that

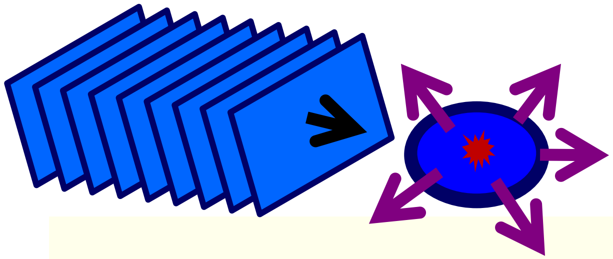
$$\frac{d\sigma}{d\Omega} = \left| f(\vec{k}_i, \hat{\Omega}) \right|^2$$

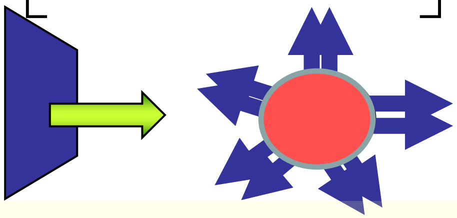
is an appropriate expression even to describe scattering of the wave packet,

we now proceed to study some important and consequential aspects of

PARTIAL WAVE ANAYLSIS

$$\psi_{\vec{k}_i}(\vec{r}; r \to \infty) \to A\left[e^{\vec{k}\bullet\vec{r}} + \frac{f(\hat{\Omega})}{r} e^{ikr}\right]$$





$$\psi_{inc}(\vec{r}; r \to \infty) \to \sum_l i^l \ (2l+1) \ P_l(\cos\theta) \ \frac{\sin(kr - \frac{l\pi}{2})}{kr}$$

$$\psi_{inc}(\vec{r}) \underset{r\to\infty}{\to} \sum_l i^l \ (2l+1) \ P_l(\cos\theta) \ \frac{e^{i\left(kr - \frac{l\pi}{2}\right)} - e^{-i\left(kr - \frac{l\pi}{2}\right)}}{2ikr}$$

$$\psi_{inc} \underset{r\to\infty}{\to} \frac{1}{2ikr} \sum_l \ (2l+1) \ \left[P_l(\cos\theta) e^{ikr} - P_l(\cos\theta)\left(-1\right)^l e^{-ikr}\right]$$

$$\psi_{inc} \underset{r\to\infty}{\to} \frac{1}{2ikr} \sum_l \ (2l+1) \ \left[P_l(\cos\theta) e^{ikr} - P_l(-\cos\theta) e^{-ikr}\right]$$

$E > 0$ continuum

in the presence of a scattering target potential

$$R'' + \frac{2}{r}R' - \frac{l(l+1)}{r^2}R + \frac{2\mu}{\hbar^2}\left[E - V(r)\right]R = 0$$

$$\mathrm{R}_{\varepsilon l}(r) = \frac{y_{\varepsilon l(r)}}{r}; \qquad \text{i.e. } y_{\varepsilon l(r)} = r\mathrm{R}_{\varepsilon l}(r)$$

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

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

When $\lim_{r\to\infty}|U(r)| = \frac{M}{r^{1+\varepsilon}}$; M: constant and $\varepsilon \rangle 0$

$$rR_\ell(k,r) = y_\ell(k,r) \xrightarrow[r\to\infty]{} kr\left[C_\ell^{(1)}(k) j_\ell(kr) + C_\ell^{(2)}(k) n_\ell(kr)\right], \quad r \gg \text{"range"}$$

of the potential

$j_\ell(kr)$: spherical Bessel functions

$n_\ell(kr)$: spherical Neumann functions

'V≠0'

$$j_l(k,r) \xrightarrow[r\to\infty]{} \frac{\sin\left(kr - \frac{l\pi}{2}\right)}{kr} \; ; \; n_l(k,r) \xrightarrow[r\to\infty]{} \frac{-\cos\left(kr - \frac{l\pi}{2}\right)}{kr}$$

$$y_\ell(k,r) \xrightarrow[r\to\infty]{} kr\left[C_\ell^{(1)}(k)\frac{\sin\left(kr - \frac{l\pi}{2}\right)}{kr} - C_\ell^{(2)}(k)\frac{\cos\left(kr - \frac{l\pi}{2}\right)}{kr}\right]$$

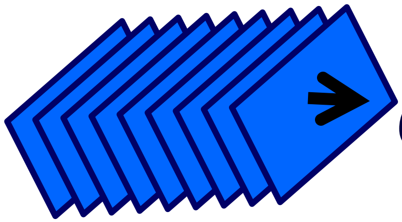
$$y_\ell(k,r) \xrightarrow[r\to\infty]{} \left[C_\ell^{(1)}(k)\sin\left(kr - \frac{l\pi}{2}\right) - C_\ell^{(2)}(k)\cos\left(kr - \frac{l\pi}{2}\right)\right]$$

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

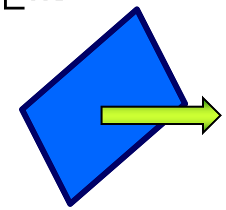
$$\tan\delta_l(k) = -\frac{C_\ell^{(2)}(k)}{C_\ell^{(1)}(k)}$$

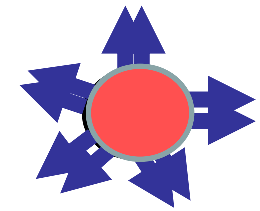
$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos\theta) j_l(kr)$$

$$e^{i\hat{k}_i \bullet \hat{r}} = 4\pi \sum_{l=0}^{\infty} i^l j_l(kr) \left[\sum_{m=-\ell}^{\ell} Y^*_{\ell m}(\hat{\mathrm{k}}_i) Y_{\ell m}(\hat{e}_r) \right]$$



$$e^{+i(kz-\omega t)} \qquad \hat{k}_i = \hat{e}_z$$





$$\psi_{Tot} \xrightarrow[r\to\infty]{} \frac{1}{2ikr} \sum_l c_l (2l+1) \left[P_l(\cos\theta) e^{i(kr+\delta_l)} - P_l(-\cos\theta) e^{-i(kr+\delta_l)} \right]$$

$$\psi^+_{Tot}(\vec{r},t)\Big]_{r\to\infty} \longrightarrow$$

$C_l = e^{i\delta_l(k)}$ describes 'collisions'

$$e^{+i(kz-\omega t)} + \frac{e^{+i(kr-\omega t)}}{r} \left\{ \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) \left[e^{2i\delta_l(k)} - 1 \right] P_l(\cos\theta) \right\}$$

Please refer to details from :

PCD STiAP Unit 6 Probing the Atom

Lecture link: http://nptel.iitm.ac.in/courses/115106057/27 & /28 & /29 & /30

$$y_l(k,r) \underset{r\to\infty}{\longrightarrow} A_l(k)\sin\left(kr - \frac{l\pi}{2} + \delta_l(k)\right)$$

$$\tan\delta_l(k) = -\frac{C_\ell^{(2)}(k)}{C_\ell^{(1)}(k)}$$

$$y_\ell(k,r) \underset{r\to\infty}{\longrightarrow} \left[C_\ell^{(1)}(k)\sin\left(kr - \frac{l\pi}{2}\right) - C_\ell^{(2)}(k)\cos\left(kr - \frac{l\pi}{2}\right)\right]$$

Linear combination of Spherical Bessel & Neumann

We can also write the same as

Linear combination of spherical ingoing waves

&

spherical outgoing waves

$$R_l(k,r) \underset{r\to\infty}{\longrightarrow} A_l(k)\frac{\sin\left[kr-\frac{l\pi}{2}+\delta_l(k)\right]}{r}$$

$$R_l(k,r) \underset{r\to\infty}{\longrightarrow} A_l(k)\frac{e^{i\left[kr-\frac{l\pi}{2}+\delta_l(k)\right]}-e^{-i\left[kr-\frac{l\pi}{2}+\delta_l(k)\right]}}{2ir}$$

$$r\,\mathrm{R}_\ell(k,r) = y_\ell(k,r) \underset{r\to\infty}{\longrightarrow} A_l(k)\frac{e^{i\left[kr-\frac{l\pi}{2}+\delta_l(k)\right]}-e^{-i\left[kr-\frac{l\pi}{2}+\delta_l(k)\right]}}{2i}$$

$$y_\ell(k,r) \underset{r\to\infty}{\longrightarrow} A_l(k)\frac{e^{ikr}e^{-i\frac{l\pi}{2}}e^{i\delta_l(k)}-e^{-ikr}e^{+i\frac{l\pi}{2}}e^{-i\delta_l(k)}}{2i}$$

$$y_\ell(k,r) \underset{r\to\infty}{\longrightarrow} \frac{A_l(k)e^{-i\delta_l(k)}e^{-i\frac{l\pi}{2}}}{2i}\left[e^{ikr}e^{i2\delta_l(k)}-e^{-ikr}e^{+il\pi}\right]$$

$$y_\ell(k,r) \underset{r\to\infty}{\longrightarrow} \frac{A_l(k)e^{-i\delta_l(k)}e^{-i\frac{l\pi}{2}}}{2i}\left[e^{ikr}e^{i2\delta_l(k)} - e^{-ikr}e^{+il\pi}\right]$$

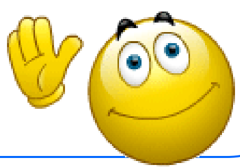
$$e^{-i\frac{l\pi}{2}} = \left(e^{-i\frac{\pi}{2}}\right)^l = (-i)^l = (-1)^l i^l; \qquad e^{il\pi} = \left(e^{i\pi}\right)^l = (-1)^l$$

$$y_\ell(k,r) \underset{r\to\infty}{\longrightarrow} \frac{A_l(k)e^{-i\delta_l(k)}(-1)^l i^l}{2i}\left[e^{ikr}e^{i2\delta_l(k)} - e^{-ikr}(-1)^l\right]$$

$$y_\ell(k,r) \underset{r\to\infty}{\longrightarrow} \tilde{A}_l(k)\left[e^{ikr}e^{i2\delta_l(k)} - e^{-ikr}(-1)^l\right]$$

Linear combination of spherical ingoing & spherical outgoing waves

$$\tilde{A}_l(k) = \frac{A_l(k)e^{-i\delta_l(k)}(-1)^l i^l}{2i}$$



Select/Special Topics *in*
'Theory of Atomic Collisions and Spectroscopy'

P. C. Deshmukh

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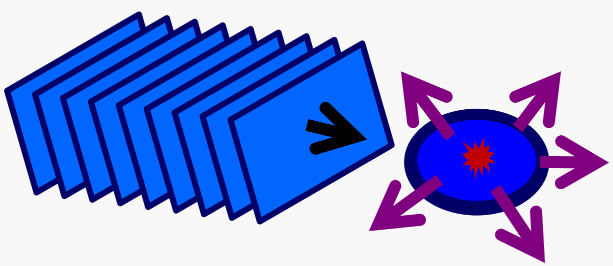
Indian Institute of Technology Madras
Chennai 600036

Lecture Number 07

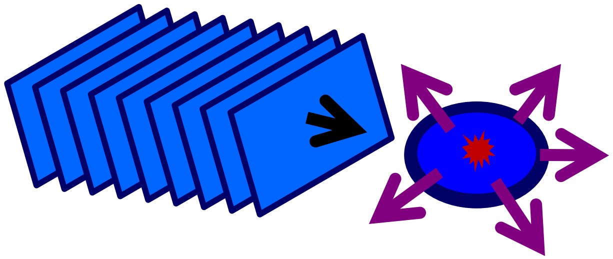
Unit 1: Quantum Theory of Collisions

OPTICAL THEOREM –
-Unitarity of the Scattering Operator



How many partial waves?
Is there an ℓ_{max}?

Primary Reference: '**Quantum Mechanics** – *Nonrelativistic theory*' **– by Landau & Lifshitz**



$$R_l(k,r) \underset{r\to\infty}{\longrightarrow} A_l(k)\frac{\sin\left[kr-\frac{l\pi}{2}+\delta_l(k)\right]}{r}$$

$$\psi^{+}_{Tot}(\vec{r},t)\Big]_{r\to\infty} \longrightarrow e^{+i(kz-\omega t)}+\frac{e^{+i(kr-\omega t)}}{r}\left\{\frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left[e^{2i\delta_l(k)}-1\right]P_l(\cos\theta)\right\}$$

$$r\,\mathrm{R}_\ell(k,r)= \; y_\ell(k,r) \underset{r\to\infty}{\longrightarrow} A_l(k)\frac{e^{i\left[kr-\frac{l\pi}{2}+\delta_l(k)\right]}-e^{-i\left[kr-\frac{l\pi}{2}+\delta_l(k)\right]}}{2i}$$

$$y_\ell(k,r) \underset{r\to\infty}{\longrightarrow} \tilde{A}_l(k)\left[e^{ikr}\,e^{i2\delta_l(k)}-e^{-ikr}(-1)^l\right]$$

Linear combination of spherical ingoing & spherical outgoing waves

$$\tilde{A}_l(k)=\frac{A_l(k)e^{-i\delta_l(k)}(-1)^l\,i^l}{2i}$$

$$e^{-i\frac{l\pi}{2}}=(-1)^l\,i^l;$$

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

$$S_l(k)=e^{i2\delta_l(k)}$$

S Matrix element

$$r\,\mathrm{R}_\ell(k,r) = \;y_\ell(k,r) \underset{r\to\infty}{\longrightarrow} A_l(k)\frac{e^{i\left[kr-\frac{l\pi}{2}+\delta_l(k)\right]}-e^{-i\left[kr-\frac{l\pi}{2}+\delta_l(k)\right]}}{2i}$$

nature *of r* $\rightarrow$ *0 solution:*

$\lim_{r\to 0} r^2V(r) = 0$ *includes coulomb*

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

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

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

←Regardless of E,m

$$R(r) = r^s\sum_{i=0}^{\infty} a_i r^i$$

$s = l \; or \; -(l+1)$:

$R(r\to 0) \to r^l \quad (\text{any } E)$

$y(r\to 0) \to r^{l+1}$

$$f_k(\theta)=\frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left[e^{2i\delta_l(k)}-1\right]P_l(\cos\theta)$$

$$f_k(\theta)=\sum_{l=0}^{\infty}(2l+1)\;a_l(k)\;P_l(\cos\theta)\rightarrow f_k(\theta):\textit{scattering amplitude}$$

$$a_l(k)=\frac{\left[e^{2i\delta_l(k)}-1\right]}{2ik}=\frac{\left[S_l(k)-1\right]}{2ik}\rightarrow a_l(k):\textit{partial wave amplitude}$$

$$a_l(k)=\frac{\cos\left[2\delta_l(k)\right]+i\sin\left[2\delta_l(k)\right]-1}{2ik}$$

$$a_l(k)=\frac{\left\{\cancel{1}-\cancel{2}\sin^2\left[\delta_l(k)\right]\right\}+i\left\{\cancel{2}\sin\left[\delta_l(k)\right]\cos\left[\delta_l(k)\right]\right\}-\cancel{1}}{\cancel{2}ik}\times\frac{(-i)}{(-i)}$$

$$a_l(k)=\frac{\left\{i\sin^2\left[\delta_l(k)\right]\right\}+\left\{\sin\left[\delta_l(k)\right]\cos\left[\delta_l(k)\right]\right\}}{k}=\frac{\sin\left[\delta_l(k)\right]e^{i\delta_l(k)}}{k}$$

$$f_k(\theta)=\sum_{l=0}^{\infty}(2l+1)\;\frac{\sin\left[\delta_l(k)\right]e^{i\delta_l(k)}}{k}\;P_l(\cos\theta)$$

$$f_k(\theta) = \sum_{l=0}^{\infty} (2l+1) \; \frac{\sin[\delta_l(k)] e^{i\delta_l(k)}}{k} \; P_l(\cos\theta)$$

$$\frac{d\sigma}{d\Omega} = f_k^*(\theta) \, f_k(\theta)$$

$$= \left\{ \sum_{l=0}^{\infty} (2l+1) \; \frac{\sin[\delta_l(k)] e^{-i\delta_l(k)}}{k} \; P_l(\cos\theta) \right\}$$

$$\times \left\{ \sum_{l'=0}^{\infty} (2l'+1) \; \frac{\sin[\delta_{l'}(k)] e^{i\delta_{l'}(k)}}{k} \; P'_l(\cos\theta) \right\}$$

$$\sigma_{Total} = \frac{2\pi}{k^2} \left\{ \begin{array}{l} \displaystyle\sum_{l'=0}^{\infty} \; \sum_{l=0}^{\infty} (2l+1)(2l'+1) \times \sin[\delta_{l'}(k)] \sin[\delta_l(k)] \\ \displaystyle\times e^{i[\delta_{l'}(k) - \delta_l(k)]} \times \int_0^{\pi} \sin\theta d\theta P_l(\cos\theta) P'_l(\cos\theta) \end{array} \right\}$$

$$\sigma_{Total} = \frac{2\pi}{k^2}\left\{ \begin{array}{l} \sum_{l'=0}^{\infty} \sum_{l=0}^{\infty} (2l+1)(2l'+1) \times \sin[\delta_{l'}(k)] \sin[\delta_l(k)] \\ \times e^{i[\delta_{l'}(k)-\delta_l(k)]} \times \int_0^{\pi} \sin\theta d\theta P_l(\cos\theta) P'_l(\cos\theta) \end{array} \right\}$$

$$\sigma_{Total} = \frac{2\pi}{k^2}\left\{ \begin{array}{l} \sum_{l'=0}^{\infty} \sum_{l=0}^{\infty} (2l+1)(2l'+1) \times \sin[\delta_{l'}(k)] \sin[\delta_l(k)] \\ \times e^{i[\delta_{l'}(k)-\delta_l(k)]} \times \frac{2}{2l+1} \delta_{ll'} \end{array} \right\}$$

$$\sigma_{Total} = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2[\delta_l(k)]$$

$$\sigma_{Total} = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2[\delta_l(k)]$$

$$\sigma_{Total} = \sum_{l=0}^{\infty}\sigma_l(k)$$

Partial wave contributions

$$\sigma_l(k) = \frac{4\pi}{k^2}(2l+1)\sin^2[\delta_l(k)]$$

$$\sigma_l(k)\Big|_{max} = \frac{4\pi}{k^2}(2l+1)$$

$$\delta_l(k) = \left(n+\frac{1}{2}\right)\pi$$

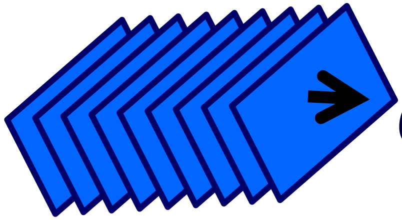
$$n = 0,\ \pm1,\ \pm2,\ \pm3,....$$

$$\sigma_l(k)\Big|_{min} = 0$$

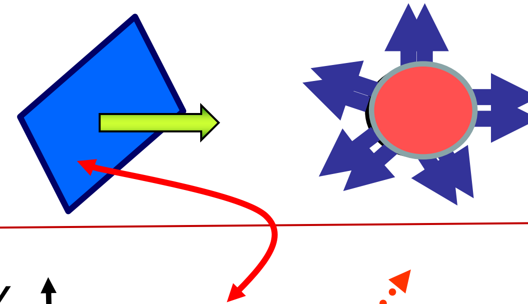
$$\delta_l(k) = n\pi$$

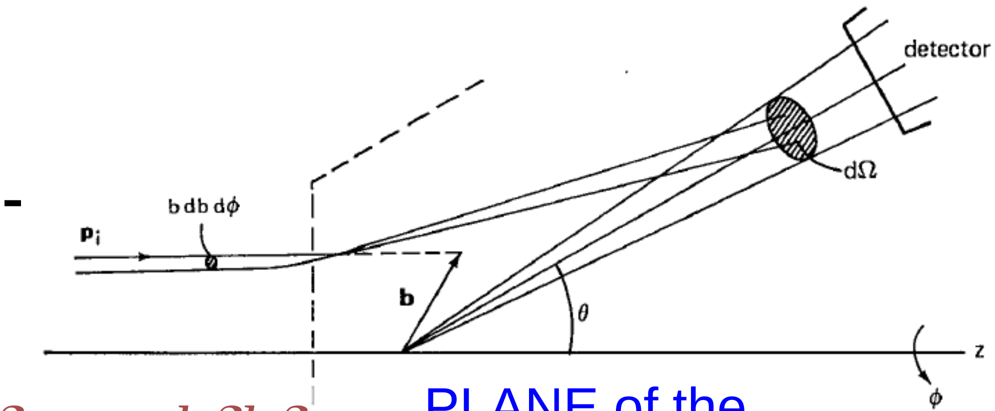
No contribution to scattering by that partial wave

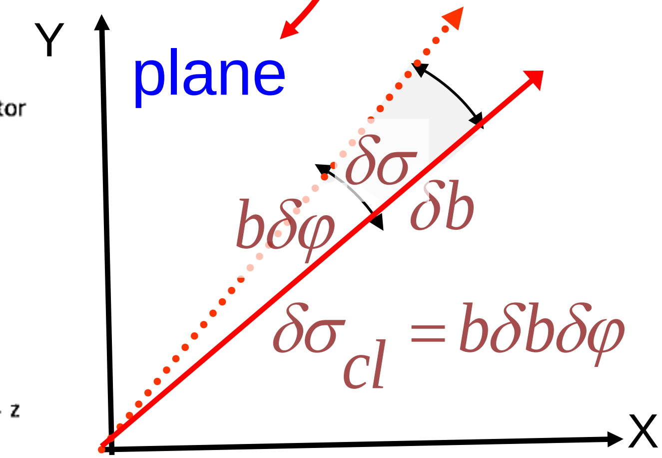
$$\sigma_{Total} = \sum_{l=0}^{\infty}\sigma_l(k) \rightarrow \text{usually, } \ l_{max} \sim ka; \ \textbf{not } \infty$$



$$e^{+i(kz-\omega t)} \quad \hat{k}_i = \hat{e}_z$$







$$\delta\sigma_{cl} = b\delta b\delta\varphi$$

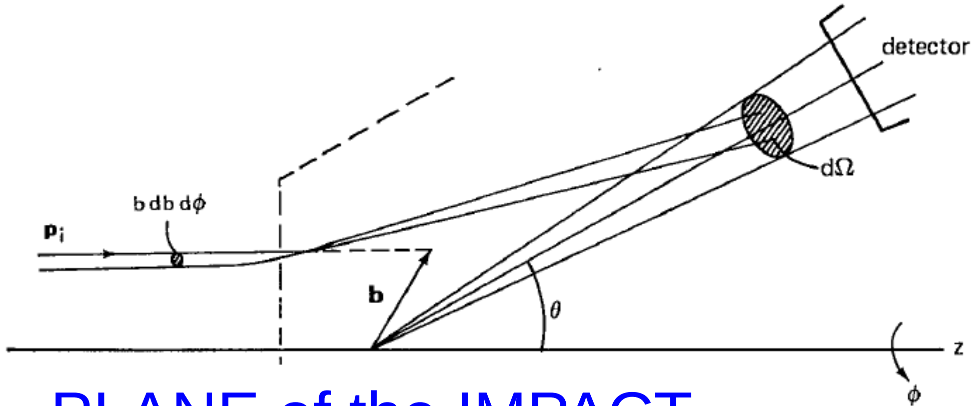
PLANE of the IMPACT PARAMETER

$$\delta\sigma_{cl} = \frac{b}{\sin\theta}\frac{\delta b}{\delta\theta}\delta\Omega$$

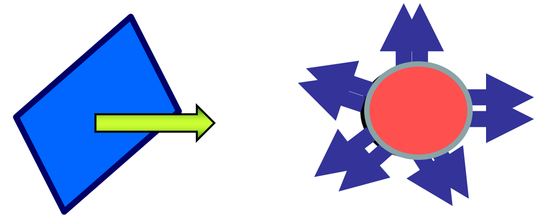
$$\delta\sigma_{cl} = b\frac{\delta b}{\delta(\cos\theta)}\delta(\cos\theta)\delta\varphi$$

$$\delta\sigma_{cl} = b\frac{\delta b}{\{-\sin\theta\delta\theta\}}\{-\sin\theta\delta\theta\}\delta\varphi$$

$$\frac{d\sigma_{cl}}{d\Omega} = \frac{b}{\sin\theta}\frac{db}{d\theta}$$



PLANE of the IMPACT PARAMETER



$$\frac{d\sigma_{cl}}{d\Omega} = \frac{b}{\sin\theta}\frac{db}{d\theta}$$

What would be the angular momentum of a classical particle at impact parameter $\vec{b}$?

$$\vec{l} = \vec{\rho} \times \vec{p} = \vec{b} \times \vec{p}$$

$$l_{\max} \sim ap = a\hbar k \text{ for } b \sim a : \text{"range"}$$

$$\hbar\sqrt{l_{\max}(l_{\max}+1)} \sim a\hbar k \quad \Rightarrow \quad l_{\max} \sim ak$$

$$\text{partial waves: } l \leq ak$$

$$a : \text{"}range\text{" of the potential}$$

Often, just 'few' partial waves suffice in the partial wave expansion

Please refer to details from :
PCD STiAP Unit 1, Lecture 5

Lecture link→ http://nptel.iitm.ac.in/courses/115106057/6

Special *further* considerations: (1) Resonances etc.
(2) V(r) falls off extremely slowly in the asymptotic region.
(3) Electron correlations.

$$f_k(\theta) = \sum_{l=0}^{\infty} (2l+1) \; \frac{\sin\left[\delta_l(k)\right] e^{i\delta_l(k)}}{k} \; P_l(\cos\theta)$$

$$\mathrm{Im}\left[\, f_k(\theta)\right] = \sum_{l=0}^{\infty} (2l+1) \; \frac{\sin^2\left[\delta_l(k)\right]}{k} \; P_l(\cos\theta)$$

for every l, **for** $\theta = 0, \;\; \cos(\theta) = 1, \; P_l(\cos\theta) = 1$

$$\mathrm{Im}\left[\, f_k(\theta = 0)\right] = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \; \sin^2\left[\delta_l(k)\right]$$

above *slide* 107 : $\sigma_{Total} = \dfrac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2\left[\delta_l(k)\right]$

$$\sigma_{Total} = \frac{4\pi}{k} \mathrm{Im}\left[\, f_k(\theta = 0)\right]$$ OPTICAL THEOREM

$$\psi(\vec{r})\underset{r\to\infty}{\to} e^{ikr\hat{n}.\hat{n}'} + \frac{f(\hat{n},\hat{n}')e^{ikr}}{r}$$

Any <u>LINEAR COMBINATION</u> of functions of the above form for different directions of incidence $\hat{n}$ will also be a solution to the scattering process.

$$\Psi(\vec{r})\underset{r\to\infty}{\to} \iint F(\hat{n})e^{ikr\hat{n}.\hat{n}'}dO + \iint F(\hat{n})\frac{f(\hat{n},\hat{n}')e^{ikr}}{r}dO$$

dO: elemental solid angle

NOTE: integration is over different directions of incidence

$$\Psi(\vec{r})\underset{r\to\infty}{\to} \iint F(\hat{n})e^{ikr\hat{n}.\hat{n}'}dO + \frac{e^{ikr}}{r}\iint f(\hat{n},\hat{n}')F(\hat{n})dO$$

Ref.: Landau & Lifshitz, NR-QM §125, page 508

$$\Psi(\vec{r})_{r\to\infty} \iint F(\hat{n})\, e^{ikr\hat{n}.\hat{n}'}\, dO + \frac{e^{ikr}}{r} \iint F(\hat{n})\, f(\hat{n},\hat{n}')\, dO$$

$e^{ikr\hat{n}.\hat{n}'}$ oscillates rapidly at large r as incident direction $\hat{n}$ changes

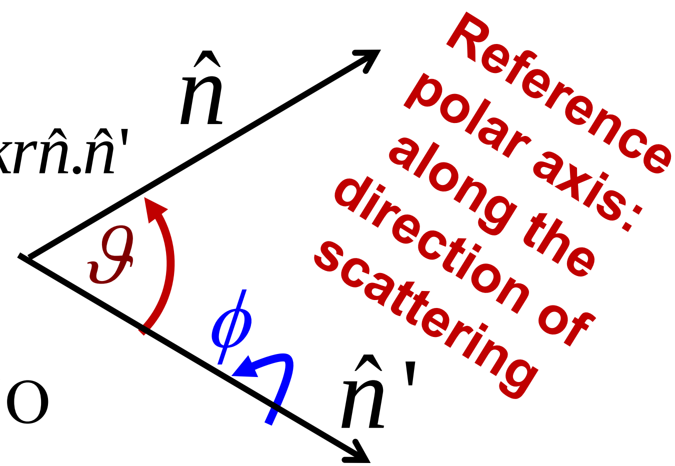
Integration is over different directions of incidence

hence $\iint F(\hat{n})\, e^{ikr\hat{n}.\hat{n}'}\, dO$ determined by $\hat{n} = \pm\hat{n}'$

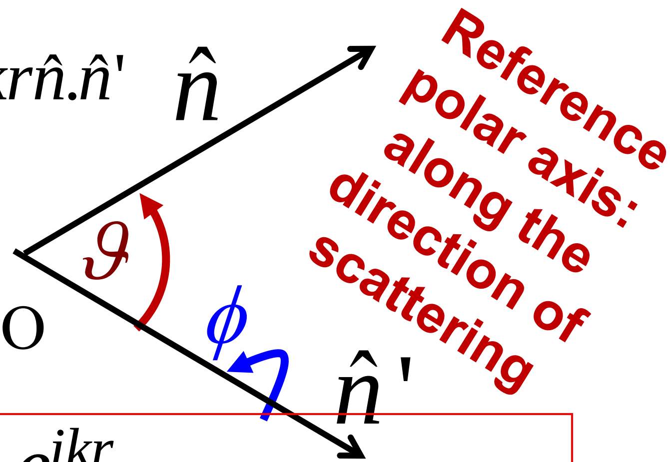
where $F(\hat{n}) \sim F(\pm\hat{n}')$

$$\Psi(\vec{r})_{r\to\infty} \int_{\vartheta=0}^{\pi} \sin\vartheta\, d\vartheta \int_{\phi=0}^{2\pi} d\phi\, F(\hat{n})\, e^{ikr\hat{n}.\hat{n}'}$$

$$+ \frac{e^{ikr}}{r} \iint F(\hat{n})\, f(\hat{n},\hat{n}')\, dO$$



$$\Psi(\vec r)\underset{r\to\infty}{\rightarrow}\int_{\vartheta=0}^{\pi}\sin\vartheta\, d\vartheta\int_{\phi=0}^{2\pi}d\phi\, F(\hat n)\,e^{ikr\hat n.\hat n'} + \frac{e^{ikr}}{r}\iint f(\hat n,\hat n')\,F(\hat n)\,dO$$



$$\Psi(\vec r)\underset{r\to\infty}{\rightarrow}2\pi\int_{\vartheta=0}^{\pi}\sin\vartheta\, d\vartheta\, F(\hat n)\,e^{ikr\hat n.\hat n'} + \frac{e^{ikr}}{r}\iint f(\hat n,\hat n')F(\hat n)\,dO$$

$$\Psi(\vec r)\underset{r\to\infty}{\rightarrow}2\pi\left.\frac{F(\hat n)\,e^{ikr\cos\vartheta}}{ikr}\right|_{\cos\vartheta=1}^{\cos\vartheta=-1} + \frac{e^{ikr}}{r}\iint f(\hat n,\hat n')F(\hat n)\,dO$$

$$\Psi(\vec r)\underset{r\to\infty}{\rightarrow}\left[-2\pi\frac{F(-\hat n')\,e^{-ikr}}{ikr}+2\pi\frac{F(\hat n')\,e^{ikr}}{ikr}\right] + \frac{e^{ikr}}{r}\iint f(\hat n,\hat n')F(\hat n)\,dO$$

$$\Psi(\vec r)\underset{r\to\infty}{\rightarrow}\frac{2\pi i}{k}\left[\frac{F(-\hat n')\,e^{-ikr}}{r}-\frac{F(\hat n')\,e^{ikr}}{r}\right] + \frac{e^{ikr}}{r}\iint f(\hat n,\hat n')F(\hat n)\,dO$$

$$\Psi(\vec{r})\underset{r\to\infty}{\to}\frac{2\pi i}{k}\left[\frac{F(-\hat{n}')e^{-ikr}}{r}-\frac{F(\hat{n}')e^{ikr}}{r}\right]+\frac{e^{ikr}}{r}\iint f(\hat{n},\hat{n}')F(\hat{n})\ dO$$

$$\Psi(\vec{r})\underset{r\to\infty}{\to}\left\{\frac{2\pi i}{k}\right\}\left[\frac{F(-\hat{n}')e^{-ikr}}{r}-\frac{F(\hat{n}')e^{ikr}}{r}+\frac{k}{2\pi i}\frac{e^{ikr}}{r}\iint f(\hat{n},\hat{n}')F(\hat{n})\ dO\right]$$

dropping the factor $\left\{\frac{2\pi i}{k}\right\}$

$$\Psi(\vec{r})\underset{r\to\infty}{\to}\frac{F(-\hat{n}')e^{-ikr}}{r}-\frac{F(\hat{n}')e^{ikr}}{r}+\frac{k}{2\pi i}\frac{e^{ikr}}{r}\iint f(\hat{n},\hat{n}')F(\hat{n})\ dO$$

ingoing Spherical wave — outgoing spherical wave

$$\Psi(\vec{r})\underset{r\to\infty}{\to}\frac{e^{-ikr}}{r}F(-\hat{n}')-\frac{e^{ikr}}{r}\left[F(\hat{n}')-\frac{k}{2\pi i}\iint f(\hat{n},\hat{n}')F(\hat{n})\ dO\right]$$

$$\Psi(\vec{r})_{r\to\infty} \frac{e^{-ikr}}{r} F(-\hat{n}') - \frac{e^{ikr}}{r}\left[F(\hat{n}') - \frac{k}{2\pi i} \iint f(\hat{n},\hat{n}') F(\hat{n})\, dO \right]$$

$$\iint f(\hat{n},\hat{n}') F(\hat{n})\, dO = 4\pi \widehat{f}\; F(\hat{n}')$$

$$\widehat{f}\; F(\hat{n}') = \frac{1}{4\pi} \iint f(\hat{n},\hat{n}') F(\hat{n})\, dO$$

definition of the operator $\widehat{f}$

$$\Psi(\vec{r})_{r\to\infty} \frac{e^{-ikr}}{r} F(-\hat{n}') - \frac{e^{ikr}}{r}\left[F(\hat{n}') - \frac{k}{2\pi i} 4\pi \widehat{f}\; F(\hat{n}') \right]$$

$$\Psi(\vec{r})_{r\to\infty} \frac{e^{-ikr}}{r} F(-\hat{n}') - \frac{e^{ikr}}{r}\left[1 + 2ki\, \widehat{f}\; \right] F(\hat{n}')$$

$$\Psi(\vec{r})\underset{r\to\infty}{\to}\frac{e^{-ikr}}{r}F(-\hat{n}')-\frac{e^{ikr}}{r}\left[1+2ki\,\widehat{f}\;\right]F(\hat{n}')$$

$$\widehat{f}\;F(\hat{n}')=\frac{1}{4\pi}\iint f(\hat{n},\hat{n}')F(\hat{n})\,dO$$

$$\Psi(\vec{r})\underset{r\to\infty}{\to}\frac{e^{-ikr}}{r}F(-\hat{n}')-\frac{e^{ikr}}{r}\;\widehat{S}\;F(\hat{n}')$$

Scattering Operator (definition) $\widehat{S}\;=\left[1+2ki\,\widehat{f}\;\right]$

Ref.: Landau & Lifshitz, NR-QM §125, Eq.125.3, page 509

Heisenberg (1943)

Scattering Operator (definition)

$$\Psi(\vec{r}) \underset{r\to\infty}{\to} \frac{e^{-ikr}}{r} F(-\hat{n}') - \frac{e^{ikr}}{r} \widehat{S} F(\hat{n}')$$

'ingoing' 'outgoing'

$$\widehat{f} F(\hat{n}') = \frac{1}{4\pi} \iint f(\hat{n}, \hat{n}') F(\hat{n}) dO$$

$$\widehat{S} = \left[1 + 2ki \widehat{f}\right]$$

$$\left\langle \frac{F(-\hat{n}')}{r} \middle| \frac{F(-\hat{n}')}{r} \right\rangle \to \text{measure of intensity of ingoing wave}$$

$$\left\langle \frac{F(\hat{n}')}{r} \middle| \widehat{S}^\dagger \widehat{S} \middle| \frac{F(\hat{n}')}{r} \right\rangle \to \text{measure of the intensity}$$

?

of the outgoing wave

Conservation of ingoing and outgoing flux $\Rightarrow \widehat{S}^\dagger \widehat{S} = 1 = \widehat{S} \widehat{S}^\dagger$

$\widehat{S}$: *unitary*

Ref.: Landau & Lifshitz, NR-QM §125, page 508

$$\Psi(\vec{r}) \underset{r\to\infty}{\to} \frac{e^{-ikr}}{r} F(-\hat{n}') - \frac{e^{ikr}}{r} \hat{S}\, F(\hat{n}')$$

$$\hat{S}^{\dagger}\hat{S} = 1$$

Scattering Operator (definition)

$$\hat{S} = \left[1 + 2ki\,\hat{f}\,\right]$$

$$\hat{f}\, F(\hat{n}') = \frac{1}{4\pi} \iint f(\hat{n}.\hat{n}') F(\hat{n})\, dO$$

$$\hat{S}^{\dagger} = \left[1 - 2ki\,\hat{f}^{\dagger}\,\right]$$

$$\hat{S}\hat{S}^{\dagger} = \left[1 + 2ki\,\hat{f}\,\right]\left[1 - 2ki\,\hat{f}^{\dagger}\,\right]$$

$$\hat{S}\hat{S}^{\dagger} = 1 - 2ki\,\hat{f}^{\dagger} + 2ki\,\hat{f} + 4k^2\,\hat{f}\,\hat{f}^{\dagger}$$

$$\hat{S}\hat{S}^{\dagger} = 1 + 2ki\left(\hat{f} - \hat{f}^{\dagger}\right) + 4k^2\,\hat{f}\,\hat{f}^{\dagger}$$

$$\hat{S}\hat{S}^{\dagger} = 1 \quad \Rightarrow \quad \left(\hat{f} - \hat{f}^{\dagger}\right) = 2ki\,\hat{f}\,\hat{f}^{\dagger}$$

Ref.: Landau & Lifshitz, NR-QM §125, page 508

$$\left(\widehat{f}-\widehat{f}^{\dagger}\right)=2ki\ \widehat{f}\ \widehat{f}^{\dagger}\qquad\Rightarrow\left(\widehat{f}-\widehat{f}^{\dagger}\right)F(\hat{n}')=2ki\ \widehat{f}\ \widehat{f}^{\dagger}F(\hat{n}')$$

$$\widehat{f}\ F(\hat{n}')-\left[\widehat{f}^{\dagger}F(\hat{n}')\right]=2ki\ \widehat{f}\ \left[\widehat{f}^{\dagger}F(\hat{n}')\right]$$

$$\widehat{f}\ F(\hat{n}')=\frac{1}{4\pi}\iint f(\hat{n},\hat{n}')F(\hat{n})\,dO$$

2nd index

Integration is over ← ***unprimed*** variables

Integration is over ***double-primed*** variables →

$$\widehat{f}^{\dagger}\ F(\hat{n}')=\frac{1}{4\pi}\iint f^{*}(\hat{n}',\hat{n}'')F(\hat{n}'')\,dO''$$

1st index

$$\frac{1}{4\pi}\iint f(\hat{n},\hat{n}')F(\hat{n})\,dO-\left[\frac{1}{4\pi}\iint f^{*}(\hat{n}',\hat{n}'')F(\hat{n}'')\,dO''\right]=$$

$$=\ 2ki\ \widehat{f}\ \left[\frac{1}{4\pi}\iint f^{*}(\hat{n}',\hat{n}'')F(\hat{n}'')\,dO''\right]$$

(The factors $\frac{1}{4\pi}$ are boxed and struck out.)

$$\iint f(\hat{n},\hat{n}')F(\hat{n})d\text{O} - \iint f^*(\hat{n}',\hat{n}'')F(\hat{n}'')d\text{O}'' =$$

$$= 2ki\ \widehat{f}\left[\iint f^*(\hat{n}',\hat{n}'')F(\hat{n}'')d\text{O}''\right]$$

$$\iint f(\hat{n},\hat{n}')F(\hat{n})d\text{O} - \iint f^*(\hat{n}',\hat{n}'')F(\hat{n}'')d\text{O}'' =$$

$$= 2ki\ \color{red}{\widehat{f}}\color{black}\left[\iint f^*(\hat{n}',\hat{n}'')\color{red}{F(\hat{n}'')}\color{black}d\text{O}''\right]$$

$$\iint f(\hat{n},\hat{n}')F(\hat{n})d\text{O} - \iint f^*(\hat{n}',\hat{n})F(\hat{n})d\text{O} =$$

$$= 2ki\ \left[\iint f^*(\hat{n}',\hat{n}'')\color{red}{\widehat{f}\ F(\hat{n}'')}\color{black}d\text{O}''\right]$$

$$\iint f(\hat{n},\hat{n}')F(\hat{n})\,d\text{O} - \iint f^*(\hat{n}',\hat{n})F(\hat{n})\,d\text{O} =$$

$$= 2ki\left[\iint f^*(\hat{n}',\hat{n}'')\left\{\widehat{f}\;F(\hat{n}'')\right\}d\text{O}''\right]$$

$$\widehat{f}\;F(\hat{n}') = \frac{1}{4\pi}\iint f(\hat{n},\hat{n}')F(\hat{n})\,d\text{O}$$

$$\widehat{f}\;F(\hat{n}'') = \frac{1}{4\pi}\iint f(\hat{n},\hat{n}'')F(\hat{n})\,d\text{O}$$

$$\iint\left[f(\hat{n},\hat{n}') - f^*(\hat{n}',\hat{n})\right]F(\hat{n})\,d\text{O} =$$

$$= 2ki\left[\iint f^*(\hat{n}',\hat{n}'')\left\{\frac{1}{4\pi}\iint f(\hat{n},\hat{n}'')F(\hat{n})\,d\text{O}\right\}d\text{O}''\right]$$

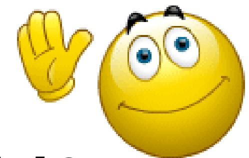
$$\iint\left[f(\hat{n},\hat{n}') - f^*(\hat{n}',\hat{n})\right]F(\hat{n})\,d\text{O} =$$

$$= \left\{\frac{ki}{2\pi}\right\}\left[\iint f^*(\hat{n}',\hat{n}'')\iint f(\hat{n},\hat{n}'')F(\hat{n})\,d\text{O}\,d\text{O}''\right]$$

$$\iint \left[f(\hat{n},\hat{n}') - f^*(\hat{n}',\hat{n}) \right] F(\hat{n})\, dO =$$

$$= \frac{ki}{2\pi} \left[\iint f^*(\hat{n}',\hat{n}'') \iint f(\hat{n},\hat{n}'') F(\hat{n})\, dO\, dO'' \right]$$

$$\iint \left[f(\hat{n},\hat{n}') - f^*(\hat{n}',\hat{n}) \right] F(\hat{n})\, dO =$$



$$= \iint \left\{ \frac{ki}{2\pi} \iint f^*(\hat{n}',\hat{n}'') f(\hat{n},\hat{n}'')\, dO'' \right\} F(\hat{n})\, dO$$

$$f(\hat{n},\hat{n}') - f^*(\hat{n}',\hat{n}) = \frac{ki}{2\pi} \iint f^*(\hat{n}',\hat{n}'') f(\hat{n},\hat{n}'')\, dO''$$

for $\hat{n}' = \hat{n}$

$$f(\hat{n},\hat{n}) - f^*(\hat{n},\hat{n}) = \frac{ki}{2\pi} \iint f^*(\hat{n},\hat{n}'') f(\hat{n},\hat{n}'')\, dO''$$

$\widehat{S}$: *unitary*

$$2i\,\mathrm{Im}\left[f(\hat{n},\hat{n}) \right] = \frac{ki}{2\pi} \iint \left| f(\hat{n},\hat{n}'') \right|^2 dO''$$

$$\left| f(\hat{n},\hat{n}'') \right|^2 = \frac{d\sigma}{dO''}$$

$$2i\,\mathrm{Im}\left[f(\hat{n},\hat{n}) \right] = \frac{ki}{2\pi} \sigma_{Total}$$

$$\sigma_{Total} = \frac{4\pi}{k} \mathrm{Im}\left[f(\hat{n},\hat{n}) \right]$$ *optical theorem*

Select/Special Topics *in*
'Theory of Atomic Collisions and Spectroscopy'

P. C. Deshmukh

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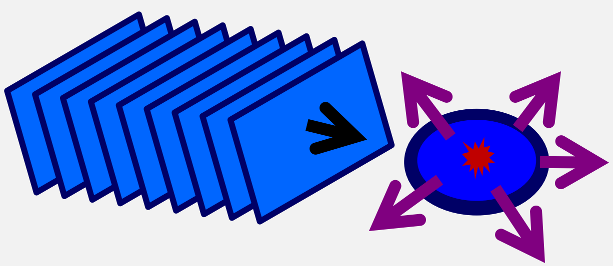
Lecture Number 08

Unit 1: Quantum Theory of Collisions



RECIPROCITY THEOREM

- from Landau & Lifshitz' NR-QM

Phase-shift analysis

- from Joachain's Quantum Collision Theory

$$\widehat{f}\ F(\hat{n}') = \frac{1}{4\pi} \iint f(\hat{n}.\hat{n}') F(\hat{n})\, dO$$

$$\widehat{S} = \left[1 + 2ki\ \widehat{f}\ \right]$$

Scattering Operator (definition)

$$\Psi(\vec{r}) \underset{r\to\infty}{\longrightarrow} \frac{e^{-ikr}}{r} F(-\hat{n}') - \frac{e^{ikr}}{r}\ \widehat{S}\ F(\hat{n}')$$

$$\Psi(\vec{r},t) \underset{r\to\infty}{\longrightarrow} \frac{e^{-ikr} e^{-i\omega t}}{r} F(-\hat{n}') - \frac{e^{ikr} e^{-i\omega t}}{r}\ \widehat{S}\ F(\hat{n}')$$

$$\Psi(\vec{r},t) \underset{r\to\infty}{\longrightarrow} \frac{e^{-i(kr+\omega t)}}{r} F(-\hat{n}') - \frac{e^{+i(kr-\omega t)}}{r}\ \widehat{S}\ F(\hat{n}')$$

$$\Psi(\vec{r},t) \underset{r\to\infty}{\rightarrow} \frac{e^{-i(kr+\omega t)}}{r} F(-\hat{n}') - \frac{e^{+i(kr-\omega t)}}{r} \hat{S}\, F(\hat{n}')$$

$$\Psi^*(\vec{r},t) \underset{r\to\infty}{\rightarrow} \frac{e^{+i(kr+\omega t)}}{r} F^*(-\hat{n}') - \frac{e^{-i(kr-\omega t)}}{r} \hat{S}^\dagger\, F^*(\hat{n}')$$

$$\Psi^*(\vec{r},-t) \underset{r\to\infty}{\rightarrow} \frac{e^{+i(kr-\omega t)}}{r} F^*(-\hat{n}') - \frac{e^{-i(kr+\omega t)}}{r} \hat{S}^\dagger\, F^*(\hat{n}')$$

$$\Psi(\vec{r}) \underset{r\to\infty}{\to} \frac{e^{-ikr}}{r} F(-\hat{n}') - \frac{e^{ikr}}{r} \hat{S} F(\hat{n}')$$

$$\Psi(\vec{r},t) \underset{r\to\infty}{\to} \frac{e^{-i(kr+\omega t)}}{r} F(-\hat{n}') - \frac{e^{+i(kr-\omega t)}}{r} \hat{S} F(\hat{n}')$$

Original function

time reversed function:

$$\Psi^*(\vec{r},-t) \underset{r\to\infty}{\to} \frac{e^{+i(kr-\omega t)}}{r} F^*(-\hat{n}') - \frac{e^{-i(kr+\omega t)}}{r} \hat{S}^* F^*(\hat{n}')$$

space part of the time-reversed function:

$$\frac{e^{+ikr}}{r} F^*(-\hat{n}') - \frac{e^{-ikr}}{r} \hat{S}^* F^*(\hat{n}')$$

space part of the time-reversed function:

$$\frac{e^{+ikr}}{r}F^*(-\hat{n}')-\frac{e^{-ikr}}{r}\widehat{S}^*\, F^*(\hat{n}')$$

$$let:\ \widehat{S}^*\, F^*(\hat{n}')=-\Phi(-\hat{n}') \rightarrow \text{definition of } -\Phi(-\hat{n}')$$

$$F^*(\hat{n}')=\left(\widehat{S}^*\right)^{-1}\widehat{S}^*\, F^*(\hat{n}')$$

$$F^*(\hat{n}')=\left(\widehat{S}^*\right)^{-1}\left[-\Phi(-\hat{n}')\right] \qquad =-\left(\widehat{S}^*\right)^{-1}\left[\Phi(-\hat{n}')\right]$$

$$F^*(\hat{n}')=-\left(\widehat{S}^*\right)^{\dagger}\left[\Phi(-\hat{n}')\right] \qquad \Rightarrow F^*(\hat{n}')=-\tilde{\widehat{S}}\left[\Phi(-\hat{n}')\right]$$

since $\left(\widehat{S}^*\right)^{\dagger}=\tilde{\widehat{S}}$

Parity:

$$F^*(-\hat{n}')=PF^*(\hat{n}')$$

$$=-P\tilde{\widehat{S}}\left[\Phi(-\hat{n}')\right]$$

$$F^*(-\hat{n}')=-P\tilde{\widehat{S}}\left[P\Phi(\hat{n}')\right]$$

$$=-P\tilde{\widehat{S}}P\;\Phi(\hat{n}')$$

space part of the time-reversed function:

$$\frac{e^{+ikr}}{r}F^*(-\hat{n}')-\frac{e^{-ikr}}{r}\ \widehat{S}^*\ F^*(\hat{n}')$$

$$F^*(-\hat{n}')=-P\tilde{\tilde{\widehat{S}}}\left[P\Phi(\hat{n}')\right]$$
$$=-P\tilde{\tilde{\widehat{S}}}P\Phi(\hat{n}')$$

space part of the time-reversed function:

$$\frac{e^{+ikr}}{r}\left[-P\tilde{\tilde{\widehat{S}}}P\Phi(\hat{n}')\right]-\frac{e^{-ikr}}{r}\ \widehat{S}^*\ F^*(\hat{n}')$$

$\widehat{S}^*\ F^*(\hat{n}')=-\Phi(-\hat{n}')\rightarrow$ definition of $-\Phi(-\hat{n}')$

space part of the time-reversed function:

$$\frac{e^{+ikr}}{r}\left[-P\tilde{\tilde{\widehat{S}}}P\Phi(\hat{n}')\right]-\frac{e^{-ikr}}{r}\ \left[-\Phi(-\hat{n}')\right]$$

space part of the time-reversed function:

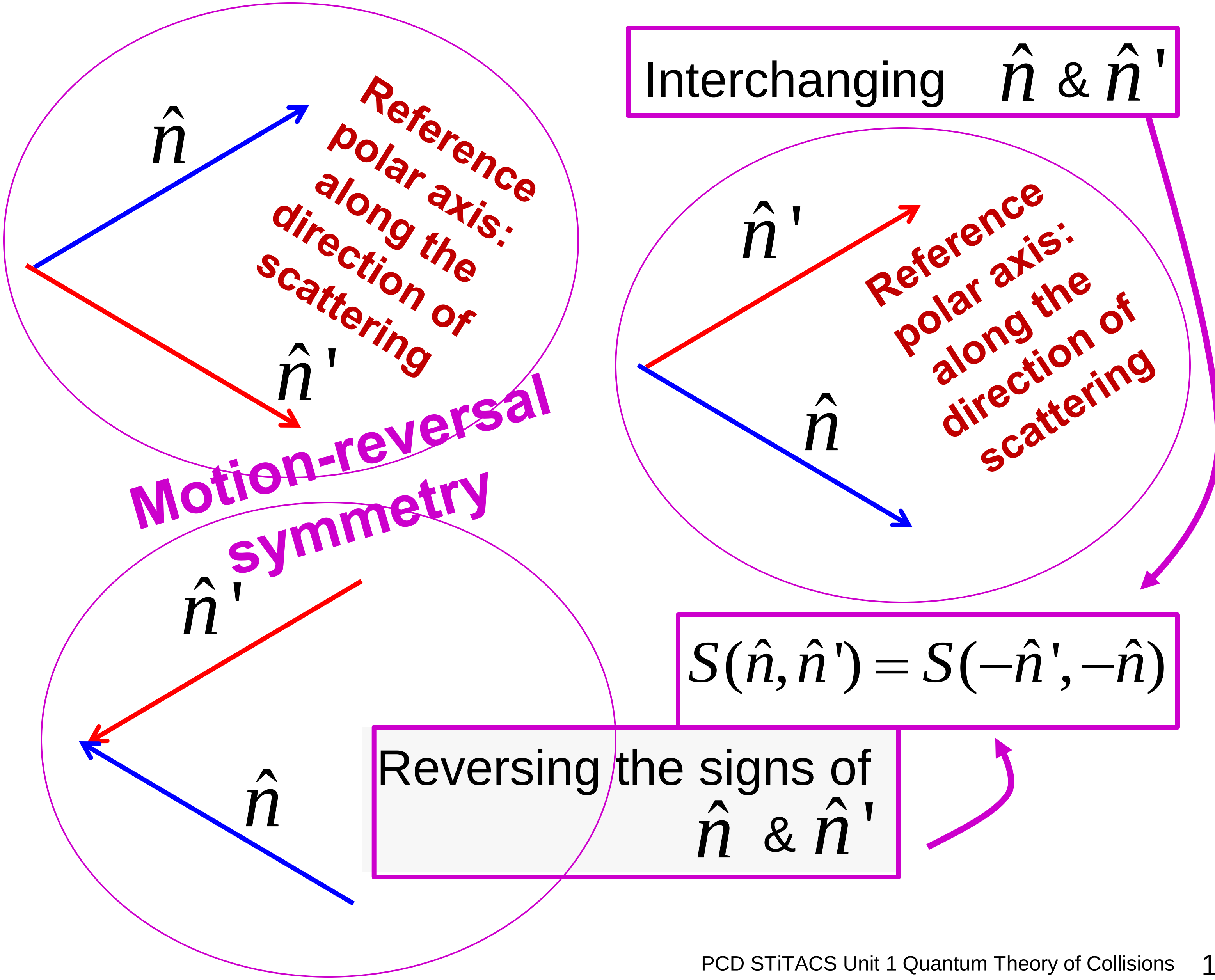
$$\frac{e^{+ikr}}{r}\left[-P\tilde{\tilde{S}}P\Phi(\hat{n}')\right]-\frac{e^{-ikr}}{r}\left[-\Phi(-\hat{n}')\right]$$

$$\frac{e^{-ikr}}{r}\left[\Phi(-\hat{n}')\right]-\frac{e^{+ikr}}{r}\left[P\tilde{\tilde{S}}P\Phi(\hat{n}')\right]$$

original function: $$\frac{e^{-ikr}}{r}F(-\hat{n}')-\frac{e^{+ikr}}{r}\hat{S}F(\hat{n}')$$

$F(\hat{n}')$ or $\Phi(\hat{n}')$ .. matter *only* of *notation* ...

$$\Rightarrow \boxed{P\tilde{\tilde{S}}P=\hat{S}}$$


Interchanging $\hat{n}$ & $\hat{n}'$
$\hat{n}$
Reference polar axis: along the direction of scattering
$\hat{n}'$
$\hat{n}'$
Reference polar axis: along the direction of scattering
$\hat{n}$
Motion-reversal symmetry
$S(\hat{n},\hat{n}') = S(-\hat{n}',-\hat{n})$
$\hat{n}'$
$\hat{n}$
Reversing the signs of $\hat{n}$ & $\hat{n}'$

interchange incidence & scattered directions

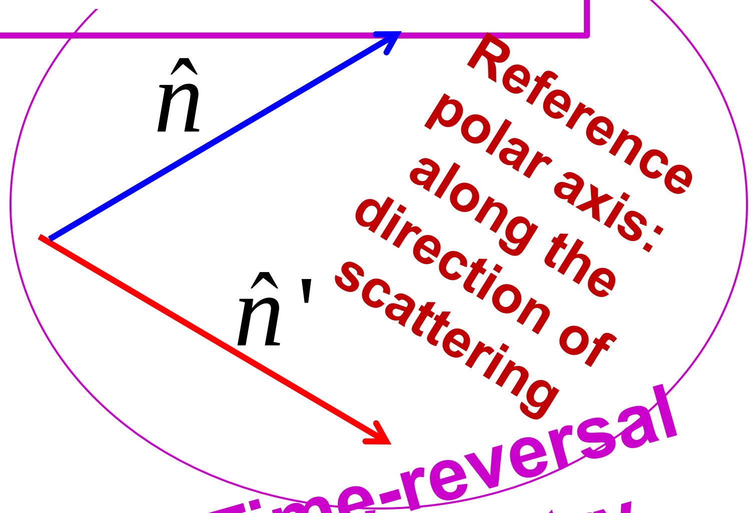
& reverse signs $S(\hat{n},\hat{n}') = S(-\hat{n}',-\hat{n})$

scattering amplitudes: $f(\hat{n},\hat{n}') = f(-\hat{n}',-\hat{n})$

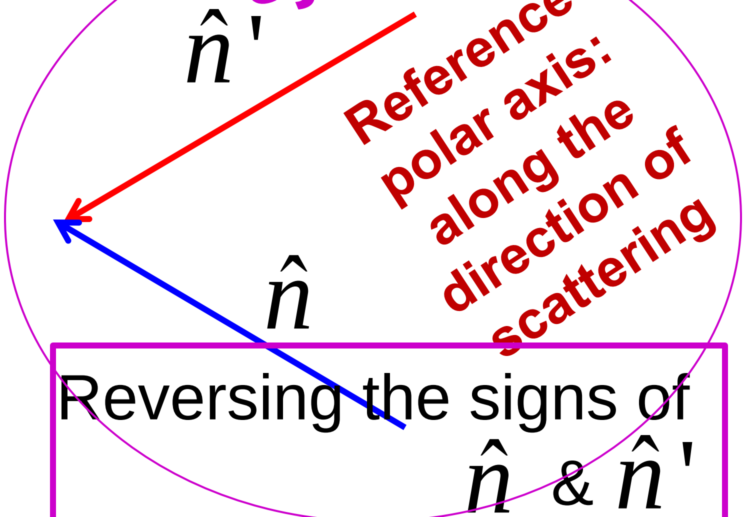
RECIPROCITY THEOREM

The scattering amplitudes for two scattering processes which are time-reversed processes of each other are the same.

$$S(\hat{n},\hat{n}') = S(-\hat{n}',-\hat{n})$$

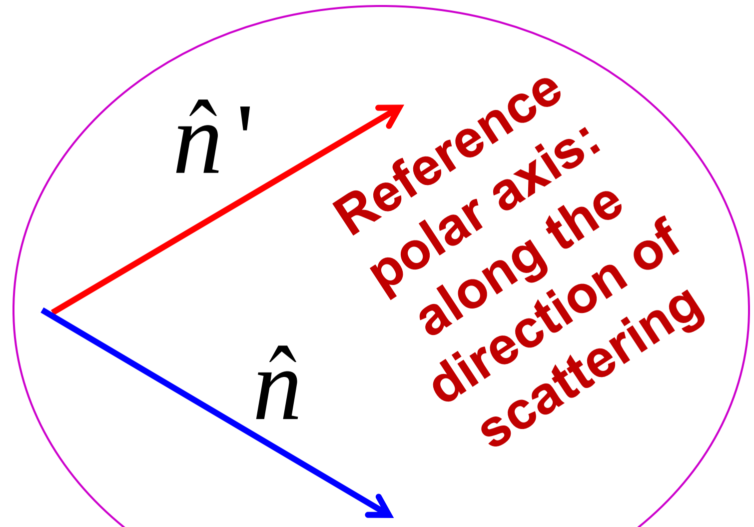


Time-reversal symmetry

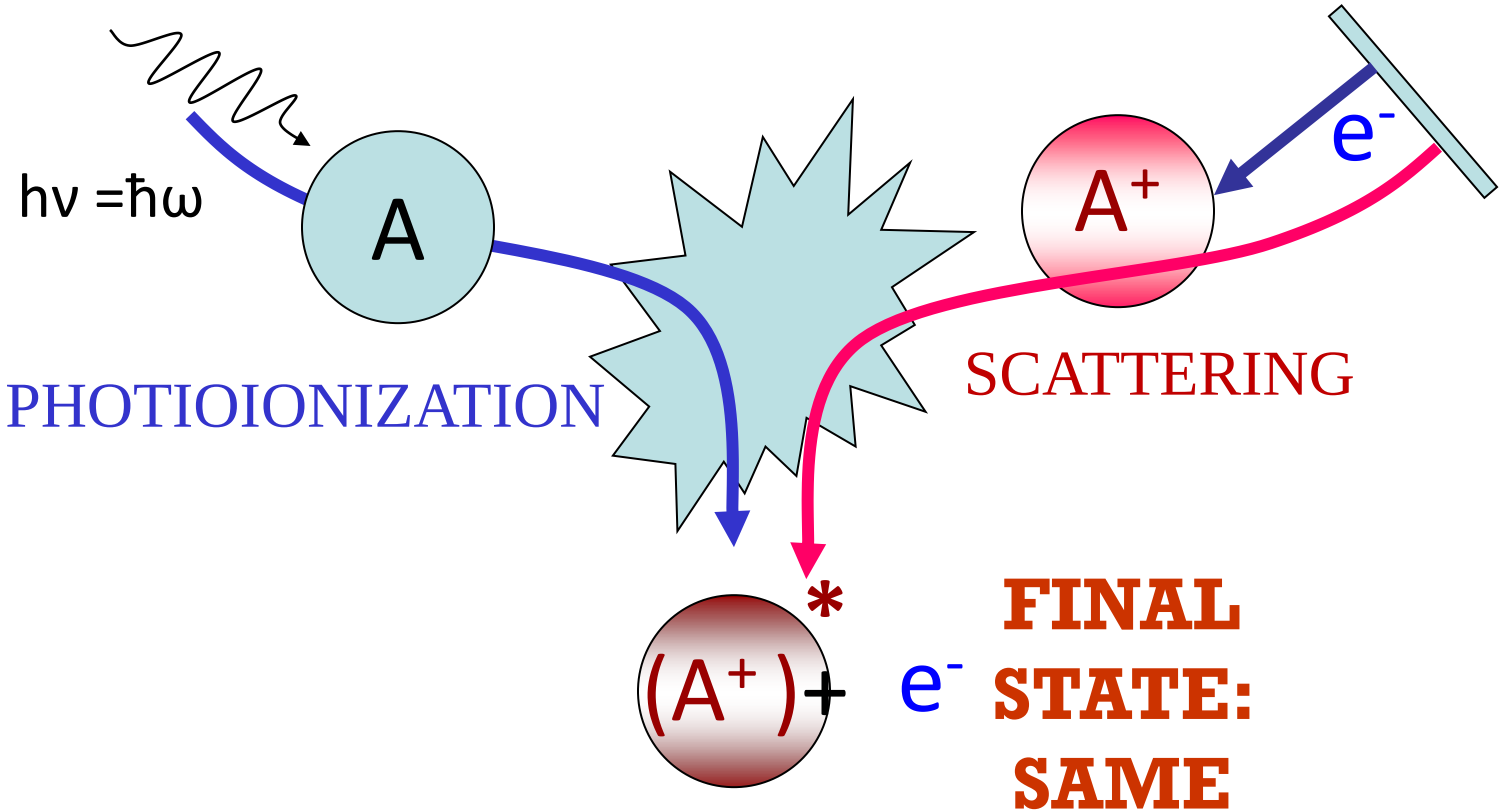


Reversing the signs of $\hat{n}$ & $\hat{n}'$

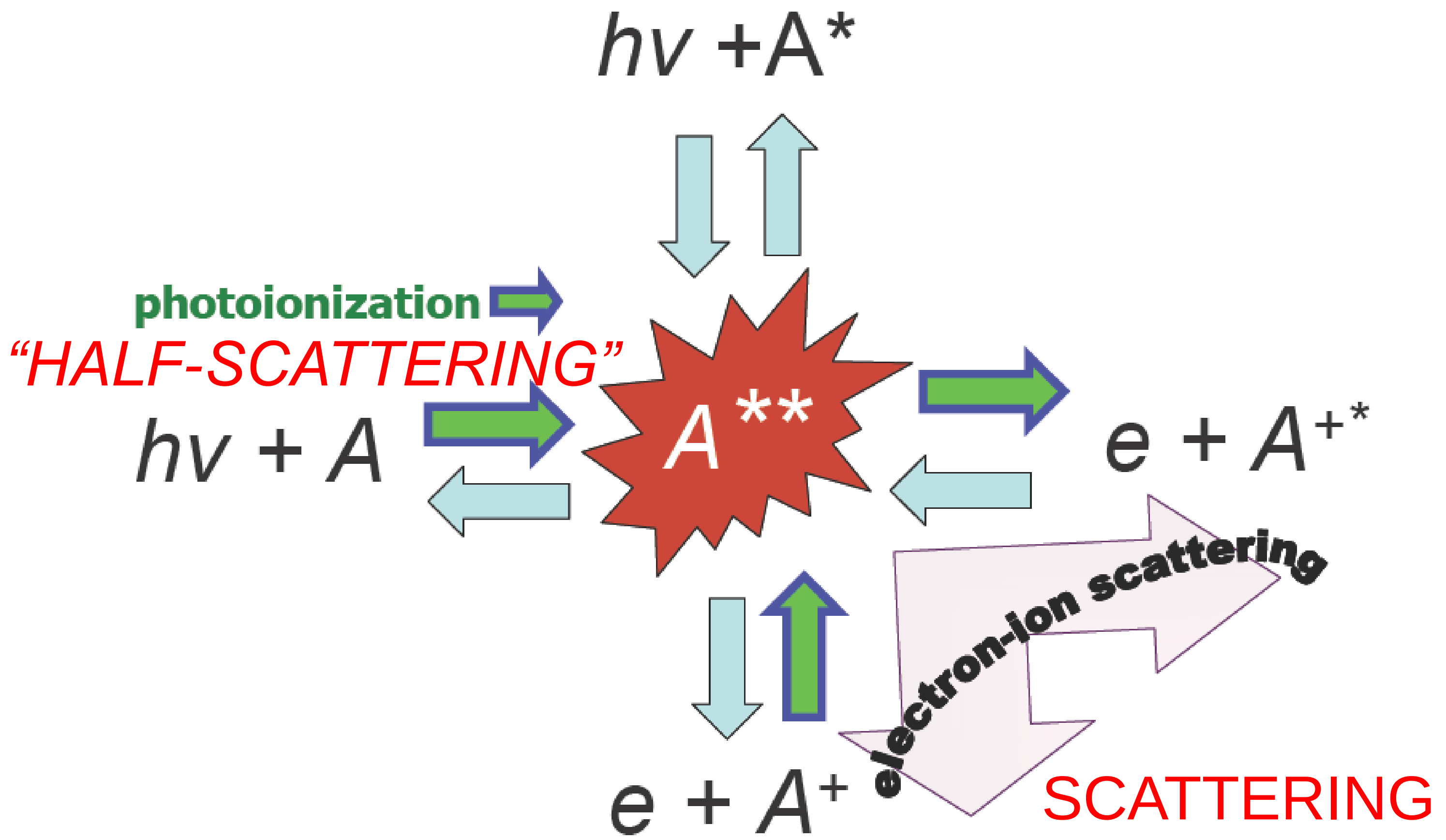
Interchanging $\hat{n}$ & $\hat{n}'$



Time-reversal interchanges the initial and final states, and reverses the direction of motion of particles in those states.



hν =ħω
A
PHOTIOIONIZATION
A+
e-
SCATTERING
*
(A+)+
e-
FINAL STATE: SAME



"Motion-Reversal"

U.Fano & A.R.P.Rau:
Theory of Atomic Collisions & Spectra

Partial wave analysis

$$\sigma_{Total} = \sum_{l=0}^{\infty} \sigma_l(k)$$

$$\sigma_l(k) = \frac{4\pi}{k^2}(2l+1)\sin^2[\delta_l(k)]$$

$$l_{\max} \sim ka$$

Consider s-wave scattering

$$\delta_{l=0}(k) \rightarrow n\pi$$

Electrons just go through the target!
- no scattering!

Ramsauer-Townsend effect

Low energy (~1eV) scattering of electrons by rare gas atoms
– Xe, Kr, Ar

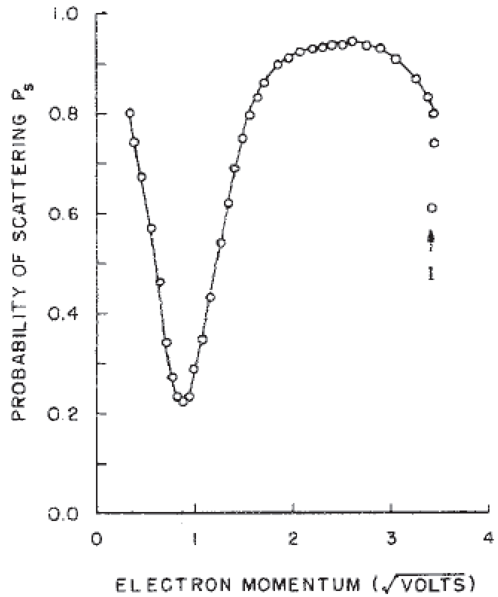


FIG. 4. The probability of scattering P_s as a function of $(V-V_s)^{1/2}$, where $V-V_s$ is the electron energy. Ionization occurs at "I".

Demonstration of Ramsauer Townsend Effect in Xenon by Kukolich – Am. J. Phys. 1968 Vol.30, No.8

$$\psi_{inc} \underset{r\to\infty}{\longrightarrow} \frac{1}{2ikr}\sum_l (2l+1) \left[P_l(\cos\theta)e^{ikr} - P_l(\cos\theta)(-1)^l e^{-ikr}\right]$$

$$\psi_{Tot}(\vec{r}) \underset{r\to\infty}{\longrightarrow} \qquad \left\{c_l^+ = e^{i\delta_l(k)}\right\}$$

$$\frac{1}{2ikr}\sum_l (2l+1)\left[P_l(\cos\theta)e^{ikr}\, e^{i2\delta_l(k)} - P_l(-\cos\theta)e^{-ikr}\right]$$

Phase shifts play a central role in quantum collision physics.

$$\psi_{inc} \underset{r\to\infty}{\longrightarrow} \frac{1}{2ikr}\sum_l (2l+1)\left[P_l(\cos\theta)e^{ikr} - P_l(\cos\theta)\left(-1\right)^l e^{-ikr}\right]$$

$$\psi_{Tot}\left(\vec{r}\right) \underset{r\to\infty}{\longrightarrow} \qquad \left\{c_l^+ = e^{i\delta_l(k)}\right\}$$

$$\frac{1}{2ikr}\sum_l (2l+1)\left[P_l(\cos\theta)e^{ikr}e^{i2\delta_l(k)} - P_l(-\cos\theta)e^{-ikr}\right]$$

Phase shifts are caused by the scattering potential,

so to study them we consider

two different scattering potentials.

$$\mathrm{R}_{\varepsilon l}(r) = \frac{y_{\varepsilon l(r)}}{r} \qquad \left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} - U(r)\right] y_l(k,r) = 0 \qquad U(r) = \frac{2mV(r)}{\hbar^2}$$

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

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

For two potentials

$$U(r) = \frac{2mV(r)}{\hbar^2}$$

$$\bar{U}(r) = \frac{2m\bar{V}(r)}{\hbar^2}$$

Normalization

$$y_l(k,r) \underset{r \to \infty}{\to} \frac{1}{k}\left[\sin\left(kr - \frac{l\pi}{2}\right) + \tan\delta_l(k)\cos\left(kr - \frac{l\pi}{2}\right)\right]$$

$$\bar{y}_l(k,r) \underset{r \to \infty}{\to} \frac{1}{k}\left[\sin\left(kr - \frac{l\pi}{2}\right) + \tan\bar{\delta}_l(k)\cos\left(kr - \frac{l\pi}{2}\right)\right]$$

$$\left[\frac{d^2}{dr^2}+k^2-\frac{l(l+1)}{r^2}-U(r)\right]y_l(k,r)=0 \quad \times\bar{y}_l(k,r)$$

Eq.A

$$\left[\frac{d^2}{dr^2}+k^2-\frac{l(l+1)}{r^2}-\bar{U}(r)\right]\bar{y}_l(k,r)=0 \quad \times y_l(k,r)$$

Eq.B

Eq.A - Eq.B

$$y_l''\bar{y}_l-\bar{y}_l''y_l-\left(U-\bar{U}\right)\bar{y}_l y_l=0$$

Wronskain of the two solutions $y_l(k,r)$ *and* $\bar{y}_l(k,r)$ *(definition):*

$$W\left[y_l(k,r),\bar{y}_l(k,r)\right]=y_l(k,r)\bar{y}_l'(k,r)-\bar{y}_l(k,r)y_l'(k,r)$$

$prime \rightarrow$ derivative with respect to r

$$-\frac{dW}{dr}-\left(U-\bar{U}\right)\bar{y}_l y_l=0$$

$$\frac{dW}{dr}=-\left(U-\bar{U}\right)\bar{y}_l y_l$$

$$\frac{dW}{dr} = -\left(U - \bar{U}\right)\bar{y}_l y_l$$

$$\int_{r=a}^{r=b} \frac{dW}{dr}\, dr = -\int_{r=a}^{r=b} \left(U - \bar{U}\right)\bar{y}_l y_l dr = -\int_{r=a}^{r=b} \bar{y}_l \left(U - \bar{U}\right) y_l dr$$

$$W\left[y_l(k,r), \bar{y}_l(k,r)\right]\Big|_a^b = -\int_{r=a}^{r=b} \bar{y}_l \left(U - \bar{U}\right) y_l dr$$

$$\left[y_l(k,r)\bar{y}_l\,'(k,r) - \bar{y}_l(k,r) y_l\,'(k,r)\right]\Big|_{r=a}^{r=b} = -\int_{r=a}^{r=b} \bar{y}_l \left(U - \bar{U}\right) y_l dr$$

$$\left[y_l(k,r)\bar{y}_l\,'(k,r) - \bar{y}_l(k,r) y_l\,'(k,r)\right]\Big|_{r=0}^{r\to\infty} = -\int_{r=0}^{r\to\infty} \bar{y}_l \left(U - \bar{U}\right) y_l dr$$

$$\left[y_l(k,r)\bar{y}_l{}'(k,r)-\bar{y}_l(k,r)y_l{}'(k,r)\right]\Big|_{r=0}^{r\to\infty}=-\int_{r=0}^{r\to\infty}\bar{y}_l\left(U-\bar{U}\right)y_l\,dr$$

$$\left[y_l(k,r)\bar{y}_l{}'(k,r)-\bar{y}_l(k,r)y_l{}'(k,r)\right]\Big|_{r\to\infty}=-\int_{r=0}^{r\to\infty}\bar{y}_l\left(U-\bar{U}\right)y_l\,dr$$

Evaluated in the asymptotic region

since

$$y_l(k,r\to 0)\to r^{l+1}\underset{r\to 0}{\to}\to 0$$

$$\bar{y}_l(k,r\to 0)\to r^{l+1}\underset{r\to 0}{\to}\to 0$$

$$y_l(k,r)\underset{r\to\infty}{\to}\frac{1}{k}\left[\sin\left(kr-\frac{l\pi}{2}\right)+\tan\delta_l(k)\cos\left(kr-\frac{l\pi}{2}\right)\right]$$

$$\bar{y}_l(k,r)\underset{r\to\infty}{\to}\frac{1}{k}\left[\sin\left(kr-\frac{l\pi}{2}\right)+\tan\bar{\delta}_l(k)\cos\left(kr-\frac{l\pi}{2}\right)\right]$$

Evaluation in the asymptotic region

$$\left[y_l(k,r)\bar{y}_l\,'(k,r)-\bar{y}_l(k,r)y_l\,'(k,r)\right]\Big|_{r\to\infty} = -\int_{r=0}^{r\to\infty}\bar{y}_l\left(U-\bar{U}\right)y_l\,dr$$

$$y_l(k,r)\underset{r\to\infty}{\rightarrow}\frac{1}{k}\left[\sin\left(kr-\frac{l\pi}{2}\right)+\tan\delta_l(k)\cos\left(kr-\frac{l\pi}{2}\right)\right]$$

$$\bar{y}_l(k,r)\underset{r\to\infty}{\rightarrow}\frac{1}{k}\left[\sin\left(kr-\frac{l\pi}{2}\right)+\tan\bar{\delta}_l(k)\cos\left(kr-\frac{l\pi}{2}\right)\right]$$

1st derivative w.r.t. r

$$\begin{cases} y_l\,'(k,r)\underset{r\to\infty}{\rightarrow}\left[\cos\left(kr-\frac{l\pi}{2}\right)-\tan\delta_l(k)\sin\left(kr-\frac{l\pi}{2}\right)\right] \\ \bar{y}_l\,'(k,r)\underset{r\to\infty}{\rightarrow}\left[\cos\left(kr-\frac{l\pi}{2}\right)+\tan\bar{\delta}_l(k)\sin\left(kr-\frac{l\pi}{2}\right)\right] \end{cases}$$

$$\left[y_l(k,r)\bar{y}_l\,'(k,r)-\bar{y}_l(k,r)y_l\,'(k,r)\right]\Big|_{r\to\infty} =$$

$$=\begin{Bmatrix}\frac{1}{k}\left[\sin\left(kr-\frac{l\pi}{2}\right)+\tan\delta_l(k)\cos\left(kr-\frac{l\pi}{2}\right)\right]\times \\ \left[\cos\left(kr-\frac{l\pi}{2}\right)-\tan\bar{\delta}_l(k)\sin\left(kr-\frac{l\pi}{2}\right)\right]\end{Bmatrix}-\begin{Bmatrix}\frac{1}{k}\left[\sin\left(kr-\frac{l\pi}{2}\right)+\tan\bar{\delta}_l(k)\cos\left(kr-\frac{l\pi}{2}\right)\right]\times \\ \left[\cos\left(kr-\frac{l\pi}{2}\right)-\tan\delta_l(k)\sin\left(kr-\frac{l\pi}{2}\right)\right]\end{Bmatrix}$$

Evaluation in the asymptotic region

$$\left[y_l(k,r)\bar{y}_l'(k,r)-\bar{y}_l(k,r)y_l'(k,r)\right]\Big|_{r\to\infty}=-\int_{r=0}^{r\to\infty}\bar{y}_l\left(U-\bar{U}\right)y_l\,dr$$

$$\left[y_l(k,r)\bar{y}_l'(k,r)-\bar{y}_l(k,r)y_l'(k,r)\right]\Big|_{r\to\infty}=$$

$$=\left\{\begin{matrix}\frac{1}{k}\left[\sin\left(kr-\frac{l\pi}{2}\right)+\tan\delta_l(k)\cos\left(kr-\frac{l\pi}{2}\right)\right]\times\\ \left[\cos\left(kr-\frac{l\pi}{2}\right)-\tan\bar{\delta}_l(k)\sin\left(kr-\frac{l\pi}{2}\right)\right]\end{matrix}\right\}-\left\{\begin{matrix}\frac{1}{k}\left[\sin\left(kr-\frac{l\pi}{2}\right)+\tan\bar{\delta}_l(k)\cos\left(kr-\frac{l\pi}{2}\right)\right]\times\\ \left[\cos\left(kr-\frac{l\pi}{2}\right)-\tan\delta_l(k)\sin\left(kr-\frac{l\pi}{2}\right)\right]\end{matrix}\right\}$$

$$\left[y_l(k,r)\bar{y}_l'(k,r)-\bar{y}_l(k,r)y_l'(k,r)\right]\Big|_{r\to\infty}=$$

$$=\frac{1}{k}\left\{\begin{matrix}\left[\sin\left(kr-\frac{l\pi}{2}\right)+\tan\delta_l(k)\cos\left(kr-\frac{l\pi}{2}\right)\right]\times\\ \left[\cos\left(kr-\frac{l\pi}{2}\right)-\tan\bar{\delta}_l(k)\sin\left(kr-\frac{l\pi}{2}\right)\right]\end{matrix}\right\}-\frac{1}{k}\left\{\begin{matrix}\left[\sin\left(kr-\frac{l\pi}{2}\right)+\tan\bar{\delta}_l(k)\cos\left(kr-\frac{l\pi}{2}\right)\right]\times\\ \left[\cos\left(kr-\frac{l\pi}{2}\right)-\tan\delta_l(k)\sin\left(kr-\frac{l\pi}{2}\right)\right]\end{matrix}\right\}$$

Evaluation in the asymptotic region

$$\left[y_l(k,r)\bar{y}_l'(k,r)-\bar{y}_l(k,r)y_l'(k,r)\right]\Big|_{r\to\infty} = -\int_{r=0}^{r\to\infty} \bar{y}_l\left(U-\bar{U}\right)y_l dr$$

$$=\frac{1}{k}\left[\begin{array}{l}\sin\left(kr-\frac{l\pi}{2}\right)\cos\left(kr-\frac{l\pi}{2}\right)-\sin^2\left(kr-\frac{l\pi}{2}\right)\tan\bar{\delta}_l(k)\\ +\tan\delta_l(k)\cos^2\left(kr-\frac{l\pi}{2}\right)\\ -\tan\bar{\delta}_l(k)\sin\left(kr-\frac{l\pi}{2}\right)\tan\delta_l(k)\cos\left(kr-\frac{l\pi}{2}\right)\end{array}\right] = \frac{1}{k}\left[\begin{array}{l}-\tan\bar{\delta}_l(k)\\ +\tan\delta_l(k)\end{array}\right]$$

$$-\frac{1}{k}\left[\begin{array}{l}\sin\left(kr-\frac{l\pi}{2}\right)\cos\left(kr-\frac{l\pi}{2}\right)-\sin^2\left(kr-\frac{l\pi}{2}\right)\tan\delta_l(k)\\ +\tan\bar{\delta}_l(k)\cos^2\left(kr-\frac{l\pi}{2}\right)\\ -\tan\bar{\delta}_l(k)\sin\left(kr-\frac{l\pi}{2}\right)\tan\delta_l(k)\cos\left(kr-\frac{l\pi}{2}\right)\end{array}\right]$$

Evaluation in the asymptotic region

$$\left[y_l(k,r)\bar{y}_l\,'(k,r)-\bar{y}_l(k,r)y_l\,'(k,r)\right]\Big|_{r\to\infty}=-\int_{r=0}^{r\to\infty}\bar{y}_l\left(U-\bar{U}\right)y_l\,dr$$

$$\frac{1}{k}\left[-\tan\bar{\delta}_l(k)+\tan\delta_l(k)\right]=-\int_{r=0}^{r\to\infty}\bar{y}_l\left(U-\bar{U}\right)y_l\,dr$$

$$\tan\delta_l(k)-\tan\bar{\delta}_l(k)=-k\int_{r=0}^{r\to\infty}\bar{y}_l(k,r)\left(U(r)-\bar{U}(r)\right)y_l(k,r)\,dr$$

$$when\ \bar{U}(r)=0\ \text{(free particle!)}$$

$$\tan\delta_l(k)=-k\int_{r=0}^{r\to\infty}\left\{rj_l(k,r)\right\}^{V=0}U(r)\left\{rR_l^{V\neq 0}(k,r)\right\}dr$$

$$\tan\delta_l(k)=-k\int_{r=0}^{r\to\infty}j_l(k,r)U(r)R_l^{V\neq 0}(k,r)r^2\,dr$$

$$Normalization:$$

$$R_l^{V\neq 0}{}_l(k,r)\underset{r\to\infty}{\longrightarrow}j_l(k,r)-\tan\delta_l(k)n_l(k,r)$$

$$\tan\delta_l(k) = -k\int_{r=0}^{r\to\infty} j_l(k,r)U(r)R_l^{V\neq 0}(k,r)r^2 dr$$

$$\tan\delta_l(k) = -\int_{r=0}^{r\to\infty} \left\{(kr)\, j_l(k,r)\right\}U(r)\left\{rR_l^{V\neq 0}(k,r)\right\}dr$$

$$rR_{kl}^{(V=0)}(r\to\infty) \to 2\left\{(kr)\, j_l(kr)\right\} \to \underset{\substack{asymptotic\\ behavior}}{\overset{r\to\infty}{\approx}} 2\sin\left(kr - l\frac{\pi}{2}\right)$$

$\mathrm{E} > 0$ continuum for $\mathrm{V} = 0$

$$\left\{\begin{array}{l} rR_l^{V\neq 0}(k,r) \underset{r\to\infty}{\longrightarrow} \sin\left[kr - \frac{l\pi}{2} + \delta_l(k)\right] \\ rR_l^{V=0}(k,r) \underset{r\to\infty}{\longrightarrow} \sin\left[kr - \frac{l\pi}{2}\right] \end{array}\right\}$$

Examine their nodal behavior

$$rR_l^{V\neq 0}(k,r) \underset{r\to\infty}{\longrightarrow} \sin\left[kr - \frac{l\pi}{2} + \delta_l(k)\right] \text{ has nodes at } kr - \frac{l\pi}{2} + \delta_l(k) = n\pi$$

$$rR_l^{V=0}(k,r) \underset{r\to\infty}{\longrightarrow} \sin\left[kr - \frac{l\pi}{2}\right] \text{ has nodes at } kr - \frac{l\pi}{2} = n\pi$$

$$n = 0,1,2,3,4,.....$$

$$rR_l^{V\neq 0}(k,r) \underset{r\to\infty}{\longrightarrow} \sin\left[kr - \frac{l\pi}{2} + \delta_l(k)\right] \rightarrow \text{ nodes @ } r = \frac{1}{k}\left[n\pi + \frac{l\pi}{2} - \delta_l(k)\right]$$

$$rR_l^{V=0}(k,r) \underset{r\to\infty}{\longrightarrow} \sin\left[kr - \frac{l\pi}{2}\right] \rightarrow \text{ nodes @ } r = \frac{1}{k}\left[n\pi + \frac{l\pi}{2}\right]$$

$$n = 0,1,2,3,4,.....$$

nodes of $R_l^{V\neq 0}(k,r)$ are pulled/pushed by $\dfrac{\delta_l(k)}{k}$

with respect to those of $R_l^{V=0}(k,r)$ depending on

$\delta_l(k) \rangle\ 0$ or $\delta_l(k) \langle\ 0$.

QUESTIONS ?
Write to:
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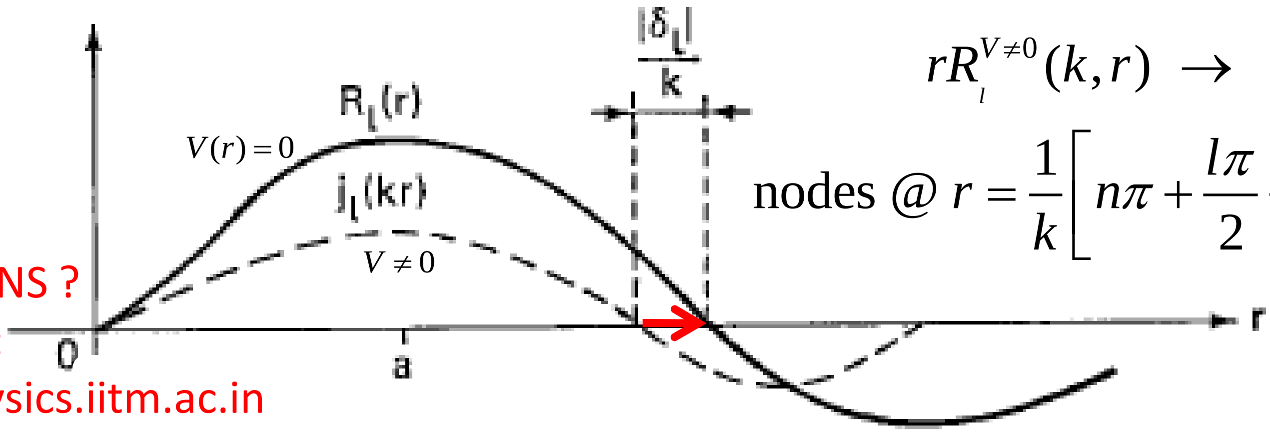
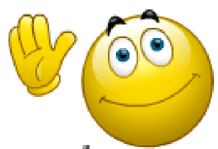


$$rR_l^{V\neq 0}(k,r) \rightarrow$$

$$\text{nodes @ } r = \frac{1}{k}\left[n\pi + \frac{l\pi}{2} - \delta_l(k)\right]$$

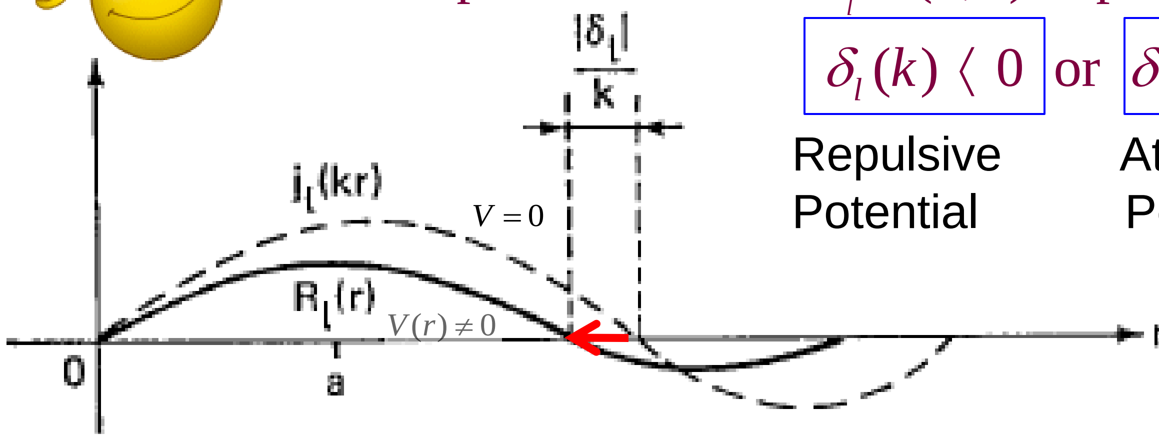


nodes of $R_l^{V\neq 0}(k,r)$ are pushed/pulled by $\dfrac{\delta_l(k)}{k}$

with respect to those of $R_l^{V=0}(k,r)$ depending on

$\delta_l(k) \langle\ 0$ or $\delta_l(k) \rangle\ 0$.

Repulsive Potential | Attractive Potential



Reference: Joachain: Quantum Collision Theory / page 80

Fig. 4.4. Schematic representation of the effect on the free radial wave $j_l(kr)$ of (a) a repulsive (positive) potential, (b) an attractive (negative) potential.

Select/Special Topics *in*
‘Theory of Atomic Collisions and Spectroscopy’

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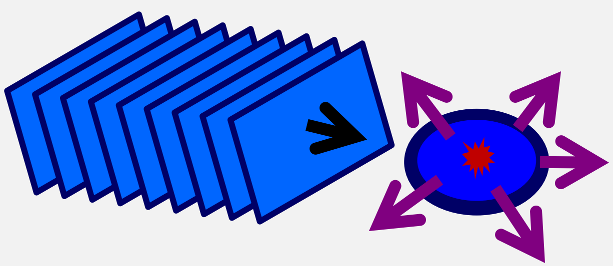
Lecture Number 09

Unit 1: Quantum Theory of Collisions

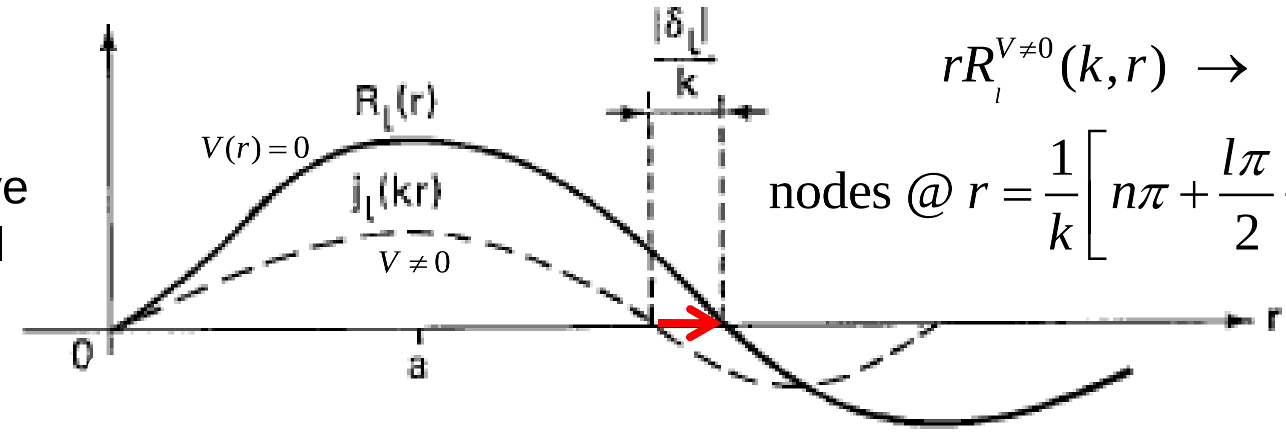


More on:

Phase-shift analysis

- from Joachain’s Quantum Collision Theory

Repulsive Potential



$rR_l^{V\neq 0}(k,r) \rightarrow$

$$\text{nodes @ } r = \frac{1}{k}\left[n\pi + \frac{l\pi}{2} - \delta_l(k)\right]$$

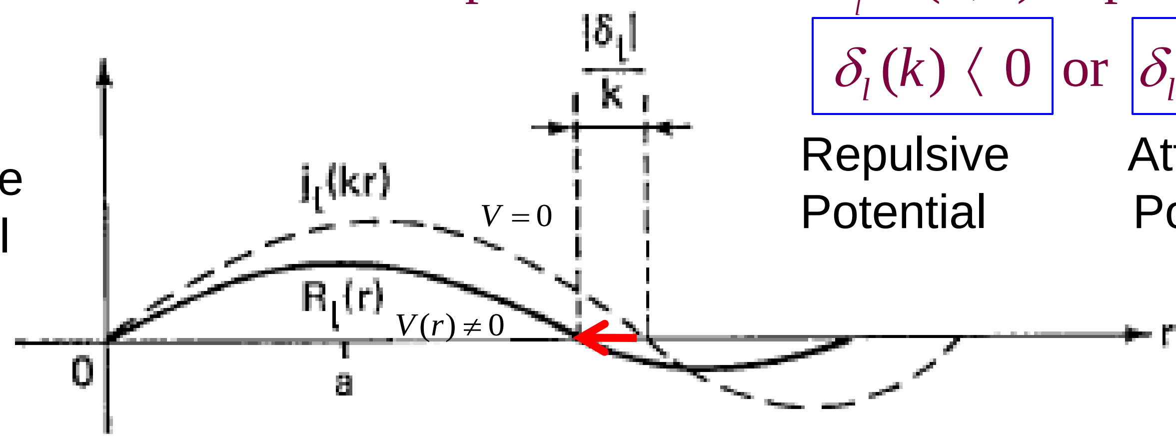
nodes of $R_l^{V\neq 0}(k,r)$ are pushed/pulled by $\dfrac{\delta_l(k)}{k}$

with respect to those of $R_l^{V=0}(k,r)$ depending on

$\boxed{\delta_l(k) \langle\ 0}$ or $\boxed{\delta_l(k)\ \rangle\ 0}$.

Repulsive Potential | Attractive Potential

Attractive Potential



Reference: Joachain: Quantum Collision Theory / page 80

Fig. 4.4. Schematic representation of the effect on the free radial wave $j_l(kr)$ of (a) a repulsive (positive) potential, (b) an attractive (negative) potential.

$$\tan \delta_l(k) = -k \int_{r=0}^{r\to\infty} j_l(k,r)U(r)R_l(k,r)r^2 dr$$

$$U(r) = U(\lambda, r)$$

$$\bar{U}(r) = U(\bar{\lambda}, r)$$

λ : coupling strength parameter

$$\tan \delta_l(k) - \tan \bar{\delta}_l(k) = -k \int_{r=0}^{r\to\infty} \bar{y}_l(k,r)\left(U(r) - \bar{U}(r)\right) y_l(k,r)dr$$

$$\frac{\tan \delta_l(k) - \tan \bar{\delta}_l(k)}{\delta\lambda} = -k \int_{r=0}^{r\to\infty} \bar{y}_l(k,r)\frac{\left(U(r) - \bar{U}(r)\right)}{\delta\lambda} y_l(k,r)dr$$

$$\frac{d}{d\lambda}\left(\tan \delta_l(k)\right) = -k \int_{r=0}^{r\to\infty} \bar{y}_l(k,r)\frac{\partial U(\lambda,r)}{\partial\lambda} y_l(k,r)dr$$

$$\frac{1}{\cos^2 \delta_l(k)} \frac{d\delta_l(k)}{d\lambda} = -k \int_{r=0}^{r\to\infty} \bar{y}_l(k,r)\frac{\partial U(\lambda,r)}{\partial\lambda} y_l(k,r)dr$$

$$\tan\delta_l(k) = -k\int_{r=0}^{r\to\infty} j_l(k,r)U(r)R_l(k,r)r^2dr$$

$$U(r) = U(\lambda, r)$$

$$\bar{U}(r) = U(\bar{\lambda}, r)$$

λ : coupling strength parameter

$$\frac{1}{\cos^2\delta_l(k)}\frac{d\delta_l(k)}{d\lambda} = -k\int_{r=0}^{r\to\infty} \bar{y}_l(k,r)\frac{\partial U(\lambda,r)}{\partial\lambda}y_l(k,r)dr$$

$$\frac{d\delta_l(k)}{d\lambda} = -k\left\{\cos^2\delta_l(k)\right\}\int_{r=0}^{r\to\infty} \bar{y}_l(k,r)\frac{\partial U(\lambda,r)}{\partial\lambda}y_l(k,r)dr$$

$$\frac{d\delta_l(k)}{d\lambda} \approx -k\{1\}\int_{r=0}^{r\to\infty} \bar{y}_l(k,r)\frac{\partial U(\lambda,r)}{\partial\lambda}y_l(k,r)dr$$

$$\frac{d\delta_l(k)}{d\lambda} \approx -k \int_{r=0}^{r\to\infty} \bar{y}_l(k,r) \frac{\partial U(\lambda,r)}{\partial \lambda} y_l(k,r)dr \qquad U(r) = U(\lambda,r)$$

λ: coupling strength parameter

$$\frac{d\delta_l(k)}{d\lambda} \approx -k \int_{r=0}^{r\to\infty} \bar{y}_l(k,r) \frac{\partial U(\lambda,r)}{\partial \lambda} \left[\bar{y}_l(k,r)\{1+...\}\right]dr$$

$$\frac{d\delta_l(k)}{d\lambda} \approx -k \int_{r=0}^{r\to\infty} [\bar{y}_l(k,r)]^2 \frac{\partial U(\lambda,r)}{\partial \lambda} dr$$

if the sign of $\left[\frac{\partial U(\lambda,r)}{\partial \lambda}\right]$ does not change in the region $0 \leq r \langle \infty$ then $\left[\frac{d\delta_l(k)}{\partial \lambda}\right]$ has opposite sign if the sign of $\left[\dfrac{\partial U(\lambda,r)}{\partial\lambda}\right]$ does not change in the region $0 \le r \langle \infty$ $\Bigg\}$ then $\Bigg\{$ $\left[\dfrac{d\delta_l(k)}{\partial\lambda}\right]$ has opposite sign

$\delta_l(k) \rightarrow$ *hitherto* defined modulo π

can now be defined as an absolute angle

by setting $\delta_l(k) = 0$ for $U = 0$, *and*

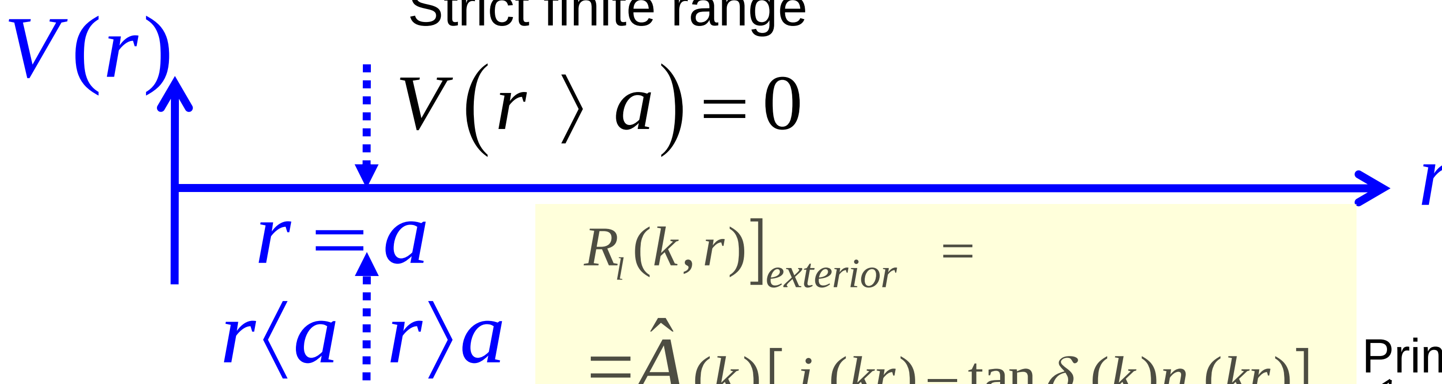
let $\delta_l(k)$ evolve continuously with

the control parameter λ to get :

$$\tan\delta_l(k) = -k \int_{r=0}^{r\to\infty} j_l(k,r)U(r)R_l(k,r)r^2 dr$$

Strict finite range

$$V(r>a)=0$$



$$\left.R_l(k,r)\right]_{exterior} = \hat{A}_l(k)\left[j_l(kr)-\tan\delta_l(k)n_l(kr)\right]$$

$R_l(k,r)$ and $\dfrac{dR_l(k,r)}{dr}$ are continuous at $r=a$.

$$\gamma_l(k)=\left[\frac{\left\{\frac{dR_l(k,r)}{dr}\right\}}{R_l(k,r)}\right]_{\text{interior}}=\left[\frac{\left\{\frac{dR_l(k,r)}{dr}\right\}}{R_l(k,r)}\right]_{\text{exterior}}=\left.\frac{\hat{A}_l(k)k\left[j_l'(kr)-\tan\delta_l(k)n_l'(kr)\right]}{\hat{A}_l(k)\left[j_l(kr)-\tan\delta_l(k)n_l(kr)\right]}\right]_{r=a}$$

Prime: derivative w.r.t. kr at $r=a$

Logarithmic derivative of the radial wave function at *r* = *a*

$$\gamma_l(k)=\frac{k\left[j_l'(ka)-\tan\delta_l(k)n_l'(ka)\right]}{\left[j_l(ka)-\tan\delta_l(k)n_l(ka)\right]}$$

Prime: derivative w.r.t. kr evaluated at $r=a$

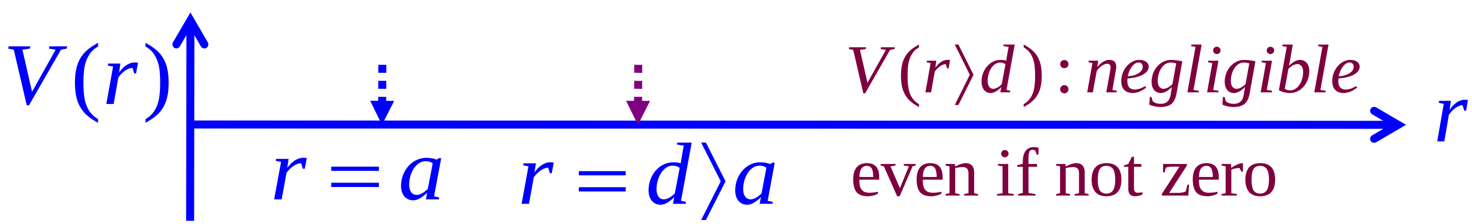
Logarithmic derivative of the radial wave function at $r = a$

$$\gamma_l(k) = \frac{k\left[j_l'(ka) - \tan\delta_l(k) n_l'(ka) \right]}{\left[j_l(ka) - \tan\delta_l(k) n_l(ka) \right]}$$

Prime: derivative w.r.t. kr

$$\tan\delta_l(k) = \frac{\left[k j_l'(ka) - \gamma_l(k) j_l(ka) \right]}{\left[k n_l'(ka) - \gamma_l(k) n_l(ka) \right]}$$

$$V(r>a) = 0$$



$$\tan\delta_l(k) = \frac{\left[k j_l'(kd) - \gamma_l(k) j_l(kd) \right]}{\left[k n_l'(kd) - \gamma_l(k) n_l(kd) \right]}$$

We shall consider $V(r>a) = 0$

$$\tan\delta_l(k) = \frac{\left[kj_l'(ka) - \gamma_l(k)\, j_l(ka)\right]}{\left[kn_l'(ka) - \gamma_l(k) n_l(ka)\right]}$$

$$q_l(k) = \frac{kj_l'(ka) / j_l(ka)}{\gamma_l(k)}$$

↑ definition : dimensionless

$$\uparrow \gamma_l(k) = \frac{kj_l'(ka) \big/ j_l(ka)}{q_l(k)}$$

$$\tan\delta_l(k) = \frac{\left[kj_l'(ka) - \left\{\dfrac{kj_l'(ka) \big/ j_l(ka)}{q_l(k)}\right\} j_l(ka)\right]}{\left[kn_l'(ka) - \left\{\dfrac{kj_l'(ka) \big/ j_l(ka)}{q_l(k)}\right\} n_l(ka)\right]}$$

cancelling k

$$\tan\delta_l(k) = \frac{\left[j_l'(ka) - \left\{\dfrac{j_l'(ka) \big/ j_l(ka)}{q_l(k)}\right\} j_l(ka)\right]}{\left[n_l'(ka) - \left\{\dfrac{j_l'(ka) \big/ j_l(ka)}{q_l(k)}\right\} n_l(ka)\right]}$$

$$\tan\delta_l(k)=\frac{j_l^{'}(ka)-\left\{\frac{j_l^{'}(ka)\big/ j_l(ka)}{q_l(k)}\right\}j_l(ka)}{n_l^{'}(ka)-\left\{\frac{j_l^{'}(ka)\big/ j_l(ka)}{q_l(k)}\right\}n_l(ka)}$$

$$\tan\delta_l(k)=\frac{j_l^{'}(ka)-\left\{\frac{j_l^{'}(ka)\big/ j_l(ka)}{q_l(k)}\right\}j_l(ka)}{n_l^{'}(ka)-\left\{\frac{j_l^{'}(ka)\big/ j_l(ka)}{q_l(k)}\right\}n_l(ka)}$$

$$\tan\delta_l(k)=\frac{j_l^{'}(ka)\left\{1-\frac{1}{q_l(k)}\right\}}{n_l^{'}(ka)-\left\{\frac{j_l^{'}(ka)\big/ j_l(ka)}{q_l(k)}\right\}n_l(ka)}$$

$$\tan\delta_l(k)=\frac{j_l^{'}(ka)\,j_l(ka)\{q_l(k)-1\}}{q_l(k)n_l^{'}(ka)\,j_l(ka)-j_l^{'}(ka)\,n_l(ka)}$$

$$\tan \delta_l(k) = \frac{j_l'(ka)\, j_l(ka)\{q_l(k)-1\}}{q_l(k)\, n_l'(ka)\, j_l(ka) - j_l'(ka)\, n_l(ka)} \xrightarrow[k\to 0]{\textit{low energy}} \; ?$$

$z = ka$

$$j_l(z) = \frac{z^l}{(2l+1)!!}\left[1 - \frac{\frac{1}{2}z^2}{1!(2l+3)} + \frac{\left(\frac{1}{2}z^2\right)^2}{2!(2l+3)(2l+5)} - \ldots\right]$$

$$(2l+1)!! = 1\times 3\times 5\times 7\times \ldots\times(2l+1)$$

$$(2l-1)!! = 1\times 3\times 5\times 7\times \ldots\times(2l-1)$$

$$n_l(z) = -\frac{(2l-1)!!}{z^{l+1}}\left[1 - \frac{\frac{1}{2}z^2}{1!(1-2l)} + \frac{\left(\frac{1}{2}z^2\right)^2}{2!(1-2l)(3-2l)} - \ldots\right]$$

$\ell > 0$

$$j_l(z) \xrightarrow[z\to 0]{} \frac{z^l}{(2l+1)!!} \qquad n_l(z) \xrightarrow[z\to 0]{} -\frac{(2l-1)!!}{z^{l+1}}$$

$$D_l = D_+ \; D_- = (2l+1)!! \; (2l-1)!!$$

$$D_{l=0} = 1$$

$$\frac{1}{D_l} = \frac{1}{(2l+1)!!(2l-1)!!} = \frac{1}{1\times3\times5\times..\times(2l+1)} \times \frac{1}{1\times3\times5\times..\times(2l-1)}$$

$$\frac{1}{D_l} = \frac{2\times4\times6\times..\times(2l)}{1\times2\times3\times4\times5\times..\times(2l+1)} \times \frac{2\times4\times6\times..\times(2l-2)}{1\times2\times3\times4\times5\times..\times(2l-1)}$$

$$\frac{1}{D_l} = \frac{2^l\times1\times2\times3\times..\times(l)}{1\times2\times3\times4\times5\times..\times(2l+1)} \times \frac{2^{l-1}\times1\times2\times3\times..\times(l-1)}{1\times2\times3\times4\times5\times..\times(2l-1)}$$

$$\frac{1}{D_l} = \frac{2^{2l-1}\times l!}{(2l+1)!} \times \frac{(l-1)!}{(2l-1)!}$$

$$D_l = \frac{(2l+1)!(2l-1)!}{2^{2l-1} l!(l-1)!}$$

$$\tan\delta_l(k) = \frac{j_l^{'}(ka)\, j_l(ka)\{q_l(k)-1\}}{q_l(k)n_l^{'}(ka)\, j_l(ka) - j_l^{'}(ka)\, n_l(ka)} \xrightarrow[k\to 0]{\textit{low energy}} ?$$

$z = ka$ $\quad$ $\ell > 0$

$$j_l(z) \underset{z\to 0}{\rightarrow} \frac{z^l}{D_+} \qquad n_l(z) \underset{z\to 0}{\rightarrow} -\frac{D_-}{z^{l+1}}$$

$$D_+ = (2l+1)!! \qquad D_- = (2l-1)!!$$

$$j_l^{'}(z) \underset{z\to 0}{\rightarrow} \frac{l z^{l-1}}{(2l+1)!!} \; ; \quad n_l^{'}(z) \underset{z\to 0}{\rightarrow} \cancel{-}\frac{(2l-1)!!\{\cancel{-}(l+1)\}}{z^{l+2}}$$

$$j_l^{'}(z) \underset{z\to 0}{\rightarrow} \frac{l z^{l-1}}{(2l+1)!!} \; ; \quad n_l^{'}(z) \underset{z\to 0}{\rightarrow} = \frac{(2l-1)!!(l+1)}{z^{l+2}}$$

$$\tan\delta_l(k) = \frac{j_l'(ka)\, j_l(ka)\{q_l(k)-1\}}{q_l(k)\, n_l'(ka)\, j_l(ka) - j_l'(ka)\, n_l(ka)} \xrightarrow[k\to 0]{\text{low energy}} ?$$

$z = ka$

$\ell > 0$

$$j_l(z) \underset{z\to 0}{\to} \frac{z^l}{D_+} \quad \text{and} \quad n_l(z) \underset{z\to 0}{\to} -\frac{D_-}{z^{l+1}}$$

$$j_l'(z) \underset{z\to 0}{\to} \frac{l z^{l-1}}{D_+} \; ; \quad n_l'(z) \underset{z\to 0}{\to} = \frac{D_-(l+1)}{z^{l+2}}$$

$$\tan\delta_l(k) \xrightarrow[k\to 0]{\substack{\text{low}\\ \text{energy}}} \frac{\left(\frac{l z^{l-1}}{D_+}\right)\left(\frac{z^l}{D_+}\right)\{q_l(k)-1\}}{q_l(k)\left(\frac{D_-(l+1)}{z^{l+2}}\right)\left(\frac{z^l}{D_+}\right) - \left(\frac{l z^{l-1}}{D_+}\right)\left(-\frac{D_-}{z^{l+1}}\right)}$$

$$\tan\delta_l(k) \xrightarrow[k\to 0]{\substack{\text{low}\\ \text{energy}}} \frac{\{q_l(k)-1\}}{D_+ D_-} \frac{l z^{l-1} \times z^l}{q_l(k)(l+1) z^{-2} + l z^{-2}}$$

$$\tan\delta_l(k) \xrightarrow[k\to 0]{\substack{\text{low}\\ \text{energy}}} \frac{q_l(k)-1}{D_+ D_-} \frac{z^{2l+1}}{q_l(k)\frac{(l+1)}{l} + 1}$$

$$\tan\delta_l(k) \underset{k\to 0}{\overset{low\ energy}{\longrightarrow}} \frac{q_l(k)-1}{D_+D_-}\frac{z^{2l+1}}{q_l(k)\frac{(l+1)}{l}+1}$$

$\ell > 0$

$$\gamma_l^{V=0}(k) = \frac{kj_l'(ka)}{j_l(ka)}$$

$$q_l(k) \underset{definition}{=} \frac{kj_l'(ka)/j_l(ka)}{\gamma_l(k)} = \frac{\gamma_l^{V=0}(k)}{\gamma_l(k)}$$

$$\gamma_l^{V=0}(k) \underset{k\to 0}{\overset{low\ energy}{\longrightarrow\longrightarrow\longrightarrow}} ?$$

$$j_l(\rho) \underset{\rho\to 0}{\to} \left[\frac{\rho^l}{D_+}\right] \overset{\rho=ka}{\to} \left[\frac{(ka)^l}{D_+}\right] \qquad j_l'(\rho) \underset{\rho\to 0}{\to} \left[\frac{l\rho^{l-1}}{D_+}\right] \overset{\rho=ka}{\to} \left[\frac{l(ka)^{l-1}}{D_+}\right]$$

$$\gamma_l^{V=0}(k) \underset{k\to 0}{\to} \frac{kl(ka)^{l-1}}{(ka)^l} = \frac{kl}{ka} = \frac{l}{a}$$

$$q_l(k\to 0) = \frac{l}{a\gamma_l(k)}$$

$$\tan\delta_l(k) \underset{k\to 0}{\overset{low\ energy}{\to}} \frac{\left(\frac{l}{a\gamma_l(k)}\right)-1}{D_+D_-}\frac{z^{2l+1}}{\left(\frac{l}{a\gamma_l(k)}\right)\left(\frac{l+1}{l}\right)+1}$$

$$\tan\delta_l(k) \underset{k\to 0}{\overset{\substack{low\\energy}}{\longrightarrow}} \frac{\left(\frac{l}{a\gamma_l(k)}\right)-1}{D_+D_-} \frac{z^{2l+1}}{\left(\frac{l}{a\gamma_l(k)}\right)\left(\frac{l+1}{l}\right)+1}$$

$z = ka$

$\ell \rangle 0$

$$\tan\delta_l(k) \underset{k\to 0}{\overset{\substack{low\\energy}}{\longrightarrow}} \frac{l-a\gamma_l(k)}{D_+D_-} \frac{z^{2l+1}}{(l+1)+a\gamma_l(k)}$$

$$\hat{\gamma}_l(k) = \lim_{k\to 0} \gamma_l(k)$$

$$\tan\delta_l(k) \underset{k\to 0}{\overset{\substack{low\\energy}}{\longrightarrow}} \frac{(ka)^{2l+1}}{D_+D_-} \frac{l-a\hat{\gamma}_l(k)}{(l+1)+a\hat{\gamma}_l(k)}$$

$$\tan\delta_l(k) \underset{k\to 0}{\overset{\substack{low\\energy}}{\longrightarrow}} (ka)^{2l+1}$$

$if\ \ a\hat{\gamma}_l = -(l+1)$

$\mapsto$ '*zero energy resonance*'

$$\tan\delta_l(k) \underset{k\to 0}{\overset{\substack{low\\energy}}{\longrightarrow}} \frac{(ka)^{2l+1}}{D_l}\frac{\left[l-a\hat{\gamma}_l\right]}{(l+1)+a\hat{\gamma}_l}$$

where $\hat{\gamma}_l \left(\underset{k\to 0}{\overset{\substack{low\\energy}}{\longrightarrow}} \right) \gamma_l(k)$

$$\mathrm{D}_l = \mathrm{D}_+ \ \mathrm{D}_- = (2l+1)!!(2l-1)!! \quad \text{for } l \rangle\ 0$$
$$= 1 \qquad\qquad\qquad \text{for } l = 0$$

RECALL:

$$f_k(\theta) = \sum_{l=0}^{\infty}(2l+1)\ a_l(k)\ P_l(\cos\theta) \rightarrow f_k(\theta): scattering\ \ amplitude$$

$$a_l(k) = \frac{\left[e^{2i\delta_l(k)}-1\right]}{2ik} = \frac{\left[S_l(k)-1\right]}{2ik} \rightarrow \boxed{a_l(k): partial\ \ wave\ \ amplitude}$$

$$\text{For small } \ \delta_l(k), \ \ \delta_l(k) \approx \tan\delta_l(k) \underset{k\to 0}{\overset{\substack{low\\energy}}{\longrightarrow}} k^{2l+1}$$

$$S_l(k) = e^{2i\delta_l(k)} \quad \rightarrow \text{S matrix element}$$

$$S_l(k) = \cos(2\delta_l) + i\sin(2\delta_l)$$

$$\approx 1 + (2i\delta_l) \quad \text{for small } \delta_l$$

$$S_l(k) \approx 1 + \left(2ic_l k^{2l+1}\right) \text{ since } \delta_l \xrightarrow[k\to 0]{\text{low energy}} k^{2l+1}$$

Partial wave amplitude

$$a_l(k) = \frac{[S_l(k) - 1]}{2ik} = \frac{\left(2ic_l k^{2l+1}\right)}{2ik} = c_l k^{2l}$$

Contribution to partial wave cross-section

$$|a_l(k)|^2 \rightarrow k^{4l}$$

Falls rapidly for small *k*, except for ℓ=0

'scattering length' → especially useful to describe low energy 's-wave only' scattering

Scattering length $\ell=0$ Low energy 's wave' scattering

definition $\alpha = -\lim_{k\to 0} \frac{\tan\delta_0(k)}{k}$ Dimension: L

Partial wave amplitude $a_l(k) = \frac{[S_l(k)-1]}{2ik} = \frac{\left[e^{2i\delta_l(k)}-1\right]}{2ik} = \frac{\cos 2\delta_l + i\sin 2\delta_l - 1}{2ik}$

$$\lim_{k\to 0} a_0(k) = \lim_{k\to 0} \frac{\cos 2\delta_0(k) + i\sin 2\delta_0(k) - 1}{2ik}$$

$$= \lim_{k\to 0} \frac{\left(\cos^2\delta_0(k) - \sin^2\delta_0(k)\right) + \left(2i\sin\delta_0(k)\cos\delta_0(k)\right) - 1}{2ik}$$

$$= \lim_{k\to 0} \frac{\left(1 - 2\sin^2\delta_0(k)\right) + \left(2i\sin\delta_0(k)\cos\delta_0(k)\right) - 1}{2ik}$$

$$\lim_{k\to 0} a_0(k) = \lim_{k\to 0} \frac{\left(-\sin^2\delta_0(k)\right) + \left(i\sin\delta_0(k)\cos\delta_0(k)\right)}{ik}$$

δ_0 : small

$$\lim_{k\to 0} a_0(k) \approx \lim_{k\to 0} \frac{i\sin\delta_0(k)}{ik} \simeq \lim_{k\to 0} \frac{i\tan\delta_0(k)}{ik} \simeq \lim_{k\to 0} \frac{\tan\delta_0(k)}{k} = -\alpha$$

$$\lim_{k\to 0} a_0(k) \simeq \lim_{k\to 0} \frac{\tan\delta_0(k)}{k} = -\alpha$$

$$f_k(\theta) = \sum_{l=0}^{\infty} (2l+1)\, a_l(k)\, P_l(\cos\theta) \rightarrow f_k(\theta): \textit{scattering amplitude}$$

$$a_l(k) = \frac{\left[e^{2i\delta_l(k)} - 1\right]}{2ik} = \frac{\left[S_l(k) - 1\right]}{2ik} \rightarrow a_l(k): \textit{partial wave amplitude}$$

Low energy 's-wave only' scattering

$$P_{l=0}(\cos\theta) = 1$$

$$f_k(\theta) = a_0(k) \underset{k\to 0}{\approx} -\alpha \qquad \Rightarrow \qquad \left|f_{k\to 0}(\theta)\right|^2 = \alpha^2$$

$$\sigma_{total} = \oiint \left|f_k(\theta)\right|^2 d\Omega = 4\pi\alpha^2$$

$$\tan\delta_l(k) = \frac{\left[kj_l^{'}(ka) - \gamma_l(k)\, j_l(ka)\right]}{\left[kn_l^{'}(ka) - \gamma_l(k) n_l(ka)\right]} \quad \text{for all } l.$$

$$\tan\delta_{l=0}(k) = \frac{\left[kj_{l=0}^{'}(ka) - \gamma_{l=0}(k)\, j_{l=0}(ka)\right]}{\left[kn_{l=0}^{'}(ka) - \gamma_{l=0}(k) n_{l=0}(ka)\right]}$$

for $\ell = 0$

$$j_0(z) = \frac{\sin z}{z} \quad ; n_0(z) = -\frac{\cos z}{z}$$

$$j_0^{'}(z) = \frac{\cos z}{z} - \frac{\sin z}{z^2}; \; n_0^{'}(z) = \frac{\sin z}{z} + \frac{\cos z}{z^2}$$

$z = ka$

$$\tan\delta_{l=0}(k) = \frac{\left[kj'_{l=0}(ka) - \gamma_{l=0}(k)\, j_{l=0}(ka)\right]}{\left[kn'_{l=0}(ka) - \gamma_{l=0}(k) n_{l=0}(ka)\right]}$$

$$j_0(z) = \frac{\sin z}{z} \quad ; n_0(z) = -\frac{\cos z}{z}$$

$$j'_0(z) = \frac{\cos z}{z} - \frac{\sin z}{z^2}; \; n'_0(z) = \frac{\sin z}{z} + \frac{\cos z}{z^2}$$

$$\gamma_0(k) = \frac{kj'_0(ka) / j_0(ka)}{q_0(k)}$$

$$\tan\delta_{l=0}(k) = \frac{\left[kj'_{l=0}(ka) - \left\{\frac{kj'_0(ka)/ j_0(ka)}{q_0(k)}\right\} j_0(ka)\right]}{\left[kn'_{l=0}(ka) - \left\{\frac{kj'_0(ka)/ j_0(ka)}{q_0(k)}\right\} n_0(ka)\right]}$$

$$\tan\delta_{l=0}(k) = \frac{\left[kj'_{l=0}(ka) q_0(k) - kj'_0(ka)\right]}{\left[kn'_{l=0}(ka) q_0(k) - kj'_0(ka)\left\{\frac{n_0(ka)}{j_0(ka)}\right\}\right]}$$

$$\tan\delta_{l=0}(k)=\frac{\left[kj'_{l=0}(ka)q_0(k)-kj'_0\left(ka\right)\right]}{\left[kn'_{l=0}(ka)q_0(k)-kj'_0\left(ka\right)\left\{\dfrac{n_0(ka)}{j_0\left(ka\right)}\right\}\right]}$$

$$\tan\delta_{l=0}(k)=\frac{kj'_{l=0}(ka)}{k}\frac{\left[q_0(k)-1\right]}{\left[n'_{l=0}(ka)q_0(k)-j'_0\left(ka\right)\left\{\dfrac{n_0(ka)}{j_0\left(ka\right)}\right\}\right]}$$

$$j_0(z)=\frac{\sin z}{z}\qquad ;\ n_0(z)=-\frac{\cos z}{z}$$

$$j'_0(z)=\frac{\cos z}{z}-\frac{\sin z}{z^2};\ n'_0(z)=\frac{\sin z}{z}+\frac{\cos z}{z^2}$$

$$\tan\delta_{l=0}(k)\underset{k\to 0}{\rightarrow}\left(\frac{\cos ka}{ka}-\frac{\sin ka}{\left(ka\right)^2}\right)\frac{\left[q_0(k)-1\right]}{\left[\left(\dfrac{\sin ka}{ka}+\dfrac{\cos ka}{\left(ka\right)^2}\right)q_0(k)-\left(\dfrac{\cos ka}{ka}-\dfrac{\sin ka}{\left(ka\right)^2}\right)\left\{-\cot\left(ka\right)\right\}\right]}$$

$$\tan\delta_{l=0}(k)\underset{k\to 0}{\to}\left(\frac{\cos\ ka}{ka}-\frac{\sin\ ka}{(ka)^2}\right)\frac{[q_0(k)-1]}{\left[\left(\frac{\sin\ ka}{ka}+\frac{\cos\ ka}{(ka)^2}\right)q_0(k)-\left(\frac{\cos\ ka}{ka}-\frac{\sin\ ka}{(ka)^2}\right)\{-\cot(ka)\}\right]}\times\frac{(ka)^2}{(ka)^2}$$

$$\tan\delta_{l=0}(k)\underset{k\to 0}{\to}(ka\cos\ ka-\sin\ ka)\frac{[q_0(k)-1]}{[(ka\sin\ ka+\cos\ ka)q_0(k)-(ka\cos\ ka-\sin\ ka)\{-\cot(ka)\}]}$$

$$\cos\theta=1-\frac{\theta^2}{2!}+\frac{\theta^4}{4!}-.....\qquad \theta\cos\theta=\theta-\frac{\theta^3}{2!}+\frac{\theta^5}{4!}-.....$$

$$\sin\theta=\theta-\frac{\theta^3}{3!}+\frac{\theta^5}{5!}-.....\qquad \theta\sin\theta=\theta^2-\frac{\theta^4}{3!}+\frac{\theta^6}{5!}-.....$$

$$\theta\cos\theta-\sin\theta=\theta-\frac{\theta^3}{2!}+..-\theta+\frac{\theta^3}{3!}..\approx\theta^3\left(\frac{1}{6}-\frac{1}{2}\right)\simeq-\frac{\theta^3}{3}$$

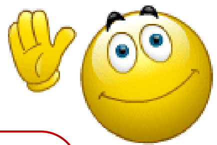
$$\theta\sin\theta+\cos\theta=\theta^2-..+1-\frac{\theta^2}{2!}..\simeq 1+\frac{\theta^2}{2}$$

$$\tan\delta_{l=0}(k)\underset{k\to 0}{\to}(ka\cos ka-\sin ka)\frac{[q_0(k)-1]}{\left[(ka\sin ka+\cos ka)q_0(k)-(ka\cos ka-\sin ka)\{-\cot(ka)\}\right]}$$

$$\theta\cos\theta-\sin\theta=\theta-\frac{\theta^3}{2!}+..-\theta+\frac{\theta^3}{3!}..\approx\theta^3\left(\frac{1}{6}-\frac{1}{2}\right)\simeq-\frac{\theta^3}{3}$$

$$\theta\sin\theta+\cos\theta=\theta^2-..+1-\frac{\theta^2}{2!}..\simeq 1+\frac{\theta^2}{2}$$

$$\tan\delta_{l=0}(k)\underset{k\to 0}{\to}\left\{-\frac{(ka)^3}{3}\right\}\frac{[q_0(k)-1]}{\left[\left\{1+\frac{(ka)^2}{2}\right\}q_0(k)-\frac{(ka)^3}{3}\{\cot(ka)\}\right]}$$



$$\cot\theta\approx\frac{1}{\theta}-\frac{1}{3}\theta-\frac{\theta^3}{45}..$$

$$\frac{(ka)^3}{3}\left\{\frac{1}{ka}-\frac{1}{3}ka-\frac{(ka)^3}{45}..\right\}\simeq\frac{1}{3}(ka)^2$$

$$\tan\delta_{l=0}(k)\underset{k\to 0}{\to}\left\{-\frac{(ka)^3}{3}\right\}\frac{[q_0(k)-1]}{\left[q_0(k)-\frac{(ka)^2}{3}\right]}$$

$$\tan\delta_{l=0}(k)\underset{k\to 0}{\to}(ka)\frac{[q_0(k)-1]}{\left[-3q_0(k)(ka)^{-2}+1\right]}$$

QUESTIONS ?

Write to: pcd@physics.iitm.ac.in

Select/Special Topics *in*
'Theory of Atomic Collisions and Spectroscopy'

P. C. Deshmukh

Department of Physics
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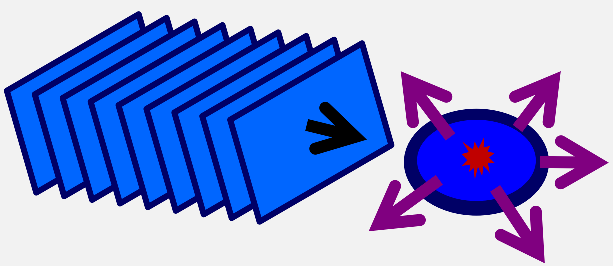
Lecture Number 10

Unit 1: Quantum Theory of Collisions



$$a\hat{\gamma}_l = -(l+1)$$

$\rightarrow$ resonant condition

in the ℓ^{th} partial wave

zero energy resonance

RECAPITULATE

From slides 165-167

$\ell > 0$

$$\tan \delta_l(k) \underset{k\to 0}{\overset{low\ energy}{\longrightarrow}} \frac{(ka)^{2l+1}}{D_+D_-} \frac{l - a\hat{\gamma}_l(k)}{(l+1)+a\hat{\gamma}_l(k)}$$

$$\tan\delta_l(k) \underset{k\to 0}{\overset{low\ energy}{\longrightarrow}} (ka)^{2l+1}$$

$S_l(k) = \cos(2\delta_l) + i\sin(2\delta_l) \approx 1 + (2i\delta_l)$ for small δ_l

$S_l(k) \approx 1 + (2ic_l k^{2l+1})$ since $\delta_l \underset{k\to 0}{\overset{low\ energy}{\longrightarrow}} k^{2l+1}$

Phase shift tends to zero (modulo π)

Partial wave amplitude

$$a_l(k) = \frac{[S_l(k)-1]}{2ik} = \frac{(2ic_l k^{2l+1})}{2ik} = c_l k^{2l}$$

$|a_l(k)|^2 \to k^{4l}$ Falls rapidly for small k, except for $\ell=0$

Slide 165

$\ell > 0$

$\ell \geq 0$

$$\tan\delta_l(k) \underset{k\to 0}{\overset{low\ energy}{\longrightarrow}} \frac{(ka)^{2l+1}}{D_+D_-} \frac{l - a\hat{\gamma}_l(k)}{(l+1) + a\hat{\gamma}_l(k)}$$

Slide 174

$\ell = 0$

$$\tan\delta_{l=0}(k) \underset{k\to 0}{\rightarrow} (ka) \frac{[q_0(k)-1]}{\left[-3q_0(k)(ka)^{-2}+1\right]}$$

$$if\ \ a\hat{\gamma}_l = -(l+1)$$

$$\mapsto 'zero\ energy\ resonance'$$

$\ell = 0$

$$\tan\delta_{l=0}(k) \underset{k\to 0}{\longrightarrow} (ka)\frac{[q_0(k)-1]}{\left[1-3q_0(k)(ka)^{-2}\right]} \quad with \quad q_0(k) = \frac{kj_0^{'}(ka)/\,j_0(ka)}{\gamma_0(k)}$$

$$j_0(z) = \frac{\sin z}{z} \quad ; \quad j_0^{'}(z) = \frac{\cos z}{z} - \frac{\sin z}{z^2}$$

$$\cos\theta = 1 - \frac{\theta^2}{2!} + \frac{\theta^4}{4!} - .....$$

$$\sin\theta = \theta - \frac{\theta^3}{3!} + \frac{\theta^5}{5!} - .....$$

$$\frac{\sin\theta}{\theta} = 1 - \frac{\theta^2}{3!} + \frac{\theta^4}{5!} - .....$$

$$\frac{\cos\theta}{\theta} = \frac{1}{\theta} - \frac{\theta}{2!} + \frac{\theta^3}{4!} - .....$$

$$\frac{\sin\theta}{\theta^2} = \frac{1}{\theta} - \frac{\theta}{3!} + \frac{\theta^3}{5!} - .....$$

$$j_0(z) = 1 - \frac{z^2}{3!} + \frac{z^4}{5!} - ..... \approx 1 - \frac{z^2}{6} + O\left(z^4\right)$$

$$j_0^{'}(z) = \left(\frac{1}{z} - \frac{z}{2!} + \frac{z^3}{4!} - ...\right) .... \left(-\frac{1}{z} + \frac{z}{3!} - \frac{z^3}{5!} - ...\right) \quad \approx z\left(\frac{1}{6} - \frac{1}{2}\right) + \left(\frac{1}{4!} - \frac{1}{5!}\right)z^3 ...$$

i.e. $$j_0^{'}(z) \simeq \left(-\frac{1}{3}\right)z + \left(\frac{1}{24} - \frac{1}{120}\right)z^3$$

$\ell = 0$

$$\tan\delta_{l=0}(k)\underset{k\to 0}{\to}(ka)\frac{[q_0(k)-1]}{\left[1-3q_0(k)(ka)^{-2}\right]}$$ *with* $$q_0(k)=\frac{kj_0^{'}(ka)/j_0(ka)}{\gamma_0(k)}$$

$$j_0(z)\simeq 1-\frac{z^2}{6}+O\left(z^4\right)$$

$$j_0^{'}(z)\simeq\left(-\frac{1}{3}\right)z+\left(\frac{1}{24}-\frac{1}{120}\right)z^3$$

$$z=ka$$

$$q_0(k\to 0)\to\frac{k\left[\frac{\left\{\left(-\frac{1}{3}\right)(ka)+\left(\frac{1}{24}-\frac{1}{120}\right)(ka)^3\right\}}{1-\frac{(ka)^2}{6}+O\left((ka)^4\right)}\right]}{\gamma_0(k)}$$

$$\frac{ka}{ka}\times$$

$$q_0(k\to 0)\to\frac{k\left\{\left(-\frac{1}{3}\right)(ka)^2+\left(\frac{4}{120}\right)(ka)^4\right\}}{\gamma_0(k)ka\left\{1-\frac{(ka)^2}{6}+O\left((ka)^4\right)\right\}}$$

$\ell = 0$

$$\tan\delta_{l=0}(k) \underset{k\to 0}{\to} (ka)\frac{\left[q_0(k)-1\right]}{\left[1-3q_0(k)(ka)^{-2}\right]} \quad \textit{with} \quad q_0(k) = \frac{kj_0^{'}(ka)/\, j_0(ka)}{\gamma_0(k)}$$

$$q_0(k\to 0) \to \frac{\left(-\frac{1}{3}\right)(ka)^2 + \left(\frac{4}{120}\right)(ka)^4}{\gamma_0(k)a\left\{1-\frac{(ka)^2}{6}+\mathrm{O}\left((ka)^4\right)\right\}} \to \frac{\left(-\frac{1}{3}\right)(ka)^2 + \left(\frac{4}{120}\right)(ka)^4}{\gamma_0(k)a}$$

$$q_0(k\to 0) \to \frac{\left(-\frac{1}{3}\right)(ka)^2 + \mathrm{O}(ka)^4}{\gamma_0(k)a}$$

$$q_0(k\to 0) \to \frac{\left(-\frac{1}{3}\right)(ka)^2}{\gamma_0(k)a}$$

$$\tan\delta_{l=0}(k) \underset{k\to 0}{\longrightarrow} (ka)\boxed{\frac{[q_0(k)-1]}{\left[1-3q_0(k)(ka)^{-2}\right]}} \quad \text{......... for } l = 0$$

$\ell = 0$

$$q_0(k\to 0) \to \left\{\frac{\left(-\frac{1}{3}\right)(ka)^2}{\gamma_0(k)a}\right\}$$

$$\frac{[q_0(k)-1]}{\left[1-3q_0(k)(ka)^{-2}\right]} \to \frac{\left\{\frac{\left(-\frac{1}{3}\right)(ka)^2}{\gamma_0(k)a}\right\}-1}{\left[1-3q_0(k)(ka)^{-2}\right]}$$

$$\to \frac{\left(-\frac{1}{3}\right)(ka)^2 - \gamma_0(k)a}{\left[1-3q_0(k)(ka)^{-2}\right]\gamma_0(k)a}$$

$$\frac{[q_0(k)-1]}{\left[1-3q_0(k)(ka)^{-2}\right]} \underset{\substack{\text{ignoring}\\ \text{weaker}\\ \text{terms}}}{\longrightarrow} \frac{-\gamma_0(k)a}{\left[1-3q_0(k)(ka)^{-2}\right]\gamma_0(k)a}$$

$$\tan\delta_{l=0}(k)\underset{k\to 0}{\to}(ka)\frac{[q_0(k)-1]}{\left[1-3q_0(k)(ka)^{-2}\right]} \quad \text{......... for } l = 0$$

$\ell = 0$

$$\frac{[q_0(k)-1]}{\left[1-3q_0(k)(ka)^{-2}\right]} \underset{\substack{\text{ignoring}\\\text{weaker}\\\text{terms}}}{\to} \frac{-\gamma_0(k)a}{\left[1-3q_0(k)(ka)^{-2}\right]\gamma_0(k)a}$$

$$\tan\delta_{l=0}(k)\underset{k\to 0}{\to}(ka)\frac{-\gamma_0(k)a}{\left[1-3q_0(k)(ka)^{-2}\right]\gamma_0(k)a} \quad \text{.... for } l = 0$$

$$\tan\delta_{l=0}(k)\underset{k\to 0}{\to}(ka)\frac{-\gamma_0(k)a}{\left[1-3q_0(k)(ka)^{-2}\right]\gamma_0(k)a} \quad \text{.... for } l = 0$$

$$\tan\delta_{l=0}(k)\underset{k\to 0}{\to}(ka)\frac{-1}{1-3q_0(k)(ka)^{-2}} \quad \text{.... for } l = 0$$

$$q_0(k)=\frac{kj_0'(ka)/j_0(ka)}{\gamma_0(k)}; \qquad q_0(k\to 0)\to\frac{\left(-\frac{1}{3}\right)(ka)^2}{\hat{\gamma}_0 a}$$

where: $\hat{\gamma}_l = \lim \gamma_l(k)$ for $l \geq 0$

$$\tan\delta_{l=0}(k)\underset{k\to 0}{\to}(ka)\frac{-1}{1-3\left[\frac{\left(-\frac{1}{3}\right)(ka)^2}{\hat{\gamma}_0 a}\right](ka)^{-2}} \quad \text{.... for } l = 0$$

$$\tan\delta_{l=0}(k) \underset{k\to 0}{\longrightarrow} (ka)\frac{-1}{1-3\left[\frac{\left(-\frac{1}{3}\right)(ka)^2}{\hat{\gamma}_0 a}\right](ka)^{-2}} \quad \text{.... for } l = 0$$

$$\tan\delta_{l=0}(k) \underset{k\to 0}{\longrightarrow} (ka)\frac{-1}{1+\left[\frac{1}{\hat{\gamma}_0 a}\right]} \quad \text{.... for } l = 0$$

$$\tan\delta_{l=0}(k) \underset{k\to 0}{\longrightarrow} (ka)\frac{-\hat{\gamma}_0 a}{[1+\hat{\gamma}_0 a]} \quad \text{.... for } l = 0$$

$$\tan\delta_l(k) \underset{k\to 0}{\overset{\substack{low\\energy}}{\longrightarrow}} \frac{(ka)^{2l+1}}{D_+D_-}\frac{l-a\hat{\gamma}_l}{(l+1)+a\hat{\gamma}_l} \quad \text{.. for } l \rangle 0$$

$$\tan\delta_{l=0}(k) \underset{k\to 0}{\longrightarrow} (ka)\frac{-\hat{\gamma}_0 a}{[1+\hat{\gamma}_0 a]} \quad \text{.... for } l = 0$$

$\ell \geq 0$

Both cases:

$$\tan\delta_l(k) \underset{k\to 0}{\overset{\substack{low\\energy}}{\longrightarrow}} \frac{(ka)^{2l+1}}{D_+D_-}\frac{l-a\hat{\gamma}_l}{(l+1)+a\hat{\gamma}_l} \quad \text{.. for } l \geq 0$$

what if: $a\hat{\gamma}_l = -(l+1) \rightarrow$ resonant condition

in the ℓ^{th} partial wave

We shall *first* consider such resonant conditions *for* $l \geq 1$.

The case $l = 0$ will be considered *later*.

first, $\ell \geq 1$

Consider the 'next' term in the low energy approximation and compare its importance with that of the consequence of the resonant condition:

$$j_l(z) = \frac{z^l}{(2l+1)!!}\left[1 - \frac{\frac{1}{2}z^2}{1!(2l+3)} + \frac{\left(\frac{1}{2}z^2\right)^2}{2!(2l+3)(2l+5)} - ....\right]$$

$$a\hat{\gamma}_l = -(l+1) \rightarrow \text{resonant condition in the } \ell^{\text{th}} \text{ partial wave}$$

$$j_l(z) \underset{z\rightarrow 0}{\rightarrow} \frac{z^l}{(2l+1)!!} + O\left(z^{l+2}\right)$$

$Corrections:\ O\left(z^{l+2}\right)$

first, $\ell \geq 1$

Recall $\gamma_l^{V=0}(k) = \frac{k j_l'(ka)}{j_l(ka)}$

Corrections: $O\left(z^{l+2}\right)$

$z = ka$

$$\gamma_l^{V=0}(k) \underset{k\to 0}{\rightarrow} \frac{kl\left(ka\right)^{l-1}}{(ka)^l} = \frac{kl}{ka} = \frac{l}{a}$$

$$q_l(k) \underset{definition}{=} \frac{\gamma_l^{V=0}(k)}{\gamma_l(k)}$$

$$q_l(k \to 0) = \frac{l/a}{\gamma_l(k)}$$

$$q_l(k \to 0) = \frac{l}{a\gamma_l(k)}$$

Next order modifications:

$$\gamma_l^{V=0}(k) \underset{k\to 0}{\rightarrow} \frac{l + O\left(k^2a^2\right)}{a}; \qquad q_l(k \to 0) = \frac{l + O\left(k^2a^2\right)}{a\gamma_l(k)}$$

first, $\ell \geq 1$

From slide 164 $\ell > 0$

recall: $\tan\delta_l(k) \underset{k\to 0}{\overset{\text{low energy}}{\longrightarrow}} \frac{q_l(k)-1}{D_+D_-} \frac{(ka)^{2l+1}}{q_l(k)\frac{(l+1)}{l}+1}$

Use next order term:

$$q_l(k\to 0) = \frac{l+O(k^2a^2)}{a\gamma_l(k)}$$

$a\hat{\gamma}_l(k\to 0) = -(l+1) \to$ resonant condition in the ℓ^{th} partial wave

$$\Rightarrow \quad q_l(k\to 0) = \frac{l+O(k^2a^2)}{[-(l+1)]}$$

$$\Rightarrow \quad \tan\delta_l(k) \underset{k\to 0}{\overset{\text{low energy}}{\longrightarrow}} \frac{\left\{\frac{l+O(k^2a^2)}{[-(l+1)]}\right\}-1}{D_+D_-} \times \frac{(ka)^{2l+1}}{\left\{\frac{l+O(k^2a^2)}{[-(l+1)]}\right\}\frac{(l+1)}{l}+1}$$

$$\ell \geq 1$$

$$\Rightarrow \tan\delta_l(k) \underset{k\to 0}{\overset{low\ energy}{\longrightarrow}} \frac{\left\{\frac{l+O(k^2a^2)}{[-(l+1)]}\right\}-1}{D_+D_-} \frac{(ka)^{2l+1}}{\left\{\frac{l+O(k^2a^2)}{[-(l+1)]}\right\}\frac{(l+1)}{l}+1}$$

$$\Rightarrow \tan\delta_l(k) \underset{k\to 0}{\overset{low\ energy}{\longrightarrow}} \frac{\left\{\frac{l+O(k^2a^2)}{[-(l+1)]}\right\}-1}{D_+D_-} \frac{(ka)^{2l+1}}{-1+\frac{O(k^2a^2)}{l}+1}$$

$$\Rightarrow \tan\delta_l(k) \underset{k\to 0}{\overset{low\ energy}{\longrightarrow}} \frac{l\left\{\frac{l+O(k^2a^2)}{[-(l+1)]}\right\}-1}{D_+D_-}(ka)^{2l-1}$$

$$\Rightarrow \tan\delta_l(k) \underset{k\to 0}{\overset{low\ energy}{\longrightarrow}} \frac{\left\{\frac{l^2}{[-(l+1)]}\right\}-1}{D_+D_-}(ka)^{2l-1}$$

Resonant contribution of the ℓ^{th} partial wave

$$\ell \geq 1$$

$$\Rightarrow \tan\delta_l(k) \underset{k\to 0}{\overset{low\ energy}{\longrightarrow}} (ka)^{2l-1}$$

$$\ell \geq 1$$

$$\tan\delta_l(k) \underset{k\to 0}{\overset{low\ energy}{\longrightarrow}} (ka)^{2l-1}$$

$$S_l(k) = e^{2i\delta_l} = \cos(2\delta_l) + i\sin(2\delta_l)$$

$$\approx 1 + (2i\delta_l) \text{ for small } \delta_l$$

$$S_l(k) \approx 1 + \left(2i\bar{d}_l k^{2l-1}\right) \text{ since } \delta_l \underset{k\to 0}{\overset{low\ energy}{\longrightarrow}} k^{2l-1}$$

$$f_k(\theta) = \sum_{l=0}^{\infty}(2l+1)\, a_l(k)\, P_l(\cos\theta) \rightarrow f_k(\theta): scattering\ amplitude$$

$$a_l(k) = \frac{\left[e^{2i\delta_l(k)} - 1\right]}{2ik} = \frac{[S_l(k) - 1]}{2ik} \rightarrow a_l(k): partial\ wave\ amplitude$$

Resonant contribution of the $\ell \geq 1$ ℓ^{th} partial wave

$$a_l(k) = \frac{\left[1 + \left(2i\bar{d}_l k^{2l-1}\right) - 1\right]}{2ik} = \bar{d}_l k^{2l-2}$$

$$f_k(\theta)=\sum_{l=0}^{\infty}(2l+1)\ a_l(k)\ P_l(\cos\theta)\rightarrow f_k(\theta): scattering\ \ amplitude$$

$$a_l(k)=\frac{\left[e^{2i\delta_l(k)}-1\right]}{2ik}=\frac{\left[S_l(k)-1\right]}{2ik}\rightarrow a_l(k): partial\ \ wave\ \ amplitude$$

Resonant contribution of the ℓ^{th} partial wave

$$\ell\geq 1$$

$$a_l(k)=\frac{\left[1+\left(2i\bar{d}_l k^{2l-1}\right)-1\right]}{2ik}=\bar{d}_l k^{2l-2}$$

$$for\ \ \ell=1: \qquad k^{2l-2}=k^0=1$$

$$\text{for } \ell=1,\ a_{l=1}(k)=\bar{d}_{l=1}$$

←What is the contribution of
←this term to the scattering amplitude?

$$\left[(2l+1)a_{l=1}(k)\ P_{l=1}(\cos\theta)\right]_{l=1}=3\bar{d}_{l=1}\cos\theta=\beta\cos\theta$$

$$f_k(\theta)=\sum_{l=0}^{\infty}(2l+1)\ a_l(k)\ P_l(\cos\theta) \rightarrow f_k(\theta): scattering\ \ amplitude$$

$$a_l(k)=\frac{\left[e^{2i\delta_l(k)}-1\right]}{2ik}=\frac{[S_l(k)-1]}{2ik} \rightarrow a_l(k): partial\ \ wave\ \ amplitude$$

We have, for ℓ=1:

$$\left[(2l+1)a_{l=1}(k)\ P_{l=1}(\cos\theta)\right]_{l=1}=\beta\cos\theta$$

We have, for ℓ=0: $\left[(2l+1)a_{l=0}(k)\ P_{l=0}(\cos\theta)\right]_{l=0}=-\alpha$

$$scattering\ \ amplitude \rightarrow f_k(\theta)=-\alpha+\beta\cos\theta$$

when $a\hat{\gamma}_{l=1}(k)=\left[-(l+1)\right]_{l=1}=-2$

resonant condition in the partial wave for $\ell=1$.

$$f_k(\theta) = \sum_{l=0}^{\infty} (2l+1)\, a_l(k)\, P_l(\cos\theta) \rightarrow f_k(\theta): scattering\ \ amplitude$$

$$a_l(k) = \frac{\left[e^{2i\delta_l(k)} - 1\right]}{2ik} = \frac{[S_l(k) - 1]}{2ik} \rightarrow a_l(k): partial\ \ wave\ \ amplitude$$

$$a_l(k) = \frac{\left[1 + \left(2i\bar{d}_l k^{2l-1}\right) - 1\right]}{2ik} = \bar{d}_l k^{2l-2}$$

$$\ell \geq 1$$

$$\text{if } \ell = 2,\ a_{l=2}(k) = \bar{d}_{l=2} k^2 \underset{k \to 0}{\longrightarrow} 0$$

$$\text{if } \ell \geq 2,\ a_{l=2}(k) \underset{k \to 0}{\longrightarrow} 0$$

Thus the utility of s-waves 'scattering length' formalism.

$$scattering\ \ amplitude \rightarrow f_k(\theta) = -\alpha + \beta\cos\theta$$

$$\text{when } a\hat{\gamma}_{l=1}(k) = \left[-(l+1)\right]_{l=1} = -2$$

resonant condition in the partial wave for $\ell = 1$.

$$\tan\delta_l(k) \underset{k\to 0}{\overset{\substack{low \\ energy}}{\longrightarrow}} \frac{(ka)^{2l+1}}{D_+D_-}\frac{l - a\hat{\gamma}_l}{(l+1)+a\hat{\gamma}_l} \quad \text{.. for } l \geq 0$$

if/when: $a\hat{\gamma}_l = -(l+1)$

$\rightarrow$ resonant condition in the ℓ^{th} partial wave

Above,

we *first* considered resonant conditions *for* $l \geq 1$.

NOW, we consider the case for $l = 0$.

For $l = 0$, $a\hat{\gamma}_l = -(l+1) = -1$

$$\tan\delta_{l=0}(k) \underset{k\to 0}{\longrightarrow} (ka)\frac{\left[q_0(k)-1\right]}{\left[1-3q_0(k)(ka)^{-2}\right]} \quad \text{......... for } l = 0$$

From slide 180

$$q_0(k\to 0) \to \frac{\left(-\frac{1}{3}\right)(ka)^2 + O(ka)^4}{\gamma_0(k)a}$$

$$\frac{\left[q_0(k)-1\right]}{\left[1-3q_0(k)(ka)^{-2}\right]} \to \frac{\dfrac{\left(-\frac{1}{3}\right)(ka)^2 + O(ka)^4}{\gamma_0(k)a} - 1}{\left[1-3q_0(k)(ka)^{-2}\right]} = \frac{\left(-\frac{1}{3}\right)(ka)^2 + O(ka)^4 - \gamma_0(k)a}{\left[1-3q_0(k)(ka)^{-2}\right]\gamma_0(k)a}$$

$$\frac{\left[q_0(k)-1\right]}{\left[1-3q_0(k)(ka)^{-2}\right]} \underset{\text{ignoring weaker terms}}{\longrightarrow} \frac{-\gamma_0(k)a}{\left[1-3q_0(k)(ka)^{-2}\right]\gamma_0(k)a}$$

$$\tan\delta_{l=0}(k) \underset{k\to 0}{\to} (ka)\frac{\left[q_0(k)-1\right]}{\left[1-3q_0(k)(ka)^{-2}\right]} \quad \text{......... for } l = 0$$

$$\frac{\left[q_0(k)-1\right]}{\left[1-3q_0(k)(ka)^{-2}\right]} \underset{\substack{\text{leading}\\ \text{terms}}}{\to} \frac{-\gamma_0(k)a}{\left[1-3q_0(k)(ka)^{-2}\right]\gamma_0(k)a}$$

$$\tan\delta_{l=0}(k) \underset{k\to 0}{\to} (ka)\frac{-\hat{\gamma}_0 a}{\left[\hat{\gamma}_0 a-3(\hat{\gamma}_0 a)q_0(k)(ka)^{-2}\right]} \quad \text{.... for } l = 0$$

$$\hat{\gamma}_0 = \lim_{k\to 0}\gamma_0(k)$$

$$\tan\delta_{l=0}(k) \underset{k\to 0}{\rightarrow} (ka)\frac{-\hat{\gamma}_0 a}{\left[\hat{\gamma}_0 a - 3(\hat{\gamma}_0 a) q_0(k)(ka)^{-2}\right]} \quad \text{.... for } l = 0$$

$$q_0(k) = \frac{k j_0'(ka) / j_0(ka)}{\gamma_0(k)}; \qquad q_0(k\to 0) \rightarrow \frac{\left(-\frac{1}{3}\right)(ka)^2 + O(ka)^4}{\hat{\gamma}_0 a}$$

when $a\hat{\gamma}_0 \neq -1$ (non-resonant), we had ignored $(ka)^4$

For $l = 0$, when $a\hat{\gamma}_{l=0} = -(l+1) = -1$ resonant part

we consider next order term in $(\text{ka})^4$

$$\tan\delta_{l=0}(k) \underset{k\to 0}{\rightarrow} (ka)\frac{-\hat{\gamma}_0 a}{\left[\hat{\gamma}_0 a - 3(\hat{\gamma}_0 a)\left\{\frac{\left(-\frac{1}{3}\right)(ka)^2 + O(ka)^4}{\hat{\gamma}_0 a}\right\}(ka)^{-2}\right]}$$

For $l=0$, when $a\hat{\gamma}_{l=0} = -(l+1) = -1$

resonant part

we consider next order term in $(\mathrm{ka})^4$

$$\tan\delta_{l=0}(k) \underset{k\to 0}{\to} (ka) \times \frac{-\hat{\gamma}_0 a}{\left[\hat{\gamma}_0 a - 3(\hat{\gamma}_0 a)\left\{\frac{\left(-\frac{1}{3}\right)(ka)^2 + O(ka)^4}{\hat{\gamma}_0 a}\right\}(ka)^{-2}\right]}$$

$$\tan\delta_{l=0}(k) \underset{k\to 0}{\to} (ka) \times \frac{1}{\left[(-1) - 3(-1)\left\{\frac{\left(-\frac{1}{3}\right) + O(ka)^2}{(-1)}\right\}\right]}$$

$$\boxed{a\hat{\gamma}_{l=0} = -(l+1) = -1}$$

$$\tan\delta_{l=0}(k) \underset{k\to 0}{\to} (ka) \times \frac{1}{\left[(-1) - 3\left(-\frac{1}{3}\right) - \left\{3 \times O(ka)^2\right\}\right]} \to \frac{1}{-3(ka)}$$

For $l=0$, $a\hat{\gamma}_{l=0} = -(l+1) = -1$

resonant part

considering the next order term in $(\mathrm{ka})^4$

$$\tan\delta_{l=0}(k) \underset{k\to 0}{\rightarrow} \frac{1}{-3(ka)}$$

$$\lim_{k\to 0} a_0(k) \simeq \lim_{k\to 0} \frac{\tan\delta_0(k)}{k} = -\alpha$$

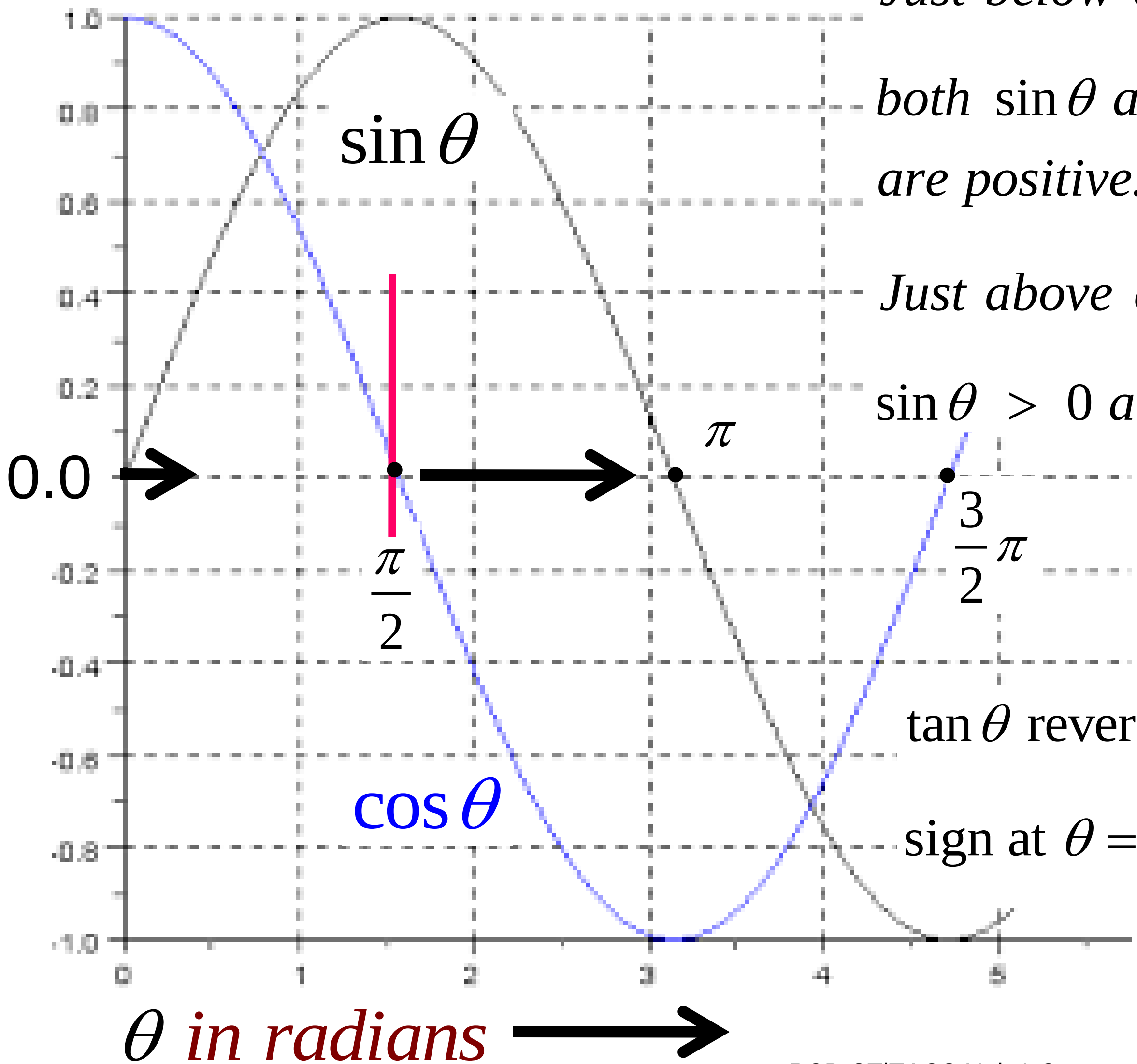
definition: scattering length

$$\lim_{k\to 0} \alpha \rightarrow \frac{1}{k^2} \quad as\ k \rightarrow 0,$$

scattering length diverges as $\frac{1}{k^2}$

$$\tan\delta_{l=0}(k) \underset{k\to 0}{\rightarrow} \textit{blows up}$$

$$\tan\delta_{l=0}(k) \rightarrow \pm\infty \text{ when } \delta_{l=0}(k) \rightarrow \pm\frac{\pi}{2}$$



$Just\ below\ \theta = \frac{\pi}{2},$

$both\ \sin\theta\ and\ \cos\theta$

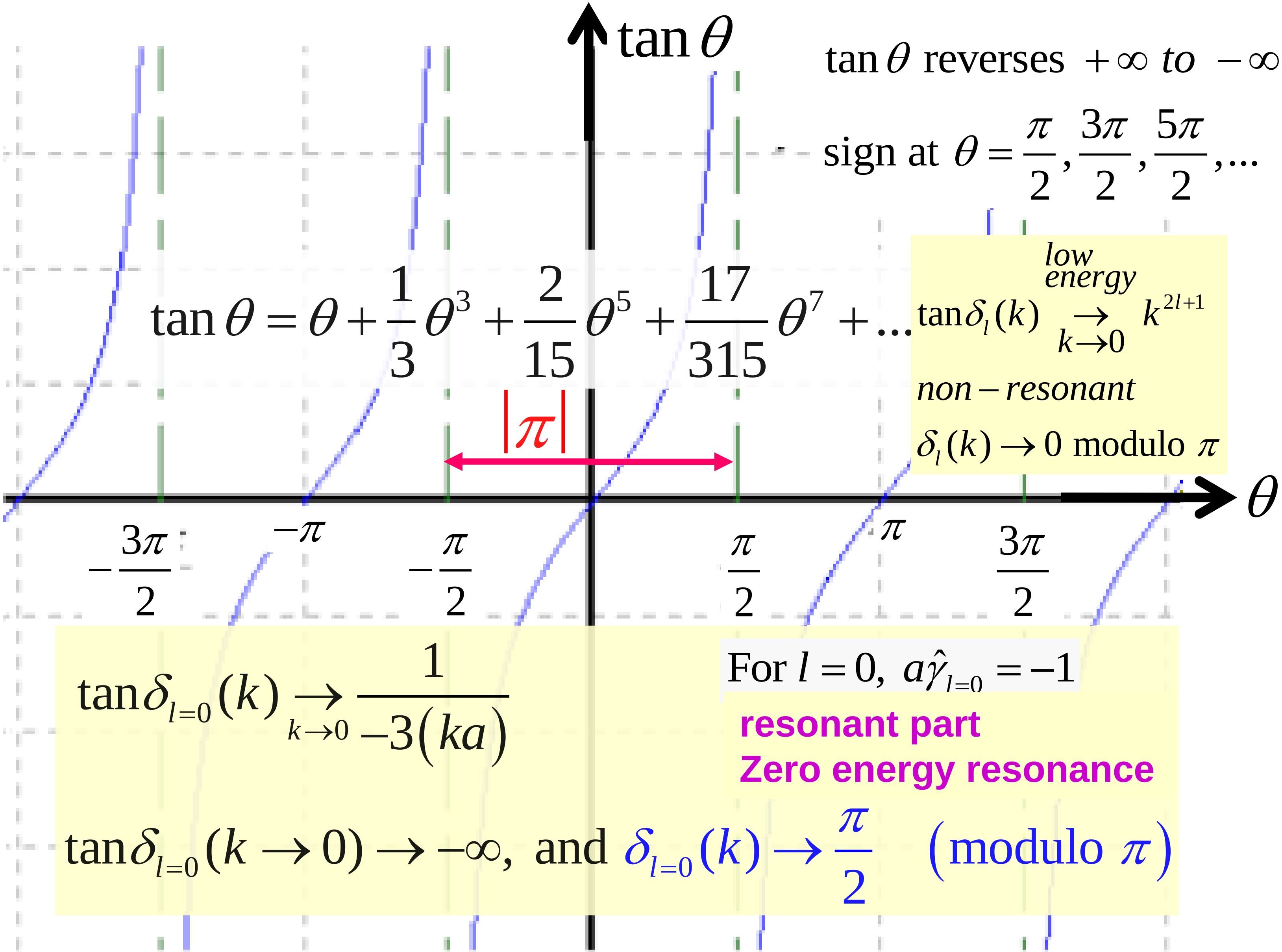
are positive.

$Just\ above\ \theta = \frac{\pi}{2},$

$\sin\theta > 0\ and\ \cos\theta < 0.$

$\tan\theta$ reverses $+\infty\ to\ -\infty$

sign at $\theta = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \ldots$



$\tan\theta$ reverses $+\infty$ *to* $-\infty$

sign at $\theta = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \ldots$

$$\tan\theta = \theta + \frac{1}{3}\theta^3 + \frac{2}{15}\theta^5 + \frac{17}{315}\theta^7 + \ldots$$

$$\tan\delta_l(k) \underset{k\to 0}{\overset{low\ energy}{\rightarrow}} k^{2l+1}$$

non – resonant

$\delta_l(k) \to 0$ modulo π

$$\tan\delta_{l=0}(k) \underset{k\to 0}{\rightarrow} \frac{1}{-3(ka)}$$

For $l=0$, $a\hat{\gamma}_{l=0} = -1$

resonant part

Zero energy resonance

$$\tan\delta_{l=0}(k\to 0) \to -\infty, \text{ and } \delta_{l=0}(k) \to \frac{\pi}{2} \quad (\text{modulo } \pi)$$

$$as\ k \to 0, \quad \delta_{l=0}(k) \to \frac{\pi}{2} \quad (\text{modulo } \pi)$$

$$f_k(\theta) = \sum_{l=0}^{\infty} (2l+1)\ a_l(k)\ P_l(\cos\theta) \to f_k(\theta): scattering\ amplitude$$

$$a_l(k) = \frac{\left[e^{2i\delta_l(k)} - 1\right]}{2ik} = \frac{\left[S_l(k) - 1\right]}{2ik} \to a_l(k): partial\ wave\ amplitude$$

$$a_0(k \to 0) = \frac{S_0(k) - 1}{2ik} \to \left[\frac{\cos 2\delta_0 + i \sin 2\delta_0 - 1}{2ik}\right]_{\delta_0 = \frac{\pi}{2}}$$

$$a_0(k \to 0) \to \left[\frac{\cos\pi + i\sin\pi - 1}{2ik}\right]_{2\delta_0 = \pi} = \frac{-1-1}{2ik} = \frac{-2}{2ik} = \frac{-1}{ik} = \frac{i}{k}$$

$\ell = 0$ $\quad a_0(k \to 0) \to \left[\dfrac{\cos\pi + i\sin\pi - 1}{2ik} \right]_{\delta_0 = \frac{\pi}{2}} = \dfrac{i}{k}$

For $l = 0$

$a\hat{\gamma}_{l=0} = -(l+1) = -1$

resonant part
Zero energy resonance

$$f_k(\theta) = \sum_{l=0}^{\infty} (2l+1)\; a_l(k)\; P_l(\cos\theta) \to f_k(\theta): \textit{scattering amplitude}$$

$$a_l(k) = \frac{\left[e^{2i\delta_l(k)} - 1\right]}{2ik} = \frac{[S_l(k) - 1]}{2ik} \to a_l(k): \textit{partial wave amplitude}$$

$\Rightarrow$

$$\sigma_{total}(k \to 0) = \oiint \left| f_k(\theta) \right|^2 d\Omega = \oiint \left| \frac{i}{k} \right|^2 d\Omega = \frac{4\pi}{k^2}$$

$$\left[f_{k\to 0}(\theta) \right]_{l=0} = \frac{i}{k}$$

$x-\sec$ blows up as $\dfrac{1}{k^2}$ $\left(\text{i.e. as } \dfrac{1}{E} \right)$ as $k \to 0$

"Zero energy resonance"

$$\delta_{l=0}(k \to 0) = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, ...$$

QUESTIONS ?

Write to: pcd@physics.iitm.ac.in

Select/Special Topics *in*
'Theory of Atomic Collisions and Spectroscopy'

P. C. Deshmukh

Department of Physics
Indian Institute of Technology Madras
Chennai 600036

Lecture Number 11

Unit 1: Quantum Theory of Collisions

Levinson's theorem

1949

Number of bound states of an attractive potential

Scattering phase shifts

For $l=0,\ a\hat{\gamma}_{l=0} = -(l+1) = -1$

resonant part

considering the next order term in $(\mathrm{ka})^4$

$$\tan\delta_{l=0}(k) \underset{k\to 0}{\to} \frac{1}{-3(ka)}$$

$$\lim_{k\to 0} a_0(k) \simeq \lim_{k\to 0} \frac{\tan\delta_0(k)}{k} = -\alpha$$

definition: scattering length

$$\lim_{k\to 0} \alpha \to \frac{1}{k^2} \quad as\ k \to 0,$$

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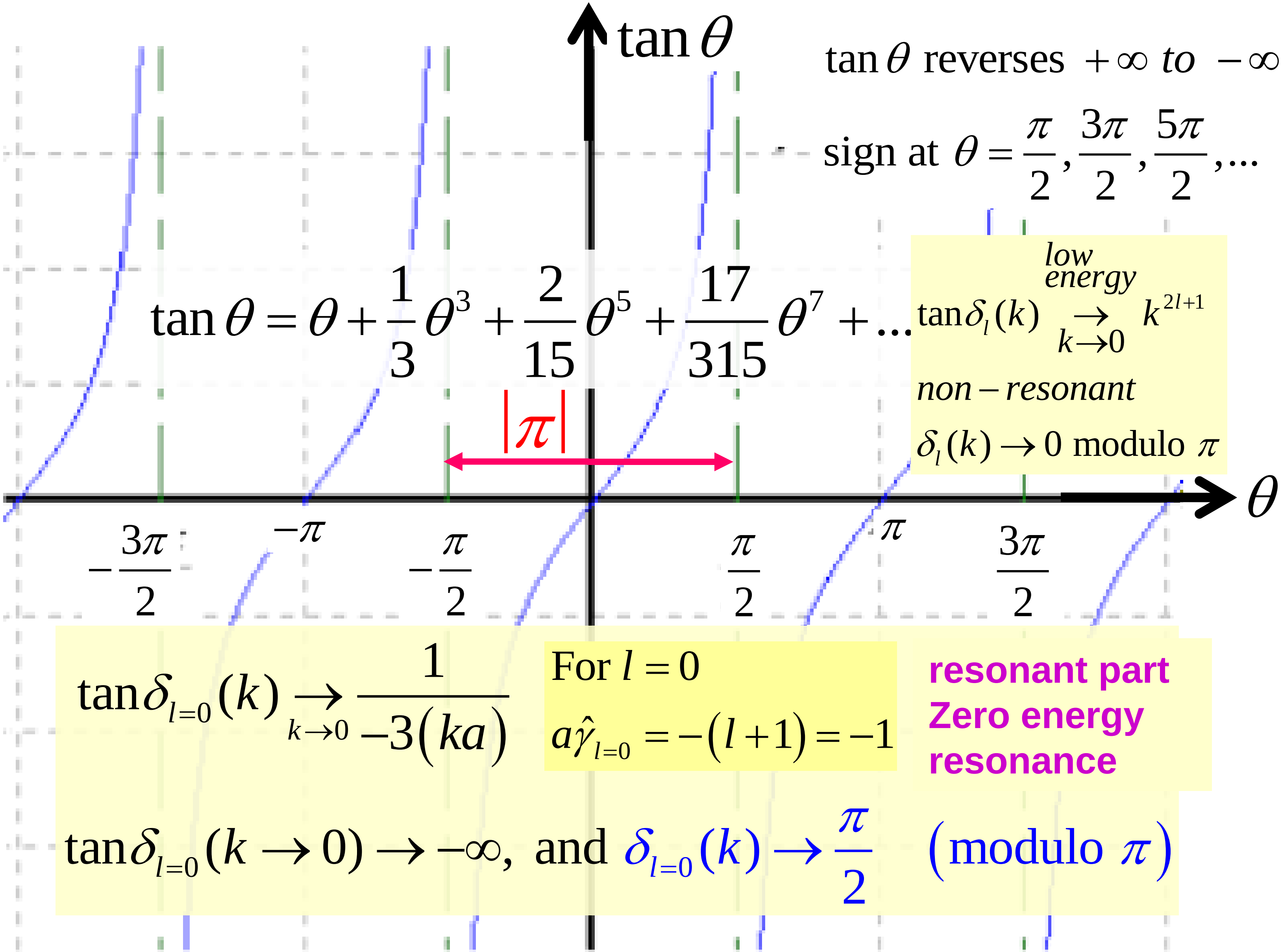


$\tan\theta$ reverses $+\infty$ *to* $-\infty$

sign at $\theta = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \ldots$

$$\tan\theta = \theta + \frac{1}{3}\theta^3 + \frac{2}{15}\theta^5 + \frac{17}{315}\theta^7 + \ldots$$

$$\tan\delta_l(k) \underset{k\to 0}{\overset{low\ energy}{\rightarrow}} k^{2l+1}$$

non – resonant

$\delta_l(k) \rightarrow 0$ modulo π

$$\tan\delta_{l=0}(k) \underset{k\to 0}{\rightarrow} \frac{1}{-3(ka)}$$

For $l = 0$

$a\hat{\gamma}_{l=0} = -(l+1) = -1$

resonant part
Zero energy
resonance

$\tan\delta_{l=0}(k \rightarrow 0) \rightarrow -\infty$, and $\delta_{l=0}(k) \rightarrow \frac{\pi}{2}$ $(\text{modulo } \pi)$

For $l=0$ when $a\hat{\gamma}_{l=0} = -(l+1) = -1$

resonant part
Zero energy resonance

$$as\ k \to 0, \quad \delta_{l=0}(k) \to \frac{\pi}{2} \qquad (\text{modulo } \pi)$$

$$f_k(\theta) = \sum_{l=0}^{\infty} (2l+1)\, a_l(k)\, P_l(\cos\theta) \to f_k(\theta) : scattering\ amplitude$$

$$a_l(k) = \frac{\left[e^{2i\delta_l(k)} - 1\right]}{2ik} = \frac{\left[S_l(k) - 1\right]}{2ik} \to a_l(k) : partial\ wave\ amplitude$$

$$a_0(k \to 0) = \frac{S_0(k) - 1}{2ik} \to \left[\frac{\cos 2\delta_0 + i \sin 2\delta_0 - 1}{2ik}\right]_{\delta_0 = \frac{\pi}{2}}$$

$$a_0(k \to 0) \to \left[\frac{\cos \pi + i \sin \pi - 1}{2ik}\right]_{2\delta_0 = \pi} = \frac{-1-1}{2ik} = \frac{-2}{2ik} = \frac{-1}{ik} = \frac{i}{k}$$

$\ell = 0$

$$a_0(k \to 0) \to \left[\frac{\cos\pi + i\sin\pi - 1}{2ik}\right]_{\delta_0 = \frac{\pi}{2}} = \frac{i}{k}$$

For $l = 0$

$a\hat{\gamma}_{l=0} = -(l+1) = -1$

resonant part
Zero energy resonance

$$f_k(\theta) = \sum_{l=0}^{\infty}(2l+1)\, a_l(k)\, P_l(\cos\theta) \to f_k(\theta): scattering\ \ amplitude$$

$$a_l(k) = \frac{\left[e^{2i\delta_l(k)} - 1\right]}{2ik} = \frac{\left[S_l(k) - 1\right]}{2ik} \to a_l(k): partial\ \ wave\ \ amplitude$$

$\Rightarrow$

$$\sigma_{total}(k \to 0) = \oiint |f_k(\theta)|^2 d\Omega = \oiint \left|\frac{i}{k}\right|^2 d\Omega = \frac{4\pi}{k^2}$$

$$\left[f_{k\to 0}(\theta)\right]_{l=0} = \frac{i}{k}$$

“Zero energy resonance”

$x-\sec$ blows up as $\frac{1}{k^2}$ $\left(\text{i.e. as } \frac{1}{E}\right)$ as $k \to 0$

$$\delta_{l=0}(k \to 0) = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, ...$$

LEVINSON's THEOREM

Kgl. Danske Videnskab. Salskab. Mat. Fys. Medd. 25 9 (1949)

reference zero of $\delta_l(k)$: $\delta_l(k \to \infty) = 0$

.... for $l = 0$:

$$\delta_0(k \to 0) = n_0 \; \pi$$

"half-bound" state

or $\delta_0(k \to 0) = \left(n_0 + \frac{1}{2}\right)\pi$ if there is a (resonant) bound state solution at zero energy.

"zero energy resonance"

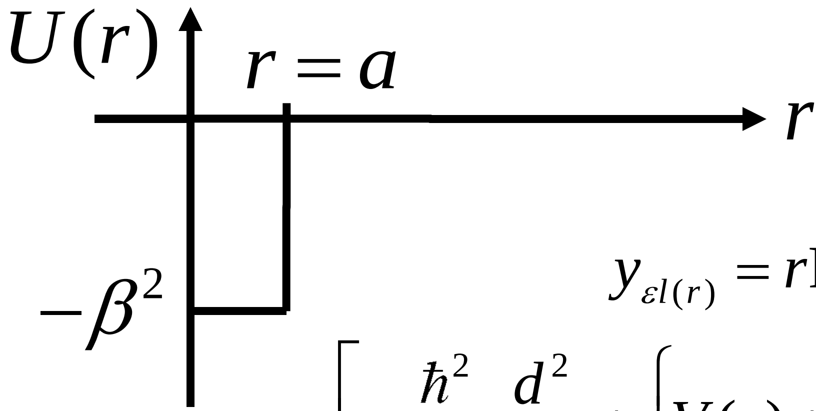
$$\sigma_{total}(k \to 0) \underset{up}{\overset{blows}{\rightarrow}} \frac{1}{k^2} \text{ when } \lambda_0 a = \sqrt{U_0}\, a = \frac{\pi}{2}$$

$$\delta_0(k \to 0) \to \frac{\pi}{2}$$

$$\delta_l(k \to 0) = n_l \; \pi \quad \text{....... for } l \geq 1$$

$$\delta_\ell(0) - \delta_\ell(\infty) = \begin{cases} (n_\ell + 1/2)\pi & \text{when } \ell = 0 \\ & \text{and a half bound state occurs} \\ n_\ell \pi & \text{the remaining cases,} \end{cases}$$

Square well attractive potential



$$U(r) = -\beta^2 \text{ for } r < a$$
$$= 0 \text{ for } r > a$$

$$y_{\varepsilon l(r)} = r\mathrm{R}_{\varepsilon l}(r)$$

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

$$\left(-\frac{2m}{\hbar^2} \right) \times$$

$$\ell = 0$$

$$U(r) = \frac{2m}{\hbar^2} V(r)$$

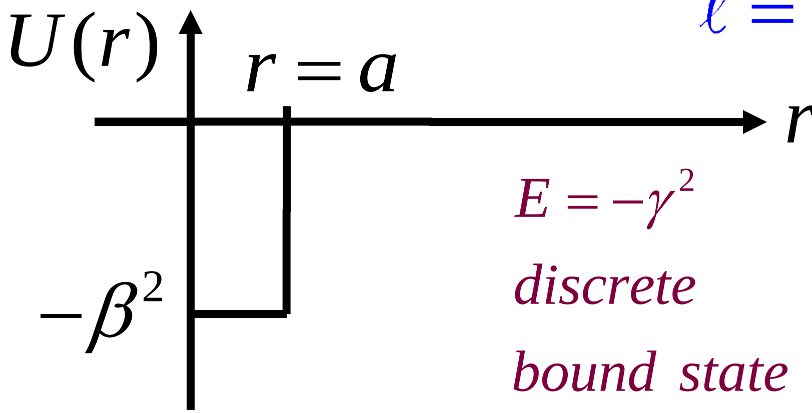
$$\left[\frac{d^2}{dr^2} + \{ -U(r) \} + \frac{2m}{\hbar^2} E \right] y_{\varepsilon l}(r) = 0$$

$$\frac{2mE}{\hbar^2} = -\gamma^2$$

discrete bound state

$$\left[\frac{d^2}{dr^2} + \{ -U(r) \} - \gamma^2 \right] y_{\varepsilon l}(r) = 0$$

Bound states of the SPHERICAL well attractive potential



$\ell = 0$ $\quad y_{\varepsilon l(r)} = r\mathrm{R}_{\varepsilon l}(r)$

$$\left[\frac{d^2}{dr^2} + \{-U(r)\} - \gamma^2\right] y_{\varepsilon l}(r) = 0$$

$E = -\gamma^2$

discrete

bound state

$$U(r) = -\beta^2 \text{ for } r < a$$
$$= 0 \text{ for } r > a$$

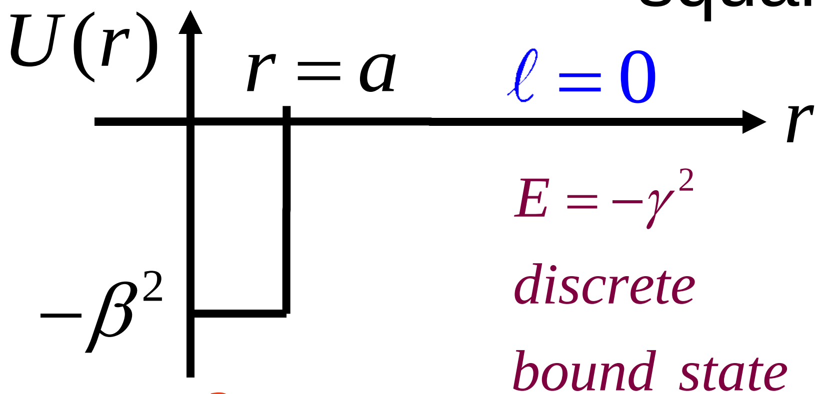
$$\left[\frac{d^2}{dr^2} + \beta^2 - \gamma^2\right] y_{\varepsilon l}(r) = 0 \quad \text{for } r < a \quad y_{\varepsilon l}(r) = \mathrm{A}\sin\left(r\sqrt{\beta^2 - \gamma^2}\right)$$

$$\left[\frac{d^2}{dr^2} - \gamma^2\right] y_{\varepsilon l}(r) = 0 \quad \text{for } r > 0 \quad y_{\varepsilon l}(r) = B\ e^{-\gamma r}$$

Continuity at $r = a \quad \Rightarrow \quad \tan\left(a\sqrt{\beta^2 - \gamma^2}\right) = -\frac{\sqrt{\beta^2 - \gamma^2}}{\gamma}$

$\tan\theta$ properties.....

DISCRETE BOUND STATES of a SPHERICAL square well attractive potential



$E=-\gamma^2$

discrete

bound state

$$U(r)=\frac{2m}{\hbar^2}V(r)$$

continuity at $r=a \quad \Rightarrow$

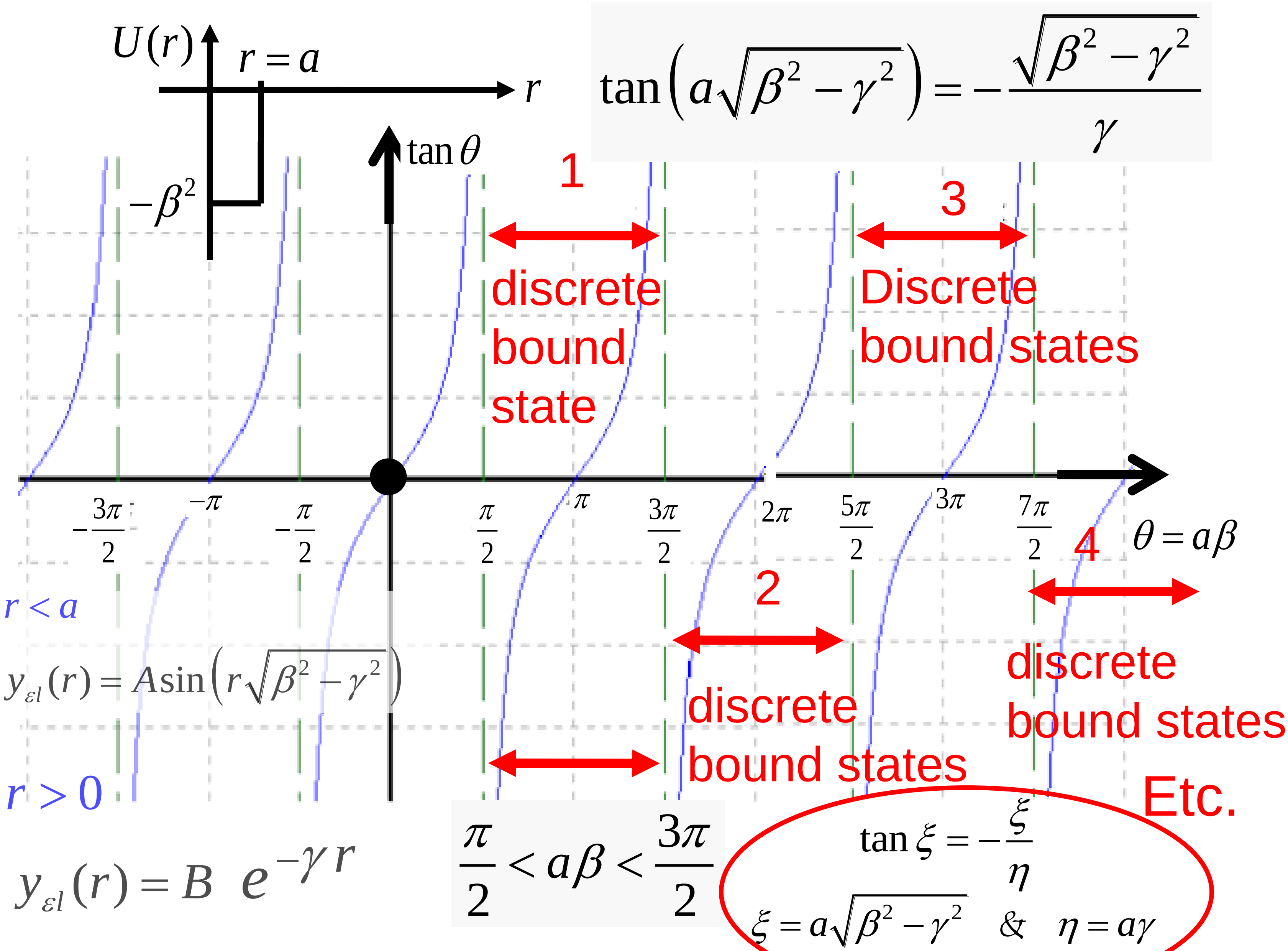
$$\tan\left(a\sqrt{\beta^2-\gamma^2}\right)=-\frac{\sqrt{\beta^2-\gamma^2}}{\gamma}$$

$$\xi=a\sqrt{\beta^2-\gamma^2} \quad \& \quad \eta=a\gamma$$

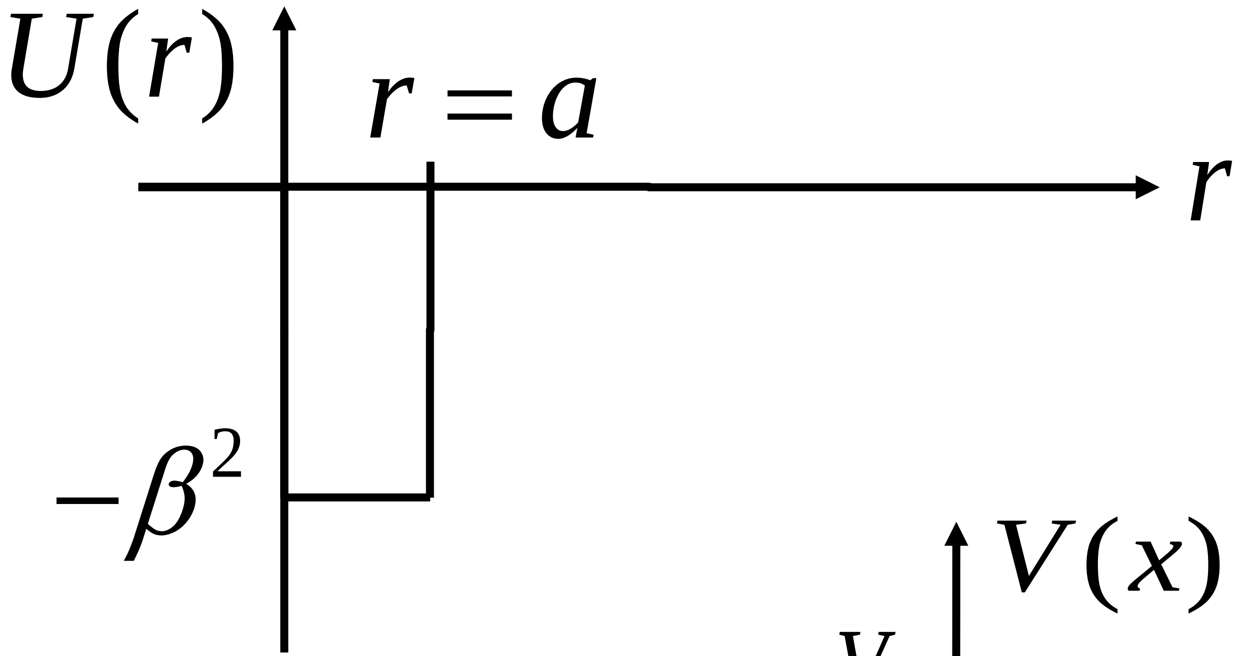
$$\tan\xi=-\frac{\xi}{\eta}$$

Bound state discrete energy levels are given by the intersection of the curves described by these two equations.

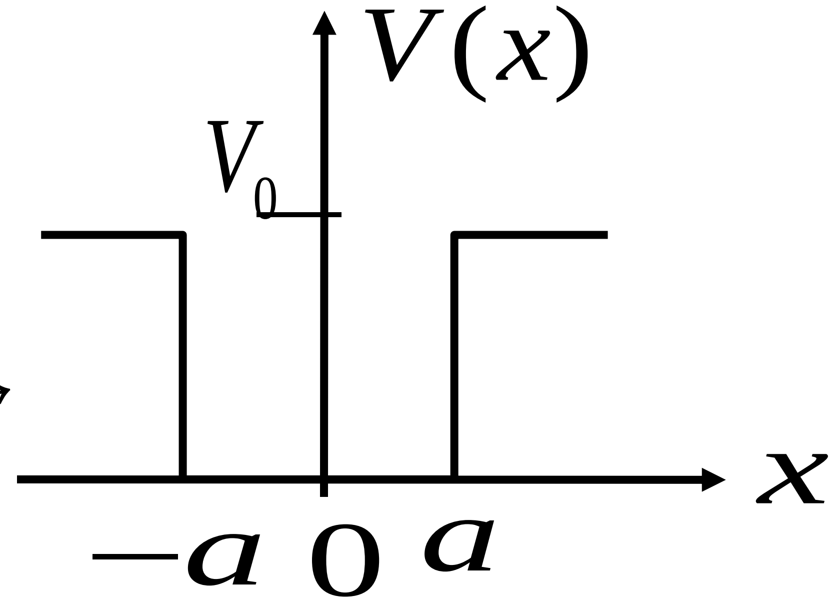
$$\xi^2+\eta^2=a^2\left(\beta^2-\gamma^2\right)+a^2\gamma^2=a^2\beta^2=U_0a^2$$

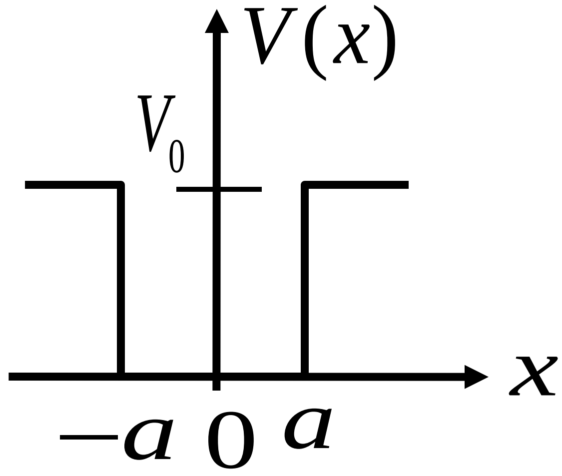


$U(r)$
$r = a$
r
$-\beta^2$
$\tan\theta$
$\tan\left(a\sqrt{\beta^2-\gamma^2}\right) = -\frac{\sqrt{\beta^2-\gamma^2}}{\gamma}$
1
discrete bound state
3
Discrete bound states
$-\frac{3\pi}{2}$
$-\pi$
$-\frac{\pi}{2}$
$\frac{\pi}{2}$
π
$\frac{3\pi}{2}$
2π
$\frac{5\pi}{2}$
3π
$\frac{7\pi}{2}$
4
$\theta = a\beta$
2
$r < a$
$y_{\varepsilon l}(r) = A\sin\left(r\sqrt{\beta^2-\gamma^2}\right)$
discrete bound states
discrete bound states
$r > 0$
Etc.
$y_{\varepsilon l}(r) = B\ e^{-\gamma r}$
$\frac{\pi}{2} < a\beta < \frac{3\pi}{2}$
$\tan\xi = -\frac{\xi}{\eta}$
$\xi = a\sqrt{\beta^2-\gamma^2}$ & $\eta = a\gamma$



We shall quickly recapitulate results from the 1-dimensional square-well problem →





I	II	III
V_0	0	V_0

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi(x)=E\psi(x)$$

$$\left.\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}+V_0\right]\psi(x)=E\psi(x)\right\}_I$$

$$\left.\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\right]\psi(x)=E\psi(x)\right\}_{II} \qquad E>0$$

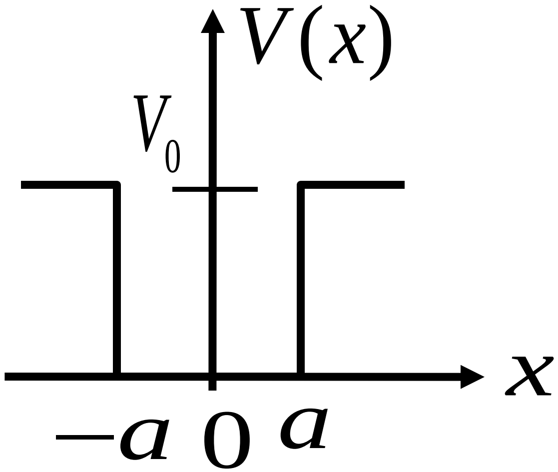
$$\left.\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}+V_0\right]\psi(x)=E\psi(x)\right\}_{III}$$

$$\psi(x)\}_I = \cancel{F}e^{-\beta x}+De^{\beta x}=De^{\beta x} \qquad \alpha=+\sqrt{\frac{2mE}{\hbar^2}}$$

$$\psi(x)\}_{II} = A\sin\alpha x + B\cos\alpha x \qquad \beta=+\sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$

$$\psi(x)\}_{III} = Ce^{-\beta x}+\cancel{G}e^{\beta x}=Ce^{-\beta x}$$

$V_0 > E$ (bound states)



I II III

V_0 0 V_0

$$\alpha = +\sqrt{\frac{2mE}{\hbar^2}}$$

$$\beta = +\sqrt{\frac{2m\left(V_0 - E\right)}{\hbar^2}}$$

$V_0 > E$ (bound states)

$$\psi(x)\}_I = De^{\beta x}$$

$$\psi(x)\}_{II} = A\sin\alpha x + B\cos\alpha x$$

$$\psi(x)\}_{III} = Ce^{-\beta x}$$

$@\, x = a:$

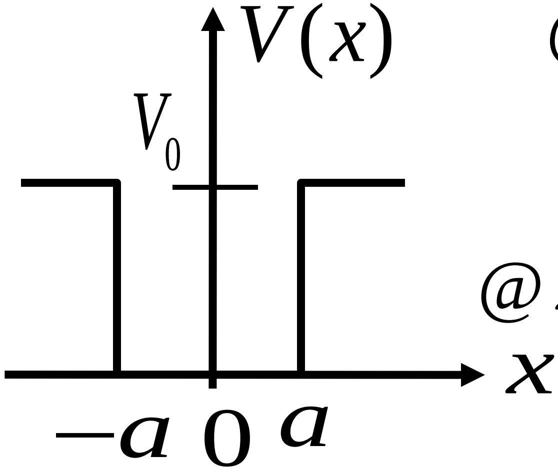
$$A\sin\alpha a + B\cos\alpha a = Ce^{-\beta a}$$

$$A\alpha\cos\alpha a - B\alpha\sin\alpha a = -\beta Ce^{-\beta a}$$

$@\, x = -a:$

$$-A\sin\alpha a + B\cos\alpha a = De^{-\beta a}$$

$$A\alpha\cos\alpha a + B\alpha\sin\alpha a = \beta De^{-\beta a}$$



$$I \quad II \quad III$$

$$V_0 \quad 0 \quad V_0$$

$$\alpha = +\sqrt{\frac{2mE}{\hbar^2}}$$

$$\beta = +\sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

$V_0 > E$ (bound states)

$$@\, x = a: \; A\sin\alpha a + B\cos\alpha a = Ce^{-\beta a}$$

$$A\alpha\cos\alpha a - B\alpha\sin\alpha a = -\beta Ce^{-\beta a}$$

$$@\, x = -a: \; -A\sin\alpha a + B\cos\alpha a = De^{-\beta a}$$

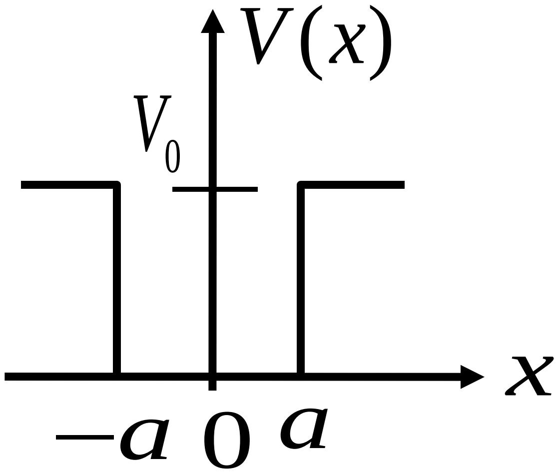
$$A\alpha\cos\alpha a + B\alpha\sin\alpha a = \beta De^{-\beta a}$$

$$2A\sin\alpha a = (C - D)e^{-\beta a}$$

$$2A\alpha\cos\alpha a = \beta(D - C)e^{-\beta a}$$

$$2B\cos\alpha a = (C + D)e^{-\beta a}$$

$$2B\alpha\sin\alpha a = \beta(C + D)e^{-\beta a}$$



$$2A\sin\alpha a = (C-D)e^{-\beta a}$$

$$2A\alpha\cos\alpha a = \beta(D-C)e^{-\beta a}$$

$$2B\cos\alpha a = (C+D)e^{-\beta a}$$

$$2B\alpha\sin\alpha a = \beta(C+D)e^{-\beta a}$$

$$\alpha = +\sqrt{\frac{2mE}{\hbar^2}}$$

$$\beta = +\sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$

$V_0 > E$ (bound states)

$A=0$ and $C=D$ whence

$$2B\cos\alpha a = 2Ce^{-\beta a}$$

$$2\alpha B\sin\alpha a = 2C\beta e^{-\beta a}$$

$$\Rightarrow \quad \boxed{\alpha\tan\alpha a = \beta}$$

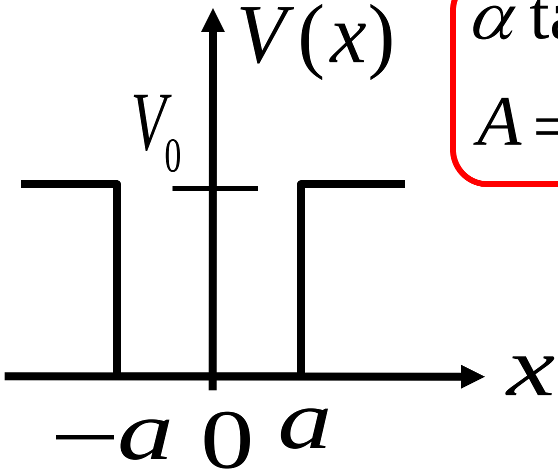
$B=0$ and $C=-D$ whence

$$2A\sin\alpha a = 2Ce^{-\beta a}$$

$$2\alpha A\cos\alpha a = -2C\beta e^{-\beta a}$$

$$\Rightarrow \frac{1}{\alpha}\tan\alpha a = -\frac{1}{\beta}$$

i.e. $\boxed{\alpha\cot\alpha a = -\beta}$



$$\alpha \tan \alpha a = \beta$$
$$A = 0 \text{ and } C = D$$

$$\alpha \cot \alpha a = -\beta$$
$$B = 0 \text{ and } C = -D$$

$$\left[\frac{1}{\alpha} \tan \alpha a = -\frac{1}{\beta}\right] \times [\alpha \tan \alpha a = \beta]$$

$$\Rightarrow \tan^2 \alpha a = -1$$

$$\alpha : imaginary \rightarrow E < 0 : contradiction$$

either

or

$$\alpha = +\sqrt{\frac{2mE}{\hbar^2}}$$

$$\beta = +\sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

$V_0 > E$ (bound states)

$$\alpha \tan \alpha a = \beta$$
$$A = 0 \text{ and } C = D$$

both ξ & η

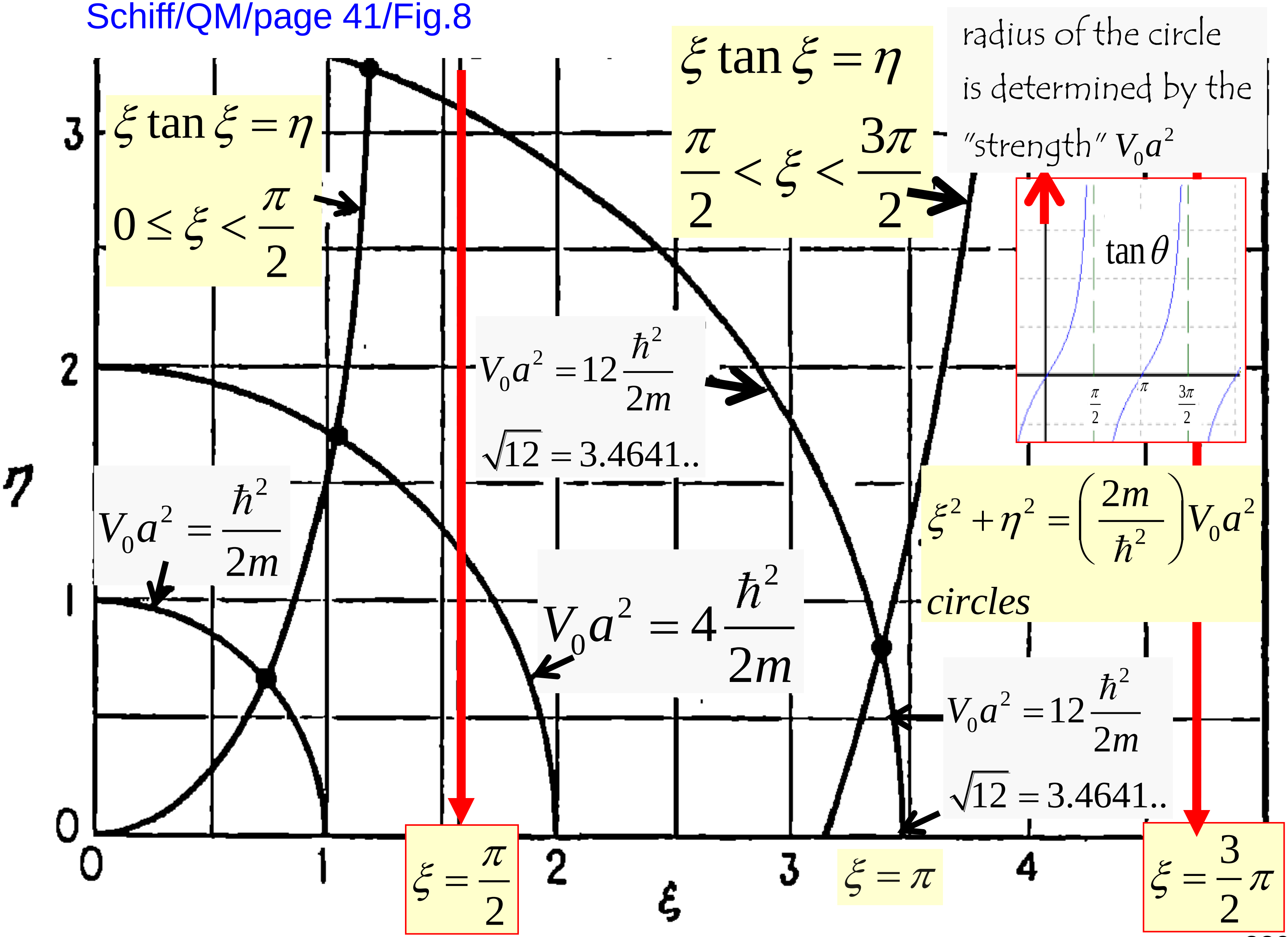
are positive

$$put: \ \xi = \alpha a$$
$$\& \ \ \eta = \beta a$$

$$\xi \tan \xi = \eta$$

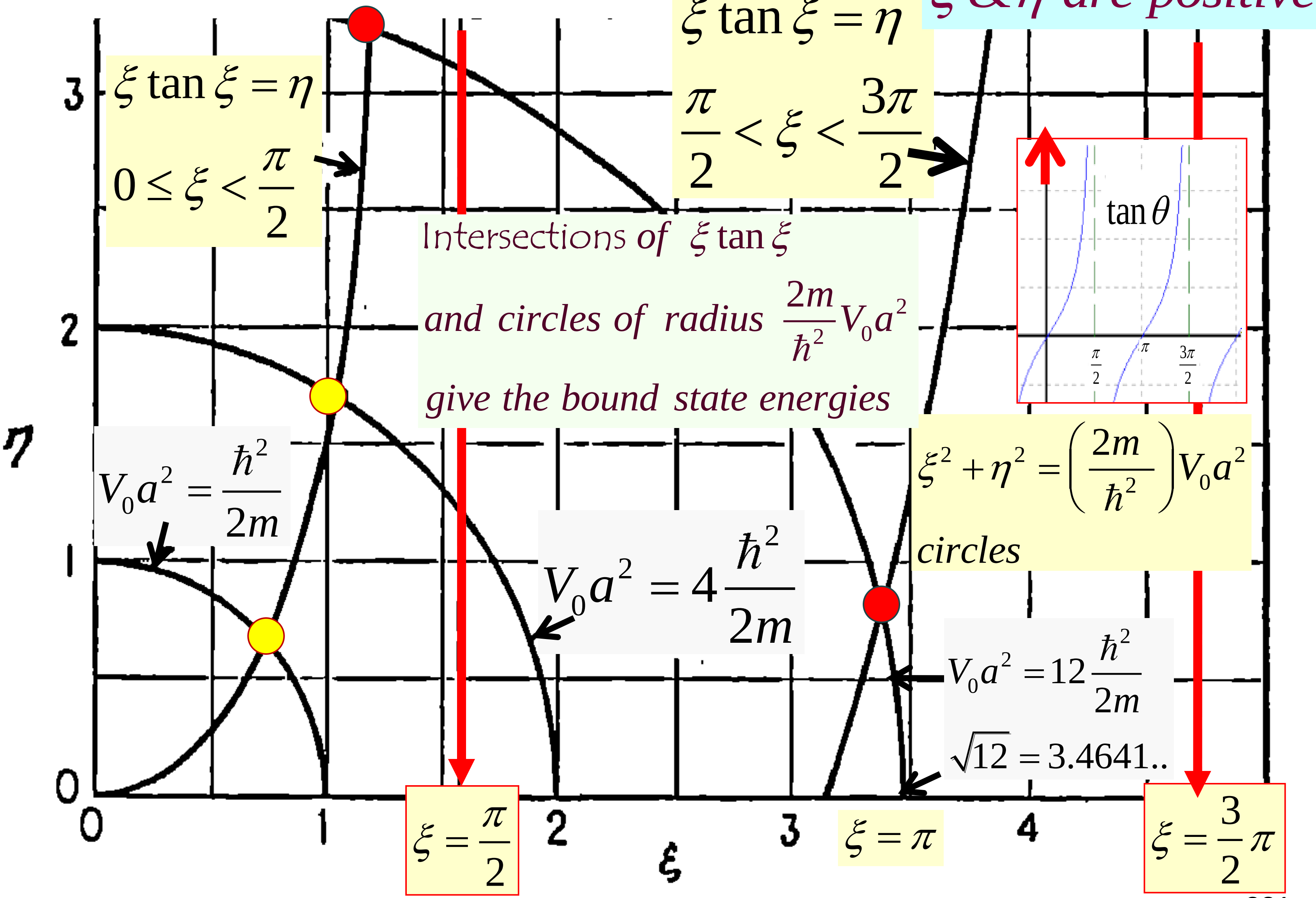
$$\xi^2 + \eta^2 = a^2 \frac{2mV_0}{\hbar^2} = \frac{2m \ V_0 a^2}{\hbar^2}$$

Schiff/QM/page 41/Fig.8

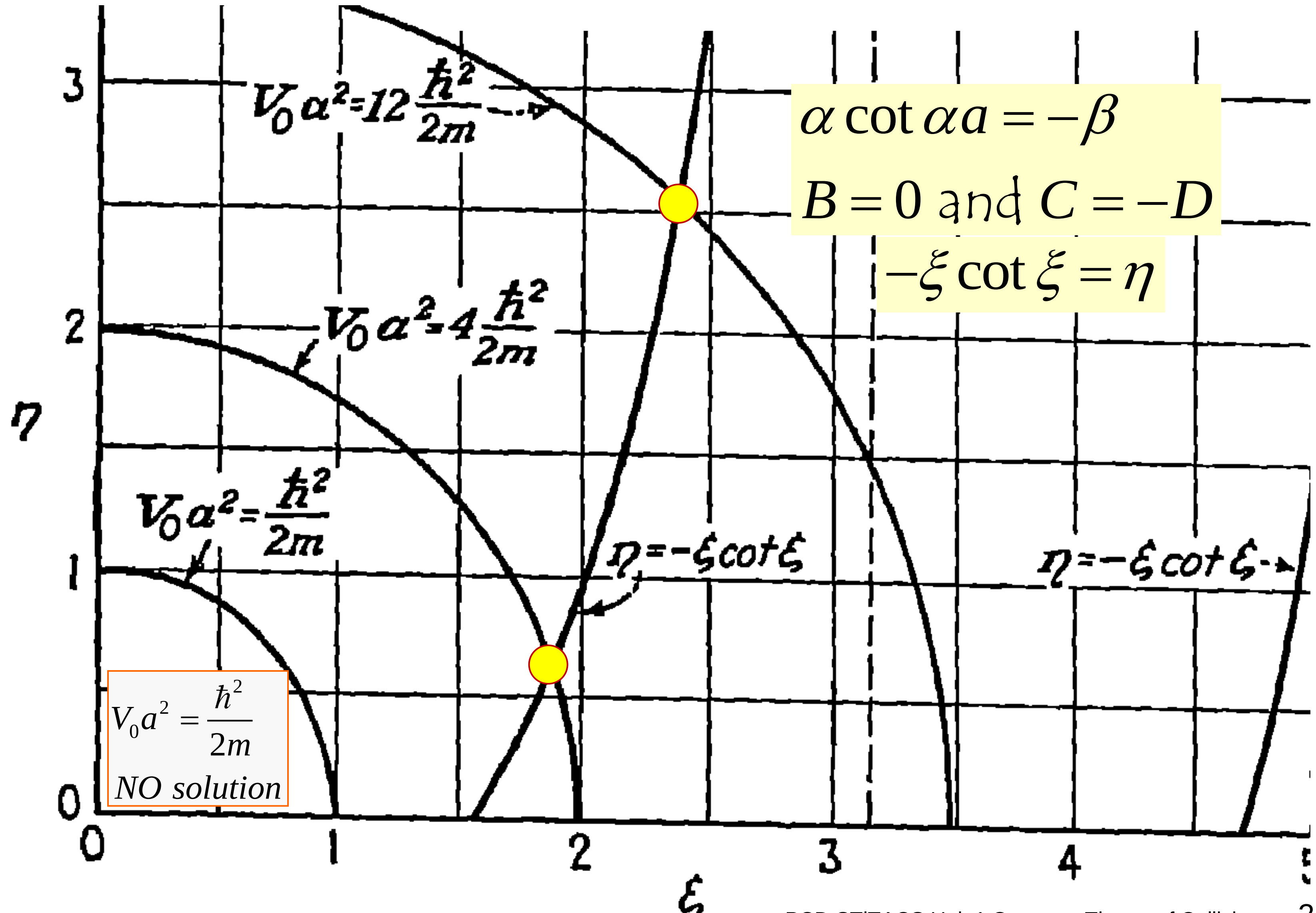


Schiff/QM/page 41/Fig.8

ξ & η *are positive*



Schiff/QM/page 42/Fig.9



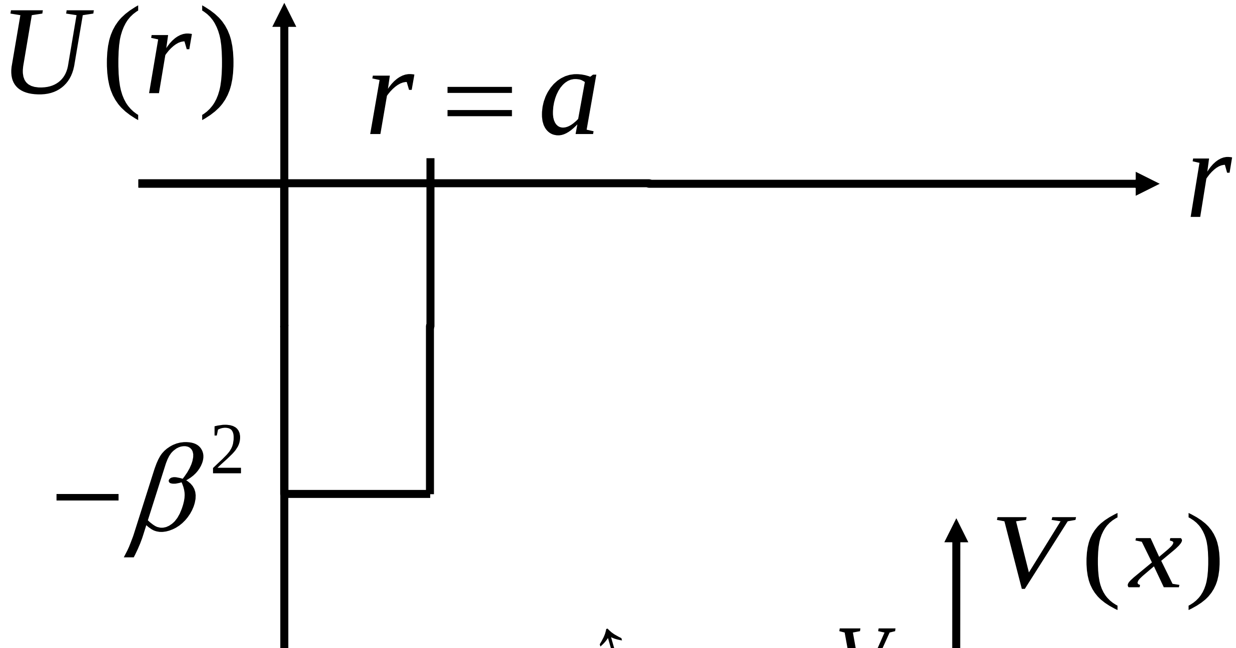
$$\alpha \cot \alpha a = -\beta$$

$$B = 0 \text{ and } C = -D$$

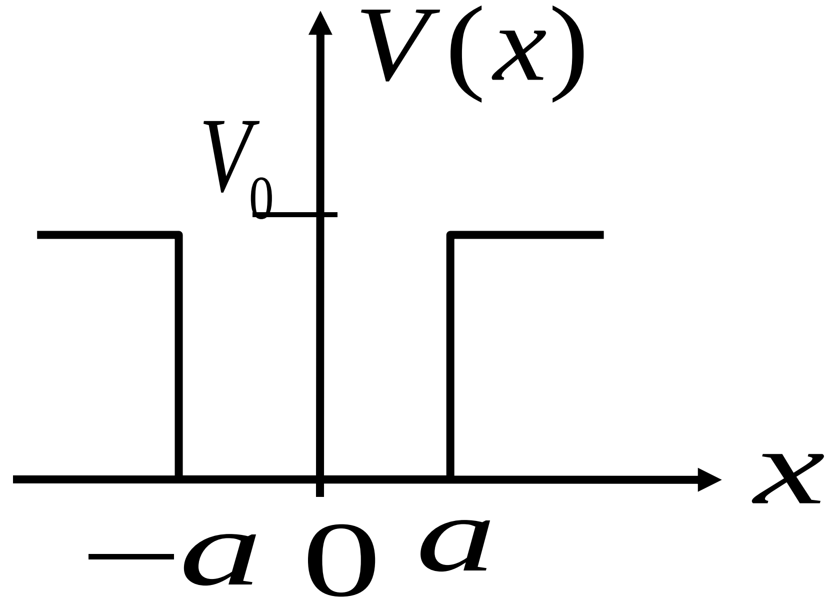
$$-\xi \cot \xi = \eta$$

$$V_0 a^2 = \frac{\hbar^2}{2m}$$

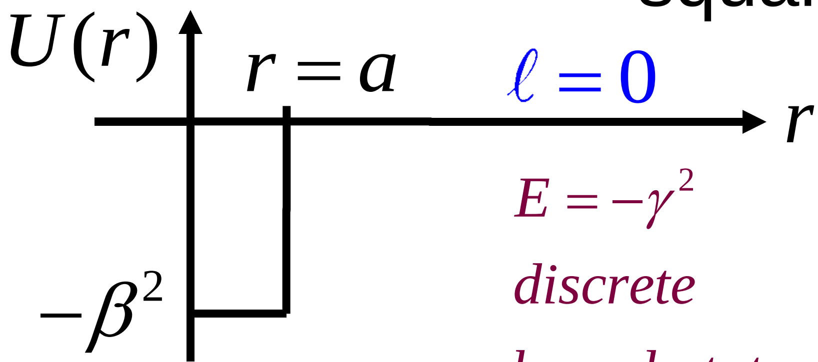
NO solution



We now go back to the ↑ SPHERICAL square-well problem.



DISCRETE BOUND STATES of a SPHERICAL square well attractive potential



$U(r)=\frac{2m}{\hbar^2}V(r)$

$\ell=0$

$E=-\gamma^2$

discrete bound state

continuity at $r=a \quad \Rightarrow$

$$\tan\left(a\sqrt{\beta^2-\gamma^2}\right)=-\frac{\sqrt{\beta^2-\gamma^2}}{\gamma}$$

$$\xi=a\sqrt{\beta^2-\gamma^2} \quad \& \quad \eta=a\gamma$$

$$\tan\xi=-\frac{\xi}{\eta}$$

Bound state discrete energy levels are given by the intersection of the curves described by these two equations.

$$\xi^2+\eta^2=a^2\left(\beta^2-\gamma^2\right)+a^2\gamma^2=a^2\beta^2=U_0a^2$$

$$\tan\xi = -\frac{\xi}{\eta}$$

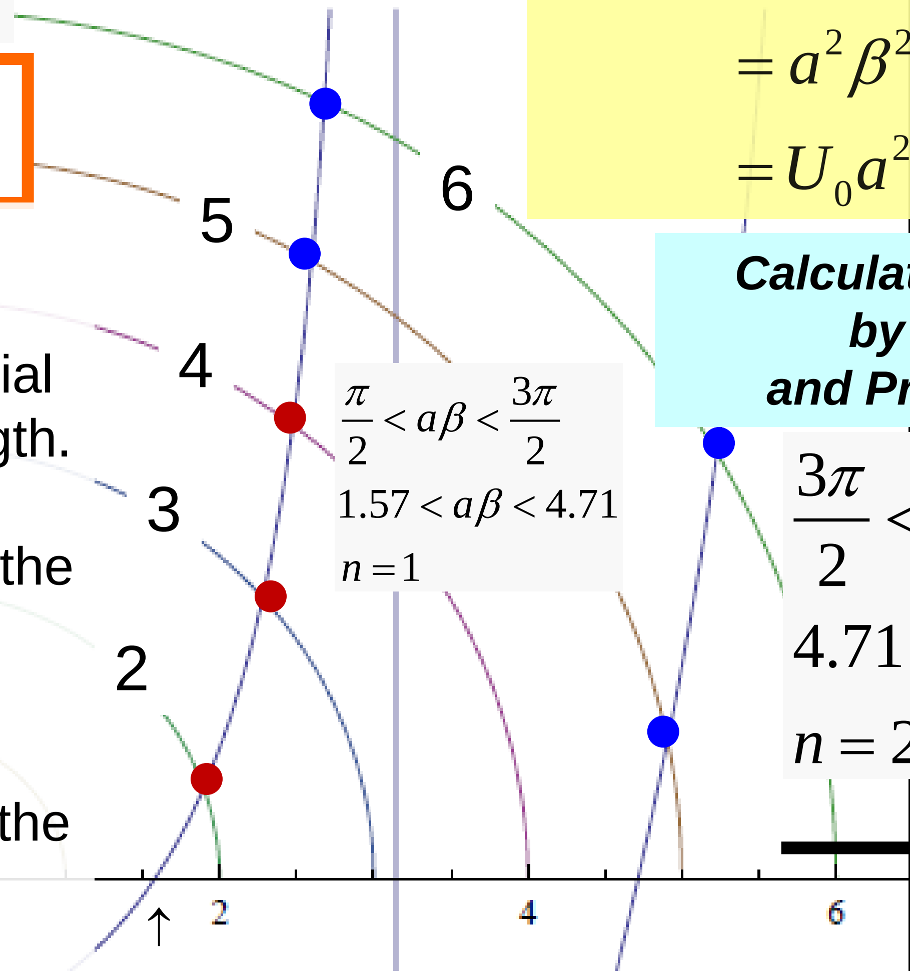
$$\eta = -\frac{\xi}{\tan\xi}$$

$$\xi^2+\eta^2 = a^2\left(\beta^2-\gamma^2\right)+a^2\gamma^2$$
$$= a^2\beta^2$$
$$= U_0 a^2$$

$$a\beta = a\sqrt{U_0}$$

Calculations and graphs by Sayantan Auddy and Pranav Manangath

Each circle represents a particular potential of a given strength. The number of times it crosses the curve $\eta = -\frac{\xi}{\tan\xi}$ gives the number of bound states the potential holds.



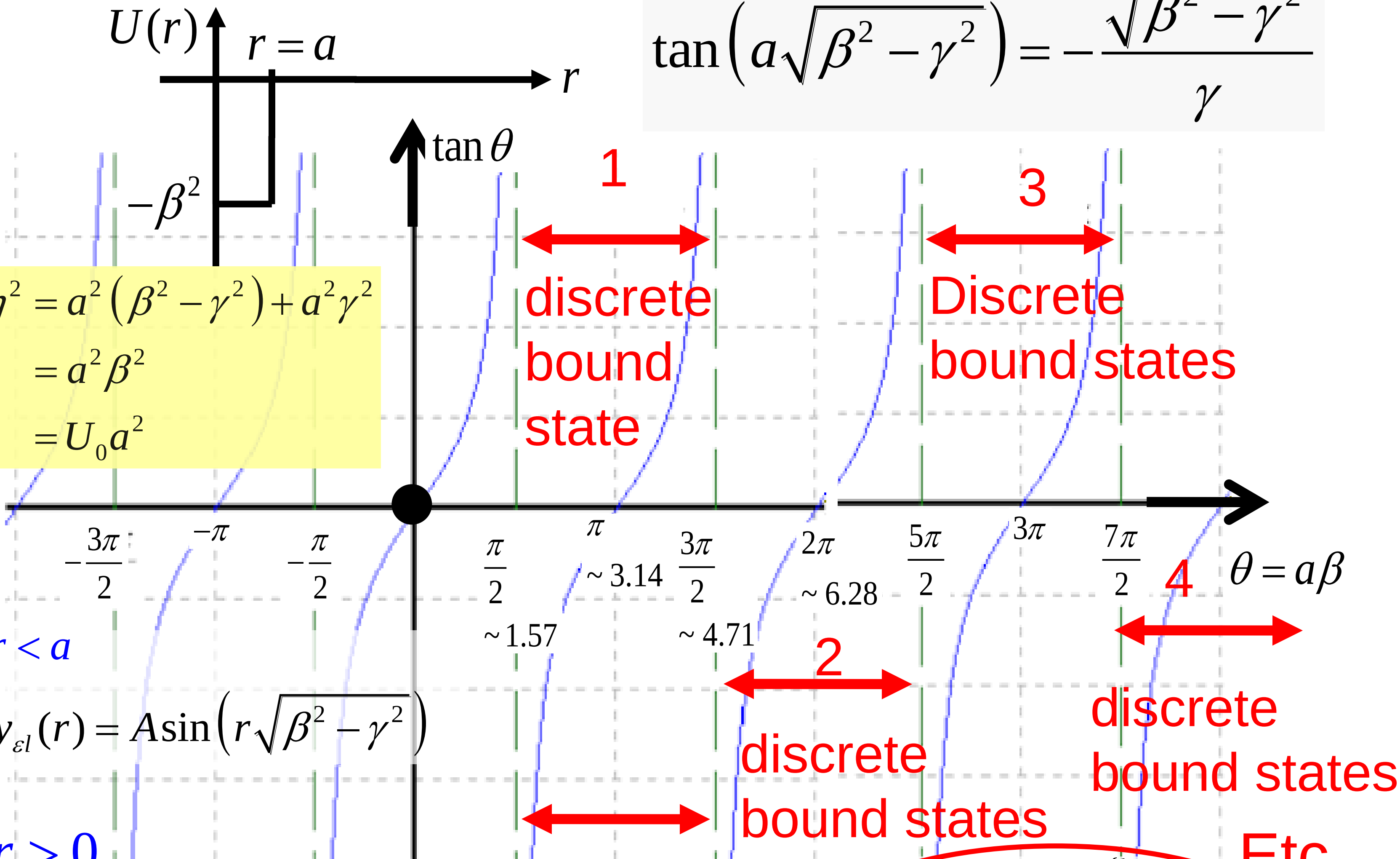
$$\frac{\pi}{2} < a\beta < \frac{3\pi}{2}$$
$$1.57 < a\beta < 4.71$$
$$n = 1$$

$$\frac{3\pi}{2} < a\beta < \frac{5\pi}{2}$$
$$4.71 < a\beta < 7.85$$
$$n = 2$$

$\rightarrow \xi$

$\uparrow$ $\frac{\pi}{2} = 1.57$

$$\tan\left(a\sqrt{\beta^2-\gamma^2}\right) = -\frac{\sqrt{\beta^2-\gamma^2}}{\gamma}$$



$$\xi^2+\eta^2 = a^2\left(\beta^2-\gamma^2\right)+a^2\gamma^2$$
$$= a^2\beta^2$$
$$= U_0 a^2$$

$r < a$

$$y_{\varepsilon l}(r) = A\sin\left(r\sqrt{\beta^2-\gamma^2}\right)$$

$r > 0$

$$y_{\varepsilon l}(r) = B\ e^{-\gamma r}$$

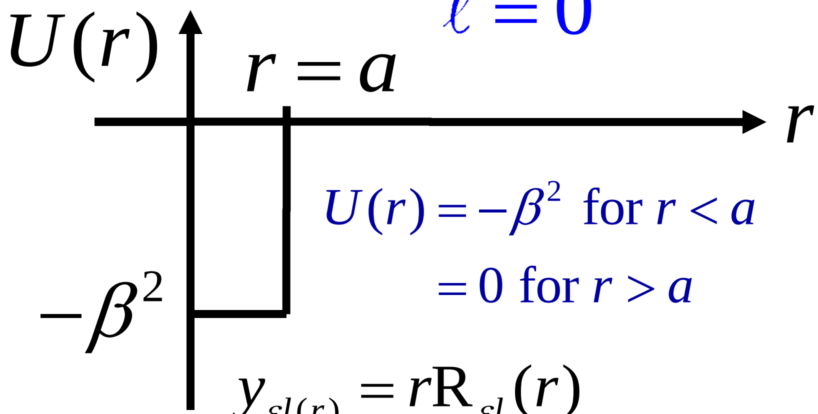
$$\frac{\pi}{2} < a\beta < \frac{3\pi}{2}$$

$$\tan\xi = -\frac{\xi}{\eta}$$

$$\xi = a\sqrt{\beta^2-\gamma^2} \quad \& \quad \eta = a\gamma$$

Etc.

We considered the bound states of a SPHERICAL well attractive potential



$\ell = 0$

$$U(r) = -\beta^2 \text{ for } r < a$$
$$= 0 \text{ for } r > a$$

$$y_{\varepsilon l(r)} = r\mathrm{R}_{\varepsilon l}(r)$$

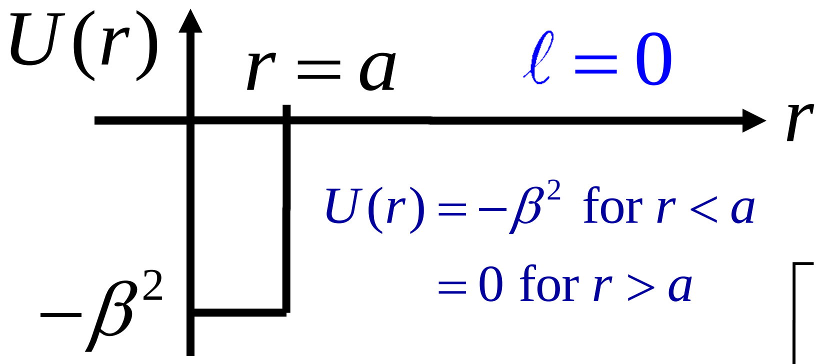
Now, we consider scattering ; continuum states

$$E = \frac{\hbar^2 k^2}{2m} > 0$$

$$U(r) = \frac{2m}{\hbar^2} V(r) \qquad \left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \left\{ V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} \right\} - E \right] y_{\varepsilon l}(r) = 0$$

$$\ell = 0 \qquad \left[\frac{d^2}{dr^2} + \{-U(r)\} + \frac{2m}{\hbar^2}E \right] y_{\varepsilon l}(r) = 0$$

$$\frac{2mE}{\hbar^2} = k^2 \qquad \left[\frac{d^2}{dr^2} + \{-U(r)\} + k^2 \right] y_{\varepsilon l}(r) = 0$$



$$U(r) = -\beta^2 \text{ for } r < a$$
$$= 0 \text{ for } r > a$$

$$\frac{2mE}{\hbar^2} = k^2 > 0$$

$$y_{\varepsilon l(r)} = r\mathrm{R}_{\varepsilon l}(r)$$

$$\left[\frac{d^2}{dr^2} + \{-U(r)\} + k^2\right] y_{\varepsilon l}(r) = 0$$

$$U(r) = \frac{2m}{\hbar^2} V(r)$$

$$\left[\frac{d^2}{dr^2} + \beta^2 + k^2\right] y_{\varepsilon l}(r) = 0 \qquad r < a \qquad y_{\varepsilon l}(r) = C\sin\left(r\sqrt{\beta^2 + k^2}\right)$$

$$\left[\frac{d^2}{dr^2} + k^2\right] y_{\varepsilon l}(r) = 0 \qquad r > a \qquad y_{\varepsilon l}(r) = D\sin\left(kr + \delta_0(k)\right)$$

Continuity at $r = a \quad \Rightarrow$

$$C\sin\left(a\sqrt{\beta^2 + k^2}\right) = D\sin\left(ka + \delta_0(k)\right)$$

$$C\sqrt{\beta^2 + k^2}\cos\left(a\sqrt{\beta^2 + k^2}\right) = Dk\cos\left(ka + \delta_0(k)\right)$$

$$C\sin\left(a\sqrt{\beta^2+k^2}\right)=D\sin\left(ka+\delta_0(k)\right)$$

$$C\sqrt{\beta^2+k^2}\cos\left(a\sqrt{\beta^2+k^2}\right)=Dk\cos\left(ka+\delta_0(k)\right)$$

$$\frac{1}{\sqrt{\beta^2+k^2}}\tan\left(a\sqrt{\beta^2+k^2}\right)=\frac{1}{k}\tan\left(ka+\delta_0(k)\right)$$

$$=\frac{1}{k}\times\frac{\tan(ka)+\tan\left(\delta_0(k)\right)}{1-\tan\left(ka\right)\tan\left(\delta_0(k)\right)}$$

$$\frac{k}{\sqrt{\beta^2+k^2}}\tan\left(a\sqrt{\beta^2+k^2}\right)-\frac{k}{\sqrt{\beta^2+k^2}}\tan\left(a\sqrt{\beta^2+k^2}\right)\tan\left(ka\right)\tan\left(\delta_0(k)\right)=$$

$$=\tan(ka)+\tan\left(\delta_0(k)\right)$$

$$-\tan\left(\delta_0(k)\right)\left\{1+\frac{k}{\sqrt{\beta^2+k^2}}\tan\left(a\sqrt{\beta^2+k^2}\right)\tan\left(ka\right)\right\}=\tan(ka)-\frac{k}{\sqrt{\beta^2+k^2}}\tan\left(a\sqrt{\beta^2+k^2}\right)$$

$$-\tan\left(\delta_0(k)\right) = \frac{\tan(ka) - \dfrac{k}{\sqrt{\beta^2+k^2}}\tan\left(a\sqrt{\beta^2+k^2}\right)}{1+\dfrac{k}{\sqrt{\beta^2+k^2}}\tan\left(a\sqrt{\beta^2+k^2}\right)\tan(ka)}$$

$$\tan\left(\delta_0(k)\right) = \frac{k\tan\left(a\sqrt{\beta^2+k^2}\right) - \sqrt{\beta^2+k^2}\tan(ka)}{\sqrt{\beta^2+k^2} + k\tan\left(a\sqrt{\beta^2+k^2}\right)\tan(ka)}$$

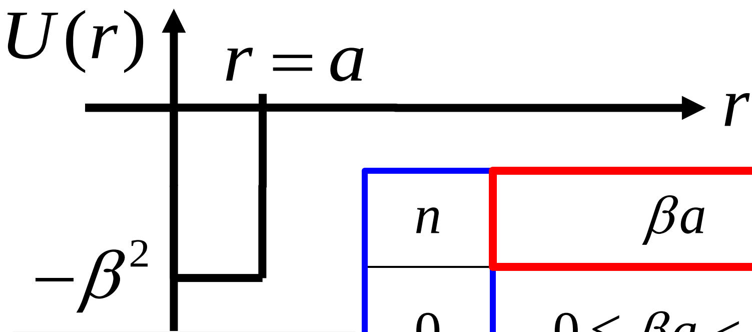
$$\frac{\tan\left(\delta_0(k)\right)}{k} = \frac{\tan\left(a\sqrt{\beta^2+k^2}\right) - \dfrac{\sqrt{\beta^2+k^2}}{k}\tan(ka)}{\sqrt{\beta^2+k^2} + k\tan\left(a\sqrt{\beta^2+k^2}\right)\tan(ka)}$$

$$\alpha = -\lim_{k\to 0}\frac{\tan\delta_0(k)}{k}$$

scattering length

$$-\alpha = \frac{a\tan(a\beta) - \beta a}{\beta a}$$

$$\alpha = a - \frac{\tan(a\beta)}{\beta}$$



Reference: ‘Quantum Theory of Scattering’ by Ta-You Wu and Takashi Ohmura (Prentice Hall, 1962) page 73

n = number of bound states

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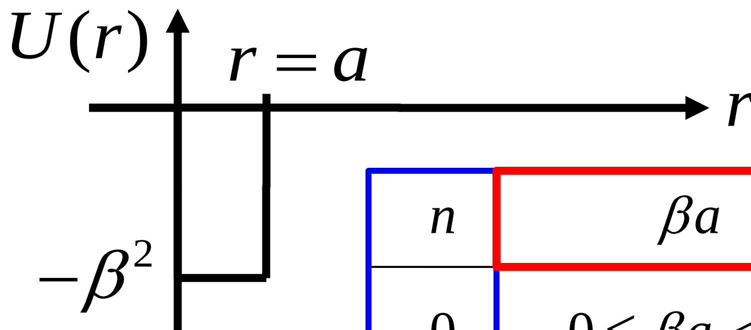
$$-\frac{1}{\alpha} = \lim_{k\to 0} k\cot\delta_0(k)$$

$$\alpha = a - \frac{\tan(a\beta)}{\beta}$$

$$\lim_{\beta\to 0}\alpha = a - \frac{\tan(a\beta)}{\beta} \simeq a - \frac{a\beta}{\beta} \to 0$$

n	βa	$k\cot\delta = x$	α	δ
0	$0 \le \beta a < \frac{\pi}{2}$	$\infty > x > 0$	$0 \ge \alpha > -\infty$	$\simeq 0$
*	$\frac{\pi}{2}$	0	$-\infty \to +\infty$	$\frac{\pi}{2}$
1	$\frac{\pi}{2} < \beta a < \pi$	$0 > x > -\infty$	$\infty > \alpha > 0$	$\simeq \pi$
1	$\pi < \beta a < \frac{3\pi}{2}$	$\infty > x > 0$	$0 > \alpha > -\infty$	$\simeq \pi$
1+*	$\frac{3\pi}{2}$	0	$-\infty \to +\infty$	$\frac{3\pi}{2}$
2	$\frac{3\pi}{2} < \beta a < 2\pi$	$0 > x > -\infty$	$\infty > \alpha > 0$	$\simeq 2\pi$
2	$2\pi < \beta a < \frac{5\pi}{2}$	$\infty > x > 0$	$0 > \alpha > -\infty$	$\simeq 2\pi$



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n	βa	Levinson's Theorem	δ
0	$0 \le \beta a < \frac{\pi}{2}$	$\delta_0(k\to 0) = 0\times\pi$	$\simeq 0$
*	$\frac{\pi}{2}$	$\delta_0(k\to 0) = \left(0+\frac{1}{2}\right)\pi$	$\frac{\pi}{2}$
1	$\frac{\pi}{2} < \beta a < \pi$	$\delta_0(k\to 0) = \pi$	$\simeq \pi$
1	$\pi < \beta a < \frac{3\pi}{2}$	$\delta_0(k\to 0) = \pi$	$\simeq \pi$
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2	$\frac{3\pi}{2} < \beta a < 2\pi$	$\delta_0(k\to 0) = 2\pi$	$\simeq 2\pi$
2	$2\pi < \beta a < \frac{5\pi}{2}$	$\delta_0(k\to 0) = 2\pi$	$\simeq 2\pi$

LEVINSON's THEOREM

Kgl. Danske Videnskab. Salskab. Mat. Fys. Medd.25 9 (1949)

zero of $\delta_l(k)$: $\quad \delta_l(k \to \infty) = 0$

.... for $l = 0$:

$$\delta_0(k \to 0) = n_0 \ \pi$$

"half-bound" state

or $\delta_0(k \to 0) = \left(n_0 + \frac{1}{2}\right)\pi$ if there is a (resonant)

"zero energy resonance"

bound state solution at zero energy.

$$\sigma_{total}(k \to 0) \underset{up}{\overset{blows}{\to}} \frac{1}{k^2} \text{ when } \lambda_0 a = \sqrt{U_0}\, a = \frac{\pi}{2}$$

$$\delta_0(k \to 0) \to \frac{\pi}{2}$$

$$\delta_l(k \to 0) = n_l \ \pi \quad \text{....... for } l \geq 1$$

$$\delta_\ell(0) - \delta_\ell(\infty) = \begin{cases} (n_\ell + 1/2)\pi & \text{when } \ell = 0 \text{ and a half bound state occurs} \\ n_\ell \pi & \text{the remaining cases,} \end{cases}$$

QUESTIONS ? Write to: pcd@physics.iitm.ac.in

Select/Special Topics *in* 'Theory of Atomic Collisions and Spectroscopy'

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Lecture Number 12

Unit 1: Quantum Theory of Collisions

More on Levinson's theorem 1949

Scattering length
Effective range

Low energy scattering **Ultra-Cold atoms**

LEVINSON's THEOREM

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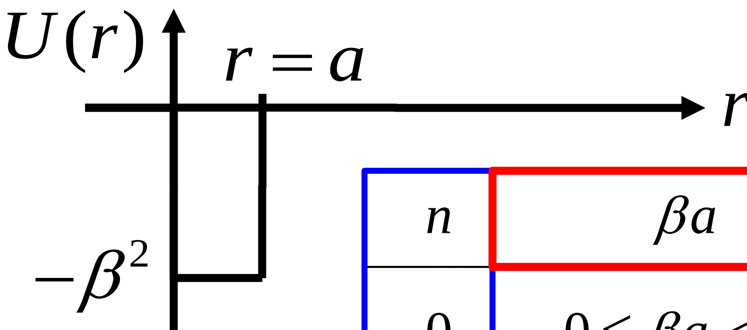

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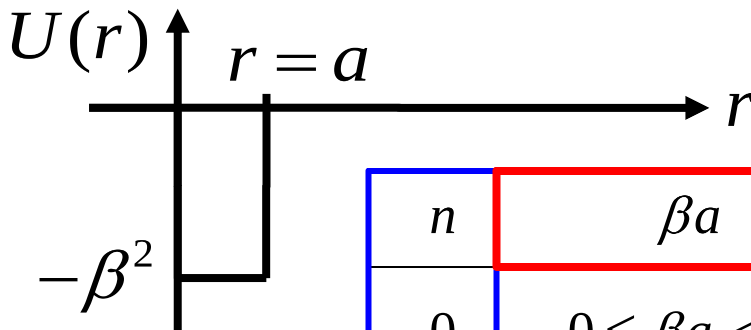

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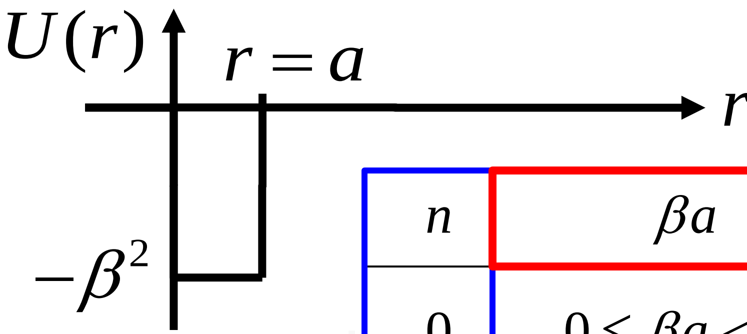
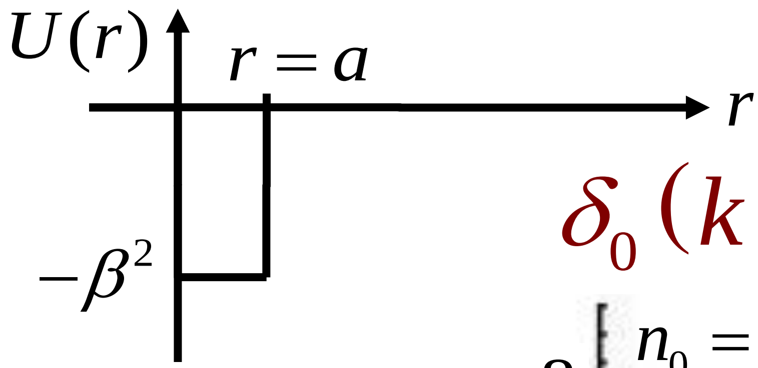


Positive α indicates a repulsive potential.

Negative α indicates an attractive potential.

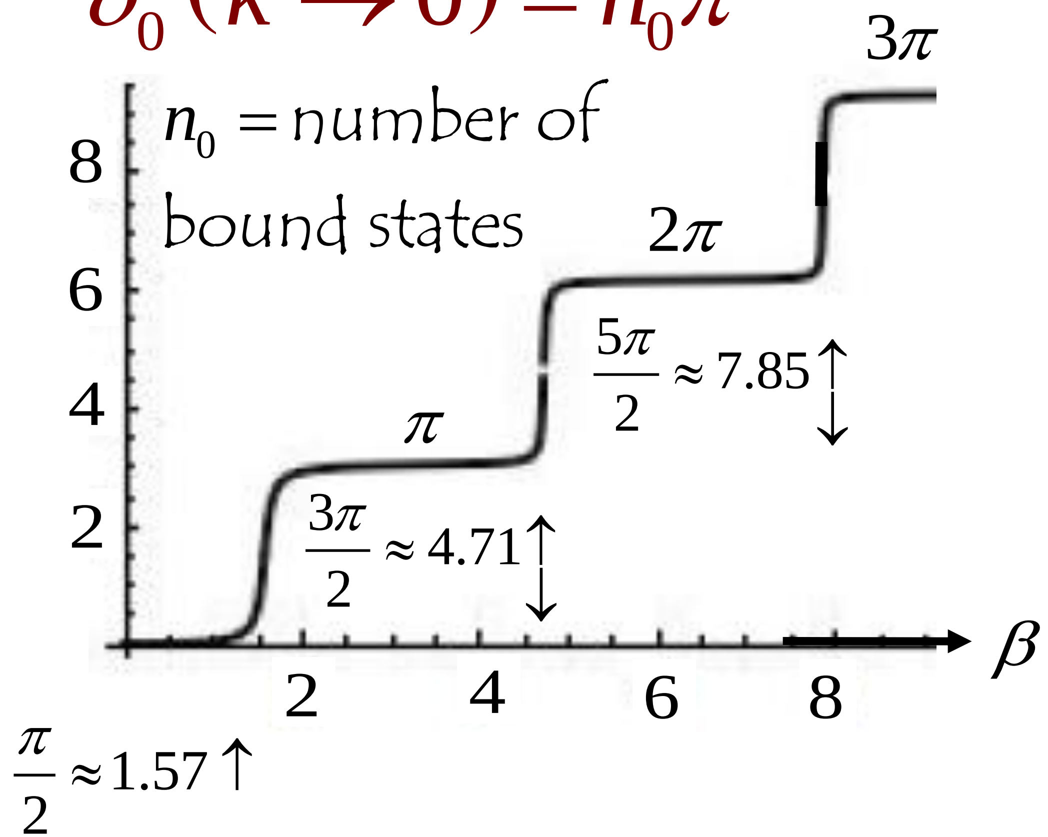
n	βa	α	δ
0	$0 \le \beta a < \frac{\pi}{2}$	*negative*	$\simeq 0$
*	$\frac{\pi}{2}$	$-\infty$ *to* $+\infty$	$\frac{\pi}{2}$
1	$\frac{\pi}{2} < \beta a < \pi$	*positive*	$\simeq \pi$
1	$\pi < \beta a < \frac{3\pi}{2}$	*negative*	$\simeq \pi$
1+*	$\frac{3\pi}{2}$	$-\infty$ *to* $+\infty$	$\frac{3\pi}{2}$
2	$\frac{3\pi}{2} < \beta a < 2\pi$	*positive*	$\simeq 2\pi$
2	$2\pi < \beta a < \frac{5\pi}{2}$	*negative*	$\simeq 2\pi$

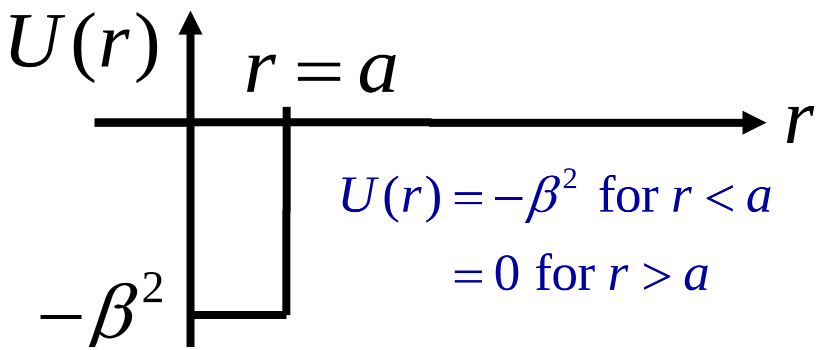
A new bound state gets formed *when* the sign of the scattering length ***is about to change*** *from* negative to positive.



$$\delta_0 (k \to 0) = n_0 \pi$$

How the s-wave phase shift changes with the strength of the potential





$$U(r) = -\beta^2 \text{ for } r < a$$
$$= 0 \text{ for } r > a$$

$$\alpha = a - \frac{\tan(a\beta)}{\beta}$$

$$\Rightarrow$$

$$\alpha = a - \frac{a\tan(a\beta)}{a\beta}$$

$$\alpha = a\left(1 - \frac{\tan(a\beta)}{a\beta}\right)$$

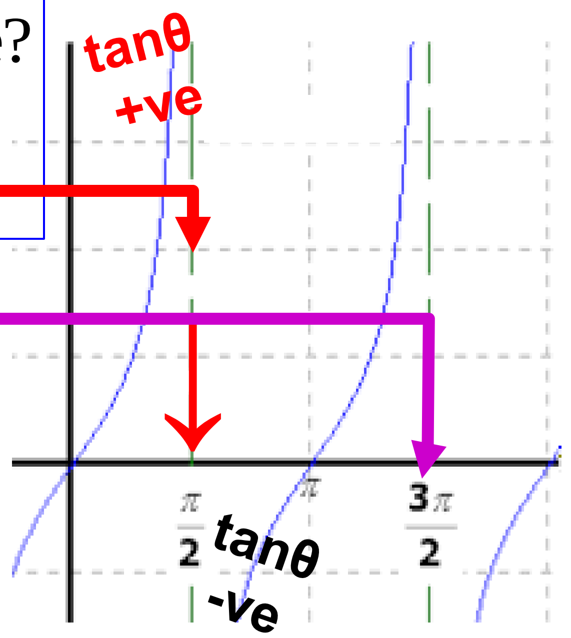
$$when \ \frac{\tan(a\beta)}{(a\beta)} > 1, \ \alpha \text{ is negative}$$

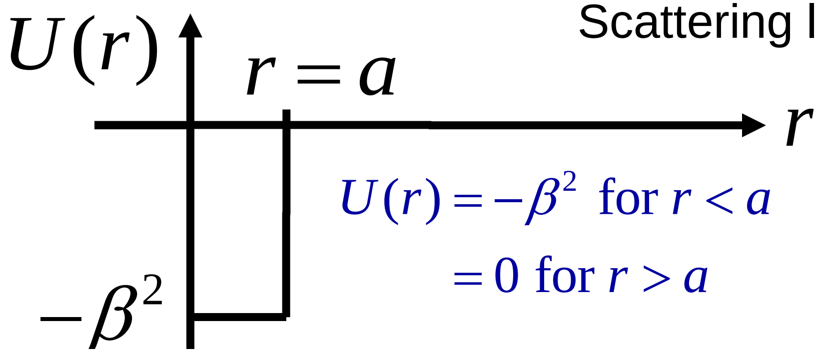
when does α get to be MOST negative?

$$when \ (a\beta) \lessapprox \frac{\pi}{2} \rightarrow 1^{st} \ bound \ state$$

$$when \ (a\beta) \lessapprox \frac{3\pi}{2} \rightarrow 2^{nd} \ bound \ state$$

$$when \ (a\beta) \lessapprox \frac{5\pi}{2} \rightarrow 3^{rd} \ bound \ state$$





$$U(r) = -\beta^2 \text{ for } r < a$$
$$= 0 \text{ for } r > a$$

Scattering length →

$$\alpha = a - \frac{\tan(a\beta)}{\beta}$$

$$\Rightarrow$$

$$\alpha = a - \frac{a\tan(a\beta)}{a\beta}$$

$$\alpha = a\left(1 - \frac{\tan(a\beta)}{a\beta}\right)$$

$$when\ \frac{\tan(a\beta)}{(a\beta)} > 1,\ \alpha \text{ is negative}$$

when does α get to be <u>MOST</u> negative?

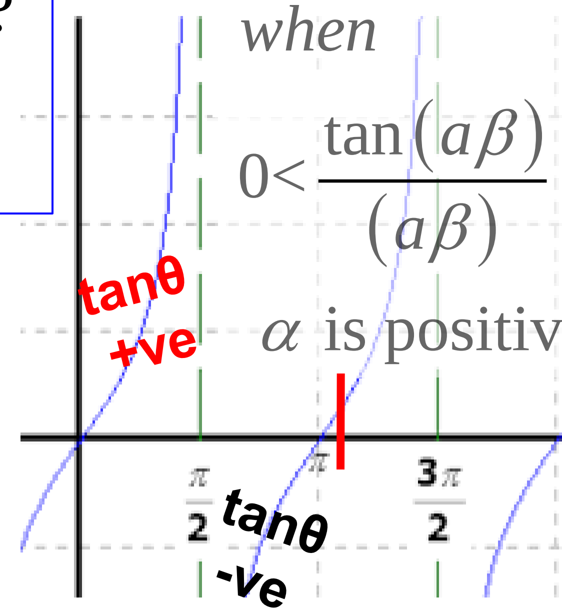
$$when\ (a\beta) \lesssim \frac{\pi}{2} \rightarrow 1^{st}\ bound\ state$$

when does α go to zero?

$$\frac{\pi}{2} < (a\beta) < \pi + \varepsilon \mapsto \alpha > 0$$

$$at\ (a\beta) = \pi + \varepsilon : \alpha \text{ changes sign } \mapsto +\ to\ -$$

$$when\ \pi + \varepsilon < (a\beta) < \frac{3\pi}{2} \mapsto \alpha < 0$$



$$when\ 0 < \frac{\tan(a\beta)}{(a\beta)} < 1,$$
$$\alpha \text{ is positive}$$

$$\frac{\pi}{2} < (a\beta) < \pi + \varepsilon \mapsto \alpha > 0$$

$$at \;\; (a\beta) = \pi + \varepsilon : \alpha \text{ changes sign } \;\; \mapsto + \; to \; -$$

$$when \;\; \pi + \varepsilon < (a\beta) < \frac{3\pi}{2} \mapsto \alpha < 0$$

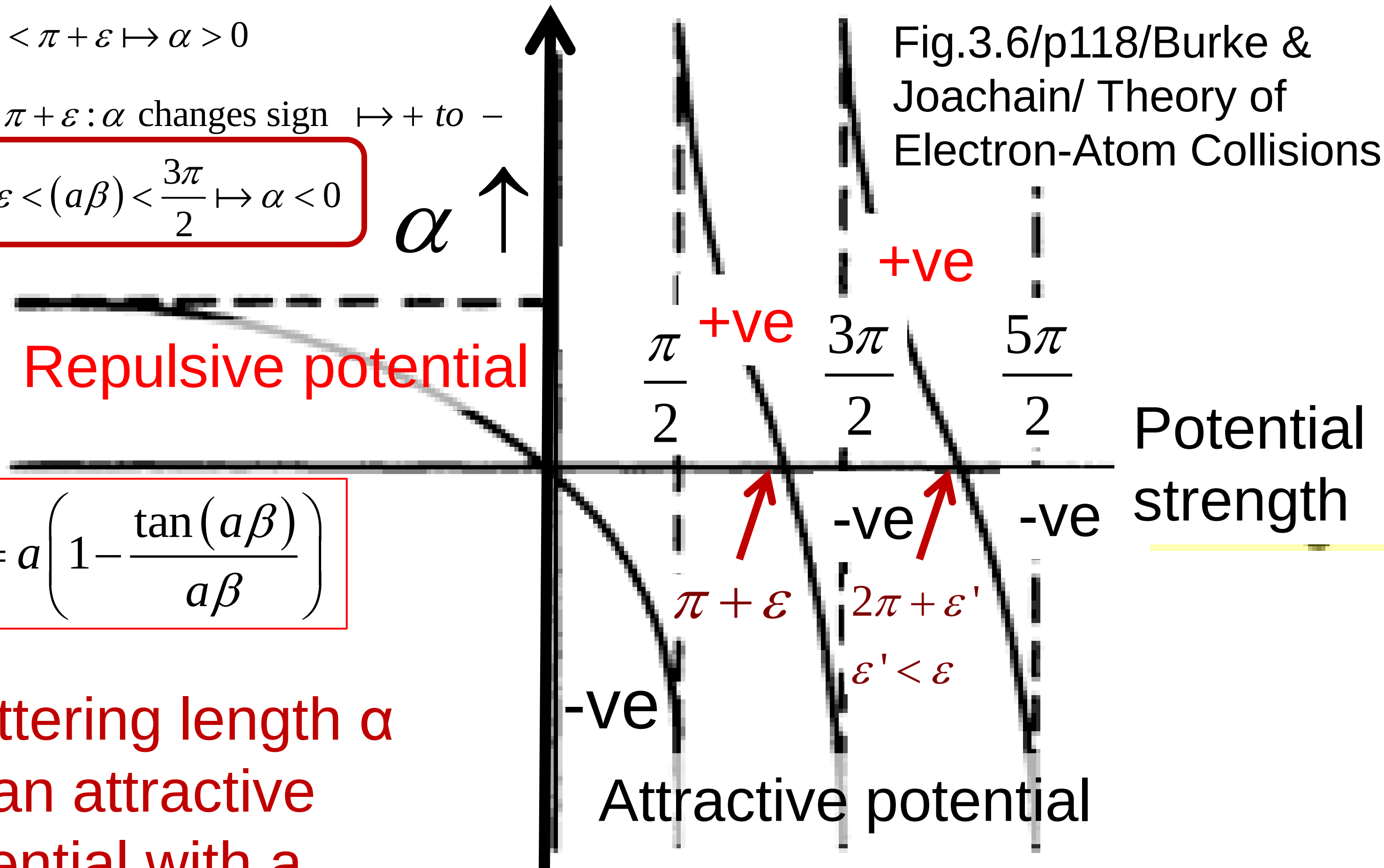


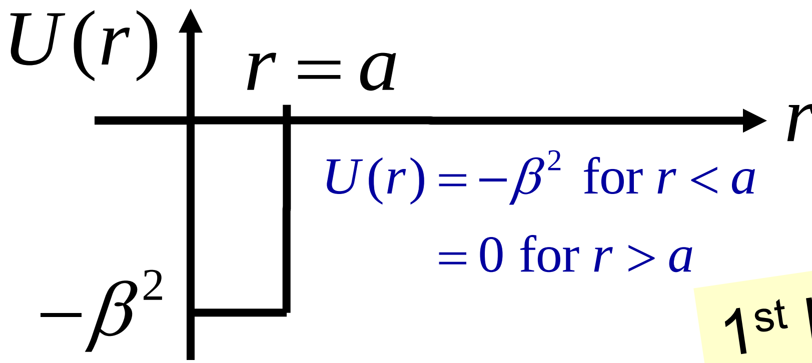
Fig.3.6/p118/Burke & Joachain/ Theory of Electron-Atom Collisions

$$\alpha = a\left(1 - \frac{\tan(a\beta)}{a\beta}\right)$$

scattering length α for an attractive potential with a finite range ‘a’

$$\alpha = a\left(1 - \frac{\tan(a\beta)}{a\beta}\right)$$

↑ *change of sign of scattering length α*



$$when \ \frac{\tan(a\beta)}{(a\beta)} > 1, \quad \alpha \text{ is negative}$$

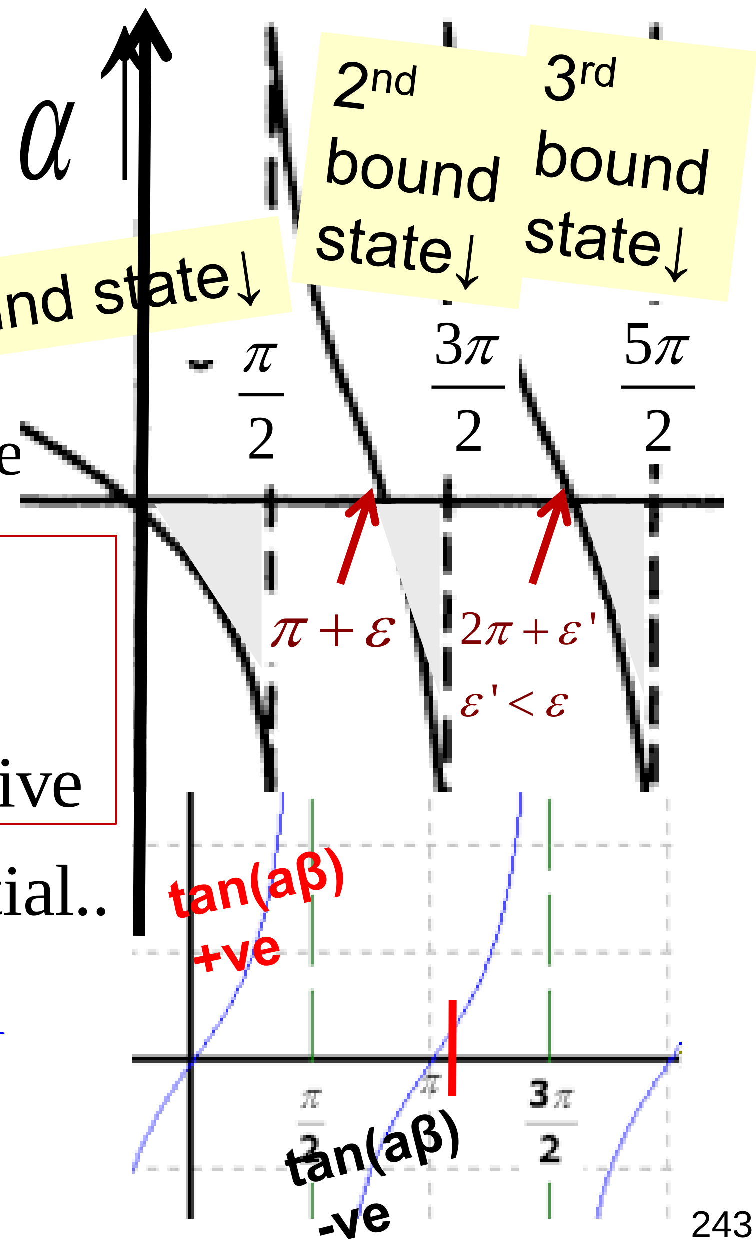
$$when \ \pi + \varepsilon < (a\beta) < \frac{3\pi}{2},$$

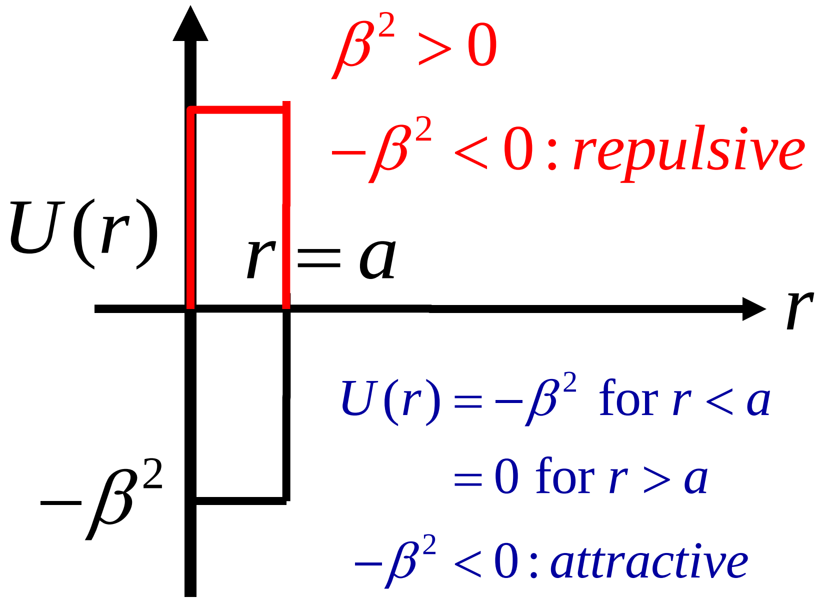
$$\alpha = a\left(1 - \frac{\tan(a\beta)}{a\beta}\right) \qquad \alpha \text{ is negative}$$

$\rightarrow$ (effective) attractive potential..

but not strong enough to bind

the next bound state



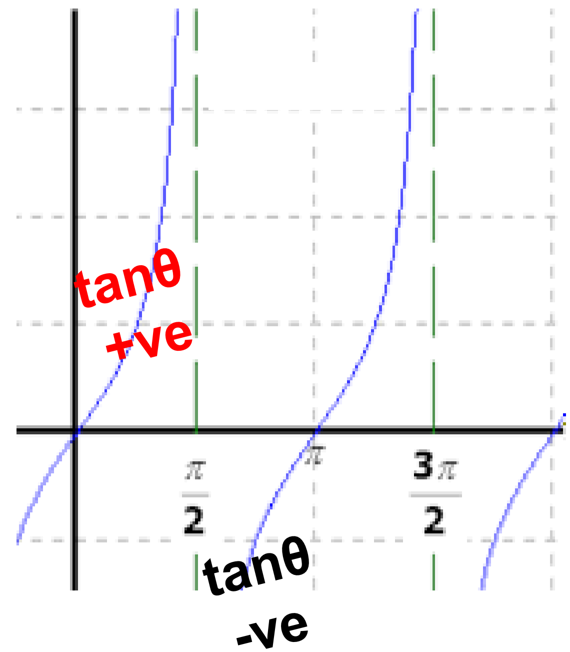


$$\alpha = a - \frac{\tan(a\beta)}{\beta}$$

$$\Rightarrow$$

$$\alpha = a - \frac{a\tan(a\beta)}{a\beta}$$

$$\alpha = a\left(1 - \frac{\tan(a\beta)}{a\beta}\right)$$



when α is positive

$\rightarrow$ (effective) repulsive potential.

$$u_{l=0}(k, r \to \infty) = A_{l=0}(k) \sin\left(kr + \delta_0(k)\right)$$

$$u_{\varepsilon,l}(r) = r R_{\varepsilon,l}(r)$$

asymptote $r \to \infty$

Low energy limit

$$u_{l=0}^{k\to 0}(k, r \to \infty) = \lim_{k\to 0} A_{l=0}(k) \sin\left(kr + \delta_0(k)\right)$$

$$k \cot\left(\delta_0(k)\right) \underset{k\to 0}{=} \frac{-1}{\alpha} \qquad \tan\left(\delta_0(k)\right) \underset{k\to 0}{\approx} -\alpha k$$

$$u_{l=0}^{k\to 0}(k, r \to \infty) = \lim_{k\to 0} A\left(kr - k\alpha\right) = \lim_{k\to 0} Ak\left(r - \alpha\right)$$

$k \to 0$

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

$$\left[\frac{d^2}{dr^2} - U(r)\right] u_{l=0}^{0}(r) = 0 \to \left[\frac{d^2}{dr^2}\right]_{r \geq a} u_{l=0}^{0}(r) = 0$$

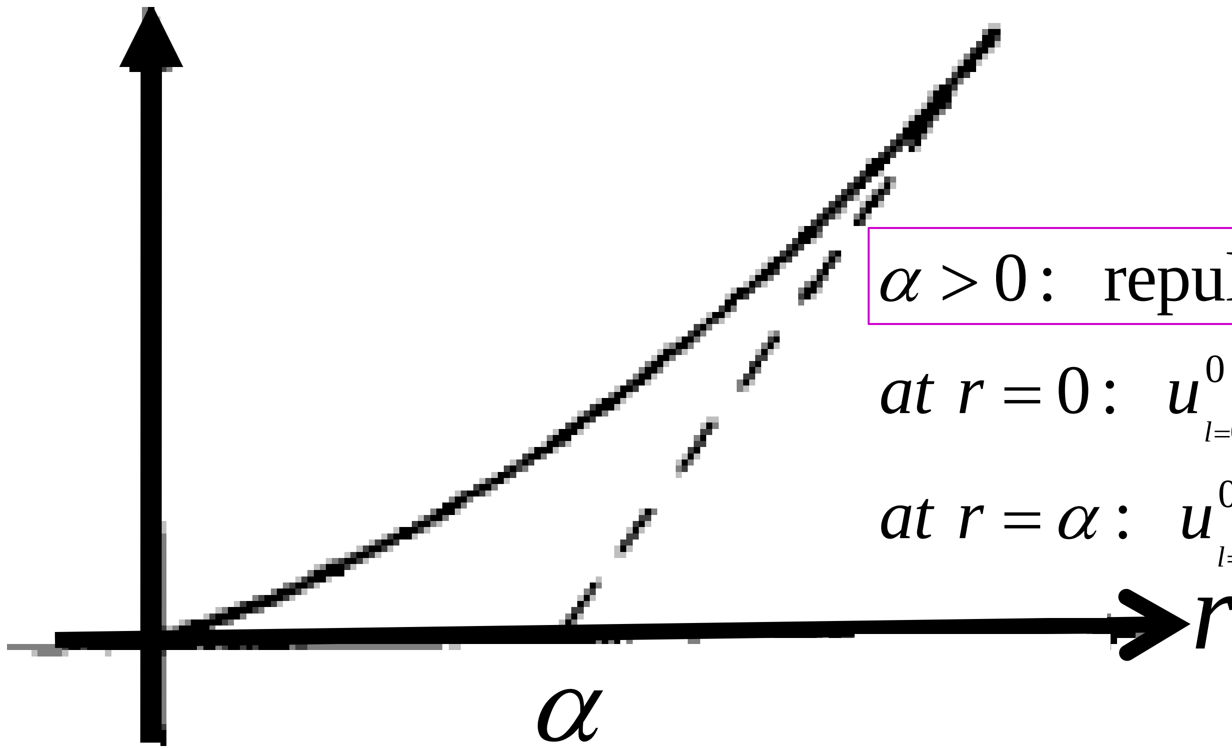
Linear relation.

α → intercept

$$u_{l=0}^{0}(r) = mr + C \quad .... \quad r \gg a$$

$$u^0_{l=0}(r) = mr + C \;= \lim_{k\to 0} Ak(r-\alpha)$$ *asymptotic behavior*

.... $r \gg a$



$\alpha > 0:$ repulsive potential

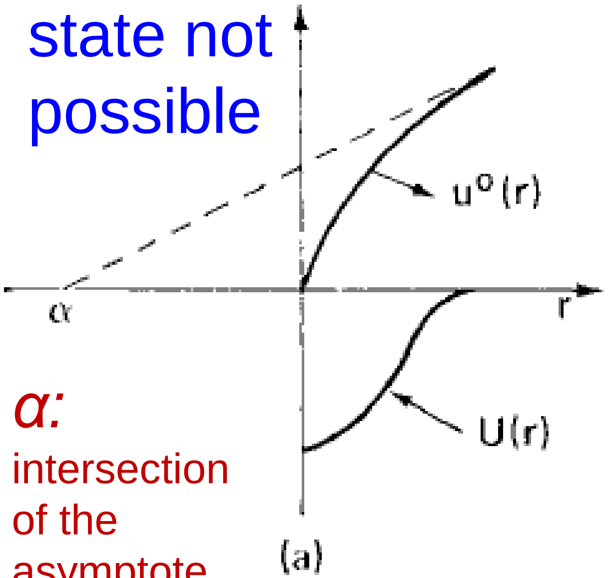
$at\; r = 0: \quad u^0_{l=0}(r) = -mk\alpha$

$at\; r = \alpha: \quad u^0_{l=0}(r) = 0$

Geometrical meaning of the scattering length α

Fig.11.11/page288/C.J.Joachain – 'Quantum Theory of Collisions'

α < 0 but bound state not possible



α: intersection of the asymptote with *r*-axis

$$u_{l=0}^{k\to 0}(k, r\to\infty) = \lim_{k\to 0} A_{l=0}(k)\sin\left(kr+\delta_0(k)\right)$$

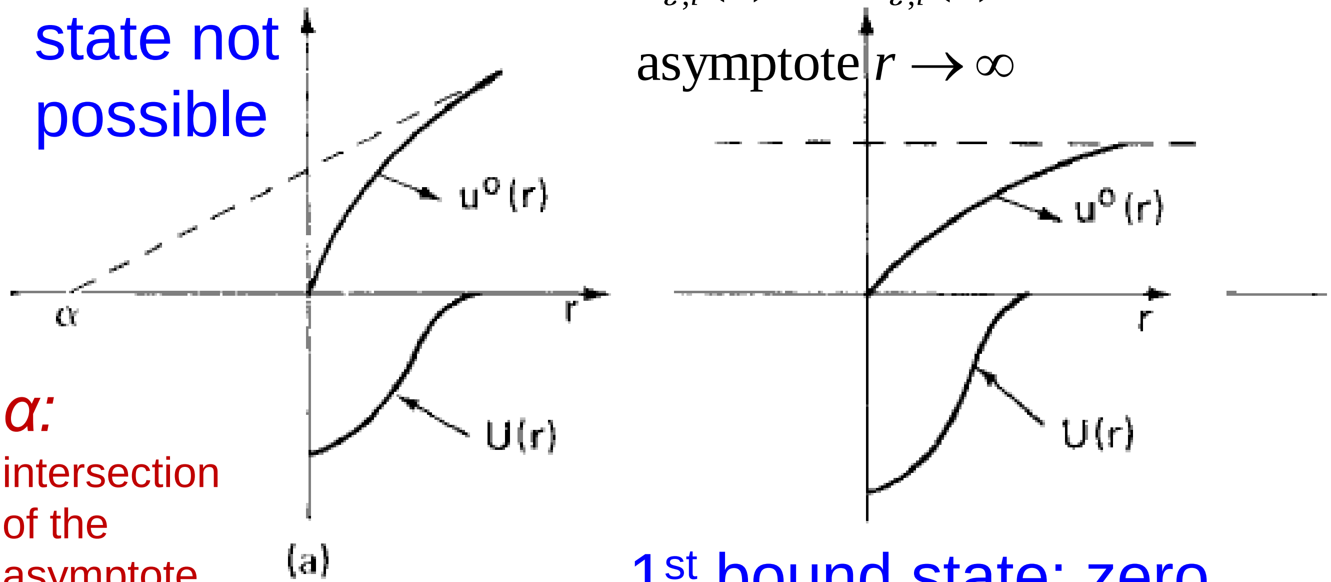
$$= \lim_{k\to 0} A\left(kr - k\alpha\right) = \lim_{k\to 0} Ak\left(r-\alpha\right)$$

Scattering length α for various attractive potentials
Fig.11.12/page289/C.J.Joachain – ‘Quantum Theory of Collisions’

α < 0 but bound state not possible

$$u_{\varepsilon,l}(r) = r\mathrm{R}_{\varepsilon,l}(r)$$

asymptote $r \to \infty$



α: intersection of the asymptote with *r*-axis

1st bound state: zero energy resonance

α→-∞ (most negative)

$$u_{l=0}^{k\to 0}(k, r\to\infty) = \lim_{k\to 0} A_{l=0}(k)\sin\left(kr + \delta_0(k)\right)$$

$$= \lim_{k\to 0} A\left(kr - k\alpha\right) = \lim_{k\to 0} Ak\left(r - \alpha\right)$$

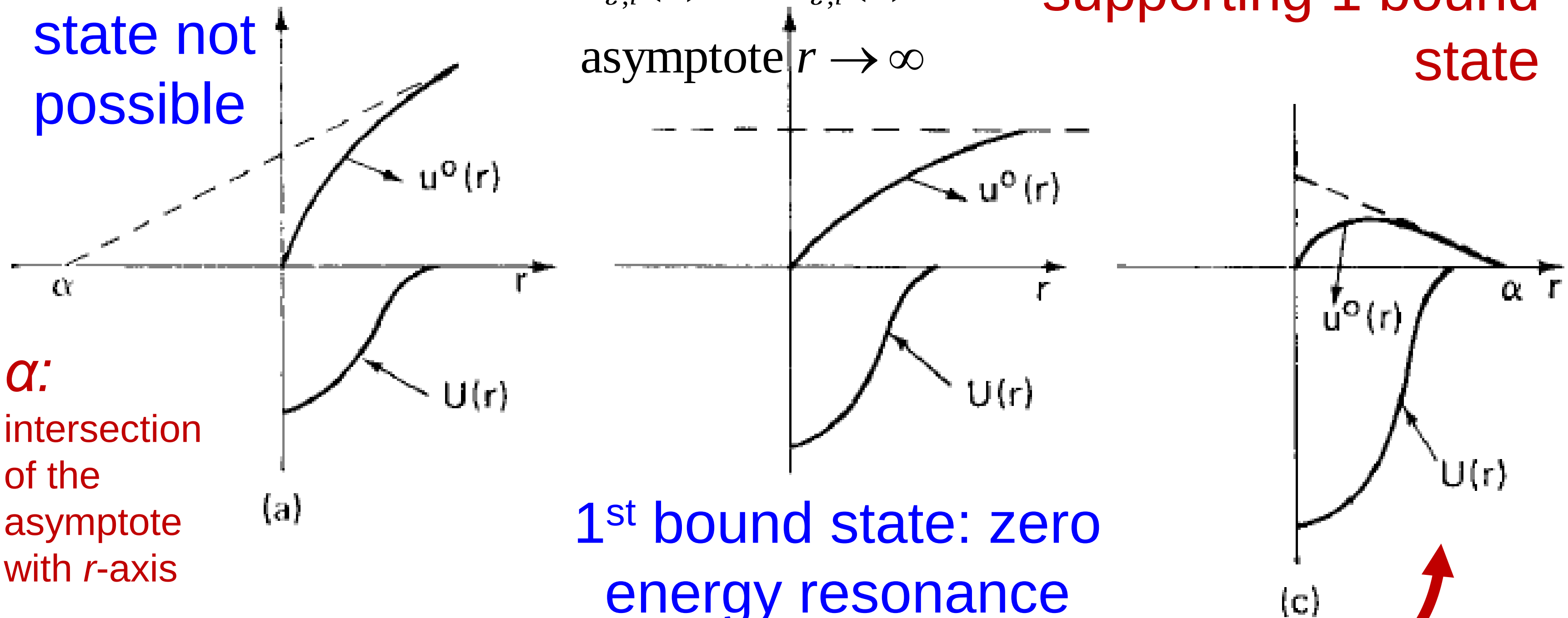
Scattering length α for various attractive potentials
Fig.11.12/page289/C.J.Joachain – ‘Quantum Theory of Collisions’

α < 0 but bound state not possible

$u_{\varepsilon,l}(r) = r\mathrm{R}_{\varepsilon,l}(r)$

asymptote $r \to \infty$

Attractive potential supporting 1 bound state



α: intersection of the asymptote with *r*-axis

1st bound state: zero energy resonance

α→-∞ (most negative)

$$u_{l=0}^{k\to 0}(k, r\to\infty) = \lim_{k\to 0} A_{l=0}(k)\sin\left(kr+\delta_0(k)\right)$$

$$= \lim_{k\to 0} A\left(kr - k\alpha\right) = \lim_{k\to 0} Ak\left(r-\alpha\right)$$

Positive *α* indicates no more bound state "repulsive" potential.

Scattering length α for various attractive potentials
Fig.11.12/page289/C.J.Joachain – 'Quantum Theory of Collisions'

The scattering length has in it vital information about the physical properties of the potential,

but it does not include details about the structure of the potential.

‘SLOW’ collisions

$$\lambda = \frac{h}{mv}: \text{ de Broglie wavelength } \rightarrow \text{large}$$

Monopole?

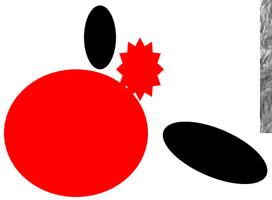
Detailed ‘structure’ of the scattering potential : IMPORTANT?

Essential focus is then on symmetry (s wave scattering) and a parameter →

→ scattering length α.

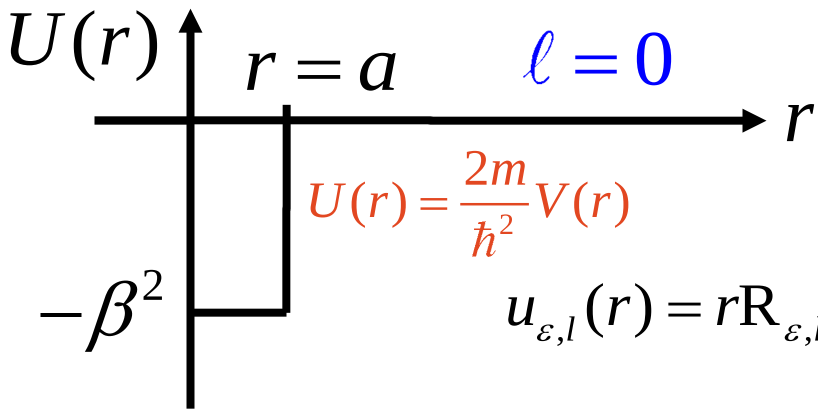
Where is the observer?

Negative
Positive



Multipole?

Charge distributions



$\ell = 0$

"EFFECTIVE RANGE"

$$U(r) = \frac{2m}{\hbar^2}V(r)$$

$$u_{\varepsilon,l}(r) = r\mathrm{R}_{\varepsilon,l}(r)$$

$$U(r) = -\beta^2 \text{ for } r<a$$
$$= 0 \text{ for } r>a$$

$$\frac{2mE}{\hbar^2} = k^2 > 0$$

PHYSICAL REVIEW VOLUME 76, NUMBER 1 JULY 1, 1949

Theory of the Effective Range in Nuclear Scattering

H. A. BETHE
*Physics Department, Cornell University, Ithaca, New York**

Neutron-Proton scattering
→Spin dependent

Theory of ultracold atomic Fermi gases

REVIEWS OF MODERN PHYSICS, VOLUME 80, OCTOBER–DECEMBER 2008

Stefano Giorgini *et al.*

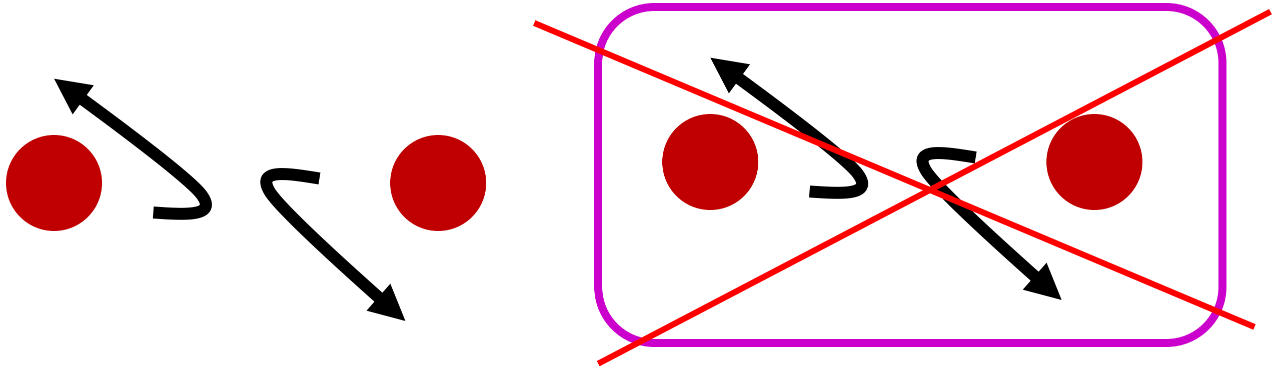
Bose atoms: quantum statistics leads to BEC phase

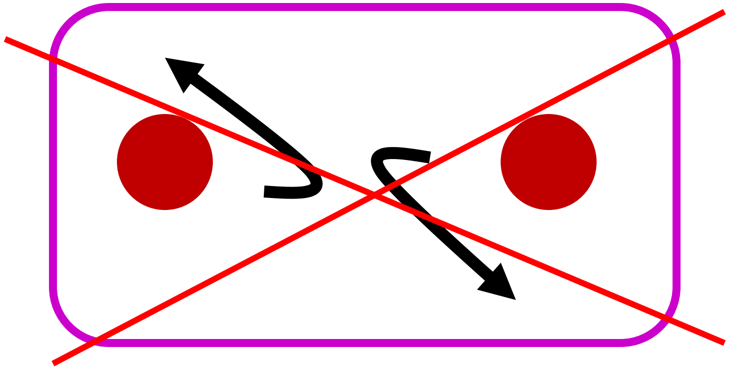
2 Fermionic cold atoms:

* BCS pairing –“Cooper pair”

* Bosonic bound-state molecule - BEC

In single-component Fermi gas, s-wave scattering is inhibited by Pauli exclusion principle.
Evaporative cooling requires collisions.





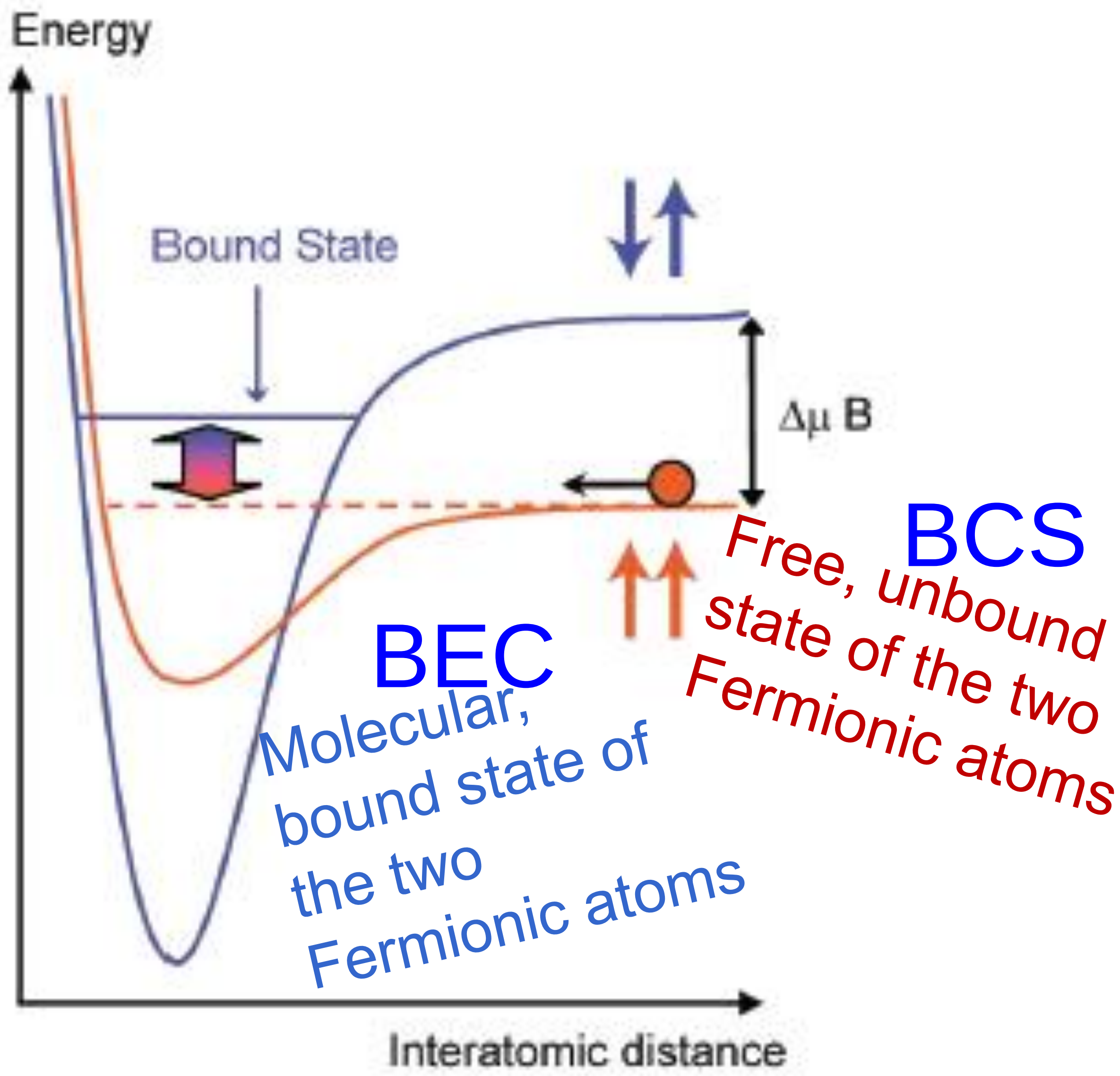
Sympathetic cooling:
Evaporate Bose atoms
and
cool Fermi atoms by enabling collisions between Bose and Fermi atoms.

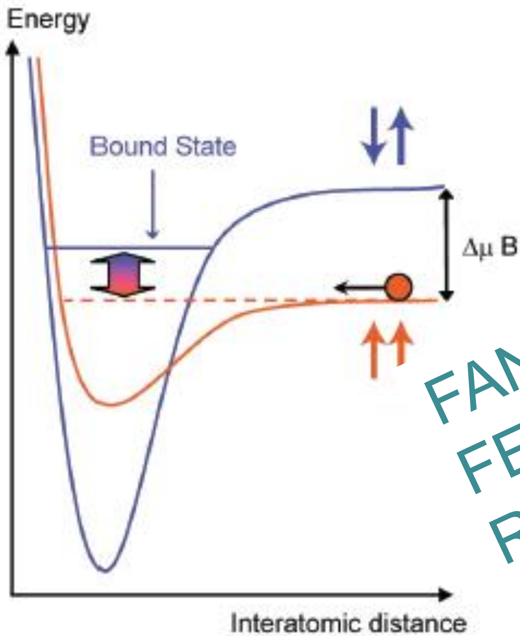
scattering length

$\alpha > 0 \quad \mapsto \quad$ repulsive interaction

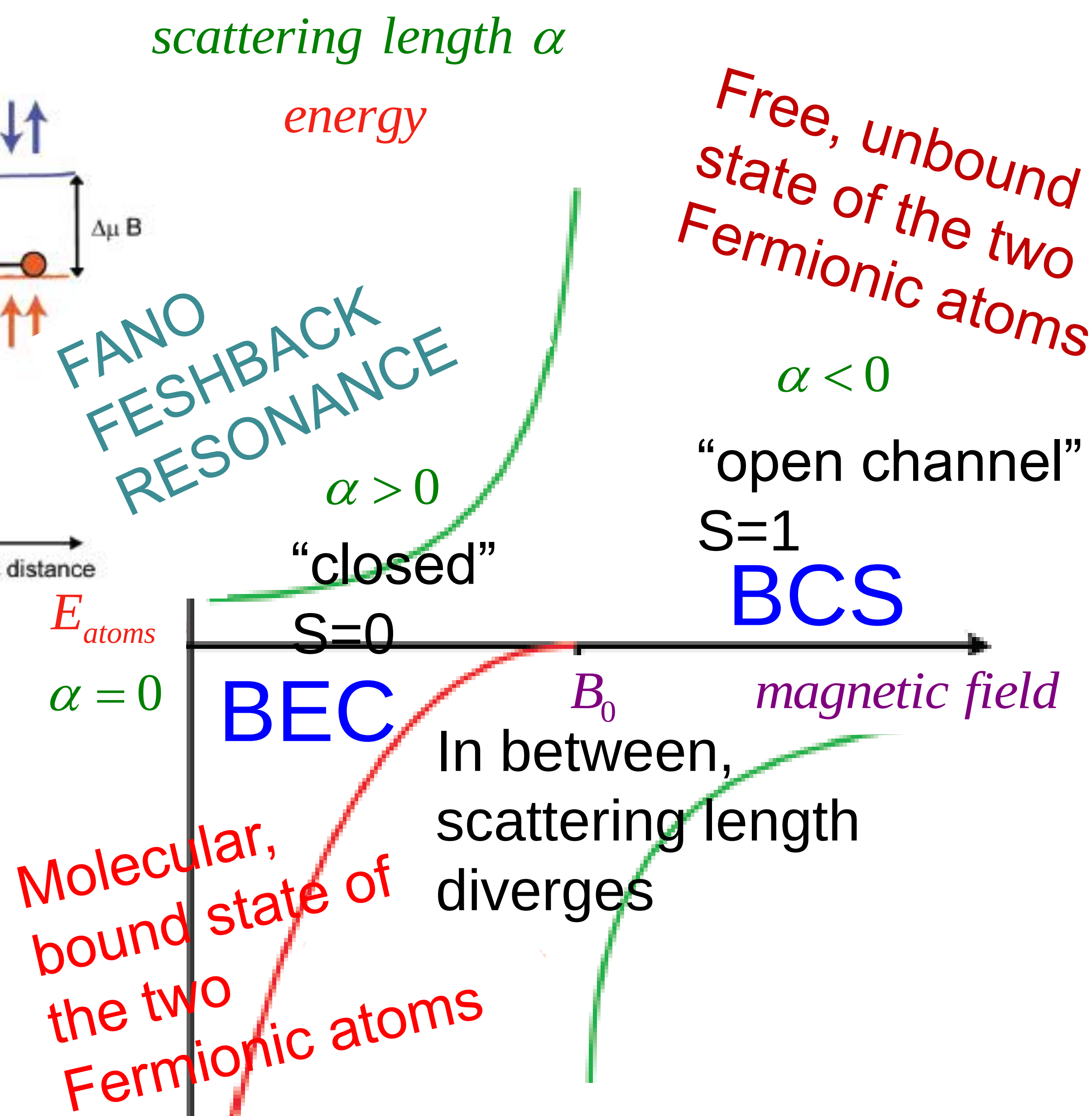
$\alpha < 0 \quad \mapsto \quad$ attractive interaction

Application: Bose Einstein Condensation of Fermionic atoms

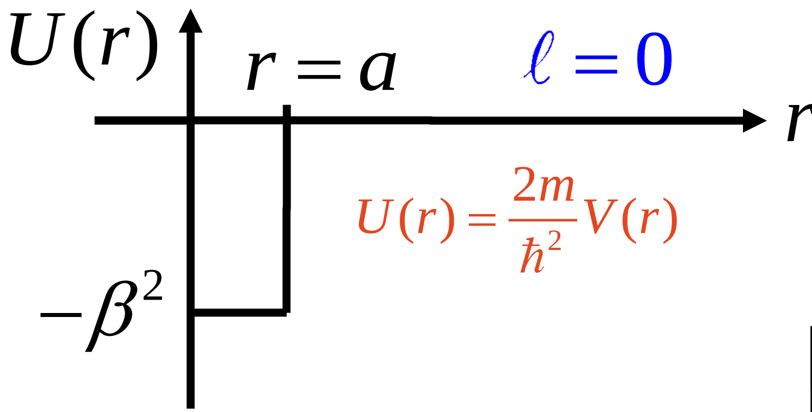

Energy
Bound State
Δμ B
Interatomic distance
BEC
Molecular, bound state of the two Fermionic atoms
BCS
Free, unbound state of the two Fermionic atoms



Ultracold, low energy s-wave scattering of two Fermionic atoms



"EFFECTIVE RANGE"



$$U(r) = \frac{2m}{\hbar^2} V(r)$$

$$U(r) = -\beta^2 \text{ for } r < a$$
$$= 0 \text{ for } r > a$$

$$\frac{2mE}{\hbar^2} = k^2 > 0$$

$$u_{\varepsilon,l}(r) = r\mathrm{R}_{\varepsilon,l}(r)$$

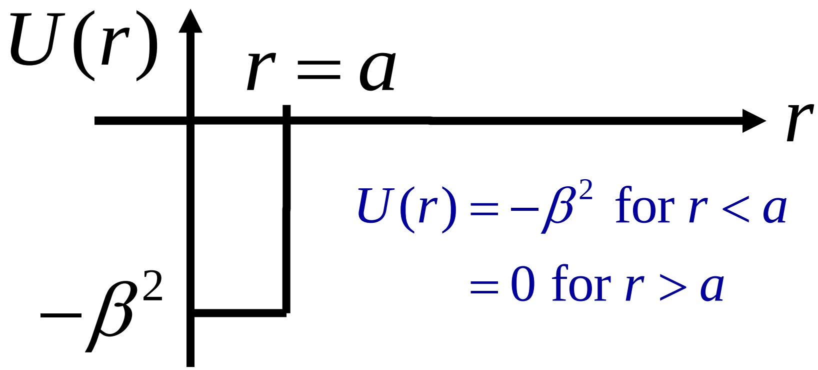
$$\left[\frac{d^2}{dr^2} + k^2 - U(r)\right] u_{\varepsilon,l=0}(r) = 0$$

$$@\,E = E_1 = \frac{\hbar^2 k_1^2}{2m}, \quad \text{the solution is } u_1(k_1, r)$$

$$@\,E = E_2 = \frac{\hbar^2 k_2^2}{2m}, \quad \text{the solution is } u_2(k_2, r)$$

$$u_1'' + k_1^2 u_1 - U(r) u_1 = 0$$
$$u_2'' + k_2^2 u_2 - U(r) u_2 = 0$$

$$u_2 u_1'' + k_1^2 u_1 u_2 - U(r) u_1 u_2 = 0$$
$$u_1 u_2'' + k_2^2 u_2 u_1 - U(r) u_2 u_1 = 0$$



$$U(r) = -\beta^2 \text{ for } r < a$$
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$$\frac{2mE}{\hbar^2} = k^2 > 0$$

$$u_{\varepsilon,l}(r) = r\mathrm{R}_{\varepsilon,l}(r)$$

$$u_2 u_1'' + k_1^2 u_1 u_2 - U(r) u_1 u_2 = 0$$
$$u_1 u_2'' + k_2^2 u_2 u_1 - U(r) u_2 u_1 = 0$$

$$u_2 u_1'' - u_1 u_2'' + \left(k_1^2 - k_2^2\right) u_1 u_2 = 0$$

$$\left[\left(u_2 u_1'\right)\Big|_0^R - \int_0^R u_2' u_1' dr \right] - \left[\left(u_1 u_2'\right)\Big|_0^R - \int_0^R u_1' u_2' dr \right] + \left(k_1^2 - k_2^2\right) \int_0^R u_1 u_2 dr = 0$$

$$\left[u_2(r) u_1'(r) - u_1(r) u_2'(r)\right]\Big|_0^R = \left(k_2^2 - k_1^2\right) \int_0^R u_1 u_2 dr$$

If $R \to \infty$

'orthogonality'

$$u_1(r=0) = 0$$
$$u_2(r=0) = 0$$

$$u_2(R) u_1'(R) - u_1(R) u_2'(R) = \left(k_2^2 - k_1^2\right) \int_0^R u_1 u_2 dr$$

$$U(r) = -\beta^2 \text{ for } r < a$$
$$= 0 \text{ for } r > a$$

$$u_{\varepsilon,l}(r) = r\mathrm{R}_{\varepsilon,l}(r)$$

$$u_2(R)u_1'(R) - u_1(R)u_2'(R) = -\left(k_1^2 - k_2^2\right)\int_0^R u_1 u_2 dr$$

Introduce functions $\psi_1(k_1, r)$ and $\psi_2(k_2, r)$ as REFERENCE funtions for comparison such that

$$u_1(k_1, r \to \infty) = \psi_1(k_1, r)$$
$$u_2(k_2, r \to \infty) = \psi_2(k_2, r)$$

$\psi_1(k_1, r)$ and $\psi_2(k_2, r)$ describe the asymptotic $r \to \infty$ behavior of $u_1(k_1, r)$ and $u_2(k_2, r)$.

Choice of normalization

$$\psi_1(k_1, r) = u_1(k_1, r \to \infty) = A_1 \sin\left(k_1 r - \delta_0\left(k_1\right)\right) = \frac{1}{\sin\left(\delta_0\left(k_1\right)\right)} \sin\left(k_1 r - \delta_0\left(k_1\right)\right)$$

$$\psi_2(k_2, r) = u_2(k_2, r \to \infty) = A_2 \sin\left(k_2 r - \delta_0\left(k_2\right)\right) = \frac{1}{\sin\left(\delta_0\left(k_2\right)\right)} \sin\left(k_2 r - \delta_0\left(k_2\right)\right)$$

$$\psi_{1,2}(k_1, r = 0) = 1$$

$$\left[u_2(r)u_1'(r) - u_1(r)u_2'(r)\right]\Big|_0^R = \left(k_2^2 - k_1^2\right)\int_0^R u_1 u_2 dr$$ Eq.1

$u_1(r=0)=0$

$u_2(r=0)=0$

$$\Rightarrow u_2(R)u_1'(R) - u_1(R)u_2'(R) = \left(k_2^2 - k_1^2\right)\int_0^R u_1 u_2 dr$$ Eq.2

$$\left[\psi_2(r)\psi_1'(r) - \psi_1(r)\psi_2'(r)\right]\Big|_0^R = \left(k_2^2 - k_1^2\right)\int_0^R \psi_1 \psi_2 dr$$ Eq.3

Eq.4

$$\left[\psi_2(R)\psi_1'(R) - \psi_1(R)\psi_2'(R)\right] - \left[\psi_2(0)\psi_1'(0) - \psi_1(0)\psi_2'(0)\right] = \left(k_2^2 - k_1^2\right)\int_0^R \psi_1 \psi_2 dr$$

$$\psi_{1,2}(k_1, r=0) = 1$$ Eq.5

$$\left[\psi_2(R)\psi_1'(R) - \psi_1(R)\psi_2'(R)\right] - \left[\psi_1'(0) - \psi_2'(0)\right] = \left(k_2^2 - k_1^2\right)\int_0^R \psi_1 \psi_2 dr$$ Eq.6

Subtract Eq.2 from 6

$$u_2(R)u_1'(R) - u_1(R)u_2'(R) = \left(k_2^2 - k_1^2\right)\int_0^R u_1 u_2 \, dr$$ Eq.2

$$\left[\psi_2(R)\psi_1'(R) - \psi_1(R)\psi_2'(R)\right] - \left[\psi_1'(0) - \psi_2'(0)\right] = \left(k_2^2 - k_1^2\right)\int_0^R \psi_1 \psi_2 \, dr$$ Eq.6

Subtract Eq.2 from 6

$$\psi_2'(0) - \psi_1'(0) = \left(k_2^2 - k_1^2\right)\int_0^R \left(\psi_1\psi_2 - u_1 u_2\right) dr$$

$$\psi_1(k_1, r) = \frac{1}{\sin\left(\delta_0\left(k_1\right)\right)} \sin\left(k_1 r - \delta_0\left(k_1\right)\right)$$

$$\psi_2(k_2, r) = \frac{1}{\sin\left(\delta_0\left(k_2\right)\right)} \sin\left(k_2 r - \delta_0\left(k_2\right)\right)$$

This equation is 'exact'.

$$\psi_1'(k_1, r)\Big|_{r=0} = \left[\frac{k_1}{\sin\left(\delta_0\left(k_1\right)\right)} \cos\left(k_1 r - \delta_0\left(k_1\right)\right)\right]\Bigg|_{r=0} = k_1 \cot\left(\delta_0\left(k_1\right)\right)$$

$$\psi_2'(k_2, r)\Big|_{r=0} = \left[\frac{1}{\sin\left(\delta_0\left(k_2\right)\right)} \sin\left(k_2 r - \delta_0\left(k_2\right)\right)\right]\Bigg|_{r=0} = k_2 \cot\left(\delta_0\left(k_2\right)\right)$$

$$k_2 \cot\left(\delta_0\left(k_2\right)\right) - k_1 \cot\left(\delta_0\left(k_1\right)\right) = \left(k_2^2 - k_1^2\right)\int_0^R \left(\psi_1\psi_2 - u_1 u_2\right) dr$$

consider now

$\lim R \rightarrow \infty$

$$k_2 \cot\left(\delta_0\left(k_2\right)\right) - k_1 \cot\left(\delta_0\left(k_1\right)\right) = \left(k_2^2 - k_1^2\right)\int_0^\infty \left(\psi_1(r,k_1)\psi_2(r,k_2) - u_1(r,k_1)u_2(r,k_2)\right)dr$$

define ρ:

$$\frac{1}{2}\rho(E_1,E_2) = \int_0^\infty \left(\psi_1(r,k_1)\psi_2(r,k_2) - u_1(r,k_1)u_2(r,k_2)\right)dr$$

$$k_2 \cot\left(\delta_0\left(k_2\right)\right) = k_1 \cot\left(\delta_0\left(k_1\right)\right) + \left(k_2^2 - k_1^2\right)\frac{1}{2}\rho(E_1,E_2)$$

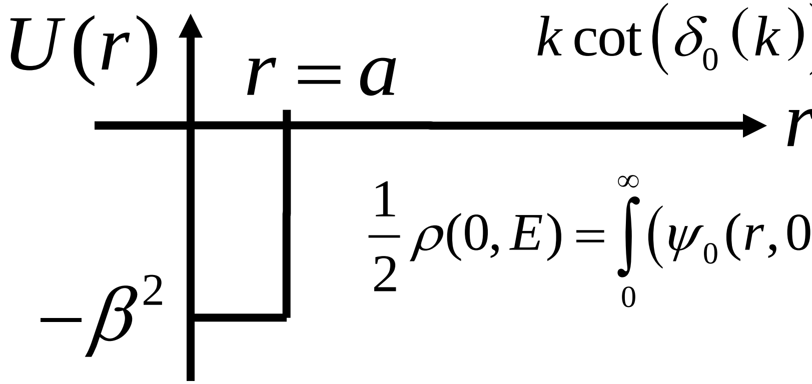
$\lim k \to 0$ scattering length (Fermi & Marshall)

$$\alpha = -\lim_{k\to 0} \frac{\tan\delta_0\left(k\right)}{k} \quad \text{i.e.} \quad -\frac{1}{\alpha} = \lim_{k\to 0} k\cot\delta_0\left(k\right)$$

$$k\cot\left(\delta_0\left(k\right)\right) = -\frac{1}{\alpha} + \frac{\rho(0,E)}{2}k^2 + O(k^4)$$

$$\frac{1}{2}\rho(0,E) = \int_0^\infty \left(\psi_0(r,0)\psi_E(r,E) - u_0(r,0)u_E(r,E)\right)dr$$

Caution! Our notation employs a symbol for scattering length that Bethe has used for its inverse!



$$k\cot\left(\delta_0(k)\right) = -\frac{1}{\alpha} + \frac{\rho(0,E)}{2}k^2 + O(k^4)$$

$$\frac{1}{2}\rho(0,E) = \int_0^\infty \left(\psi_0(r,0)\psi_E(r,E) - u_0(r,0)u_E(r,E)\right)dr$$

$$\psi_1(k_1,r) = u_1(k_1, r\to\infty) = \frac{1}{\sin\left(\delta_0(k_1)\right)}\sin\left(k_1 r - \delta_0(k_1)\right)$$

$$\psi_2(k_2,r) = u_2(k_2, r\to\infty) = \frac{1}{\sin\left(\delta_0(k_2)\right)}\sin\left(k_2 r - \delta_0(k_2)\right)$$

ψ's and u's differ only in the range of the scattering potential.

$$\left(\psi_0(r,0)\psi_E(r,E) - u_0(r,0)u_E(r,E)\right) \not\approx 0$$

ONLY in the *small r* region of the scattering potential.

In *small-r* region, wave-functions are (*nearly*) INDEPENDENT of energy.

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

$small - r$

$k^2 \ll |U(r)|$

In *small-r* region, wave-functions are (*nearly*) INDEPENDENT of energy.

$$small-r$$

$$k^2 \ll |U(r)|$$

$$\left(\psi_0(r,0)\psi_E(r,E)-u_0(r,0)u_E(r,E)\right)\approx\psi_0(r,E=0)^2-u_0(r,E=0)^2$$

in the *small r* region

Short range atomic properties are (*nearly*) INDEPENDENT of energy.

$$\frac{1}{2}\rho(0,E)\approx\frac{1}{2}\rho(0,0)=\frac{1}{2}r_0=\int_0^\infty\left[\psi_0(r,E=0)^2-u_0(r,E=0)^2\right]dr$$

$\rho(0,0)$: *effective range* of the potential

$\rightarrow$ independent of energy

$$k\cot\left(\delta_0(k)\right)\underset{k\rightarrow 0}{=}-\frac{1}{\alpha}+\frac{r_0}{2}k^2+O(k^4)$$

Caution! Our notation employs a symbol for scattering length that Bethe has used for its inverse!

$$k\cot\left(\delta_0(k)\right) \underset{k\to 0}{=} \frac{-1}{\alpha}+\frac{r_0}{2}k^2 \qquad\qquad \cot\left(\delta_0(k)\right) \underset{k\to 0}{=} \frac{-1}{k\alpha}+\frac{r_0}{2}k$$

$$a_0(k)=\frac{\left[S_0(k)-1\right]}{2ik}=\frac{\cos\left(2\delta_0\right)+i\sin\left(2\delta_0\right)-1}{2ik}$$

$$=\frac{\cos\left(2\delta_0\right)+i2\sin\left(\delta_0\right)\cos\left(\delta_0\right)-1}{2ik}\simeq\frac{\sin\left(\delta_0\right)}{k}$$

Partial wave amplitude

$$\Rightarrow\left|f_{k\to 0}(\theta)\right|^2=\frac{\sin^2\delta_0}{k^2}\simeq\frac{\tan^2\delta_0}{k^2}$$

$$\Rightarrow\sigma=4\pi\frac{\sin^2\delta_0}{k^2}\simeq 4\pi\frac{\sin^2\delta_0}{k^2\left(\sin^2\delta_0+\cos^2\delta_0\right)}=4\pi\frac{1}{\left(k^2+k^2\cot^2\delta_0\right)}$$

$$\cot\left(\delta_0(k)\right) \underset{k\to 0}{=} \frac{-1}{k\alpha} + \frac{r_0}{2}k \quad \text{and} \quad \sigma = \frac{4\pi}{k^2\left(1+\cot^2\delta_0\right)}$$

$$\Rightarrow \sigma = \frac{4\pi}{\left(k^2 + k^2\left(\frac{-1}{k\alpha} + \frac{r_0}{2}k\right)^2\right)} \qquad \Rightarrow \sigma = \frac{4\pi}{\left(k^2 + k^2\left(\frac{-2+\alpha r_0 k^2}{2k\alpha}\right)^2\right)}$$

$$\Rightarrow \sigma = \frac{4\pi}{\left(k^2 + \left(\frac{4-4\alpha r_0 k^2 + \alpha^2 r_0^2 k^4}{4\alpha^2}\right)\right)} = \frac{4\pi}{\left(\frac{4k^2\alpha^2 + 4 - 4\alpha r_0 k^2 + \alpha^2 r_0^2 k^4}{4\alpha^2}\right)}$$

$$\Rightarrow \sigma = \frac{4\pi}{k^2 + \alpha^{-2} - k^2\alpha^{-1}r_0 + \frac{1}{4}r_0^2 k^4}$$

Bethe's α is inverse of the scattering length

$$\Rightarrow \sigma = \frac{4\pi\alpha^2}{1 + k^2\alpha\left(\alpha - r_0\right) + \left(\frac{1}{2}\alpha r_0\right)^2 k^4}$$

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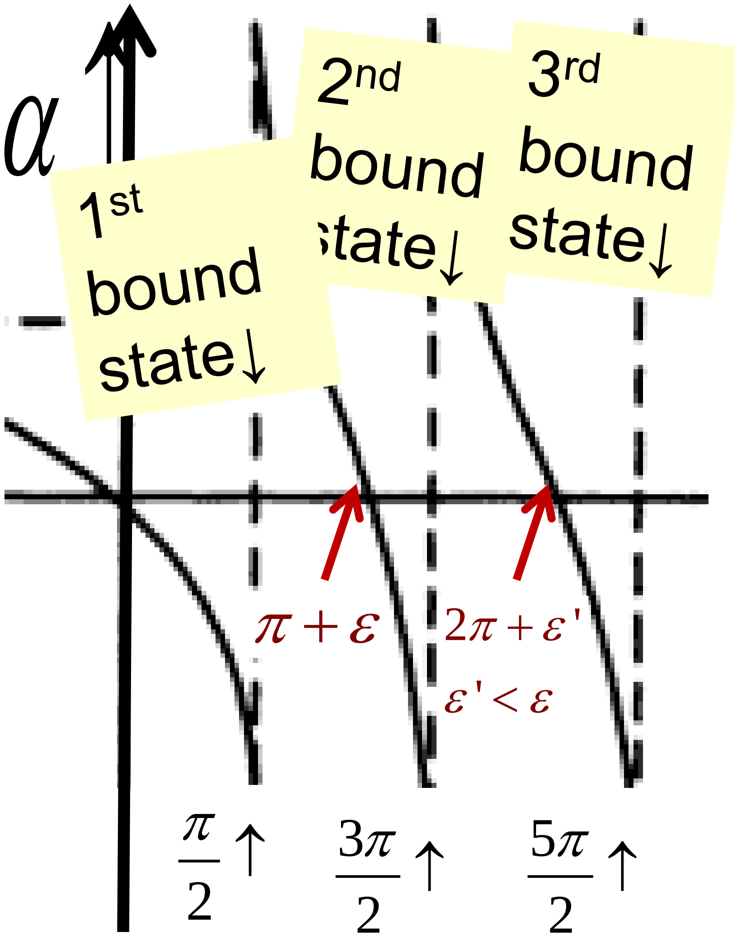
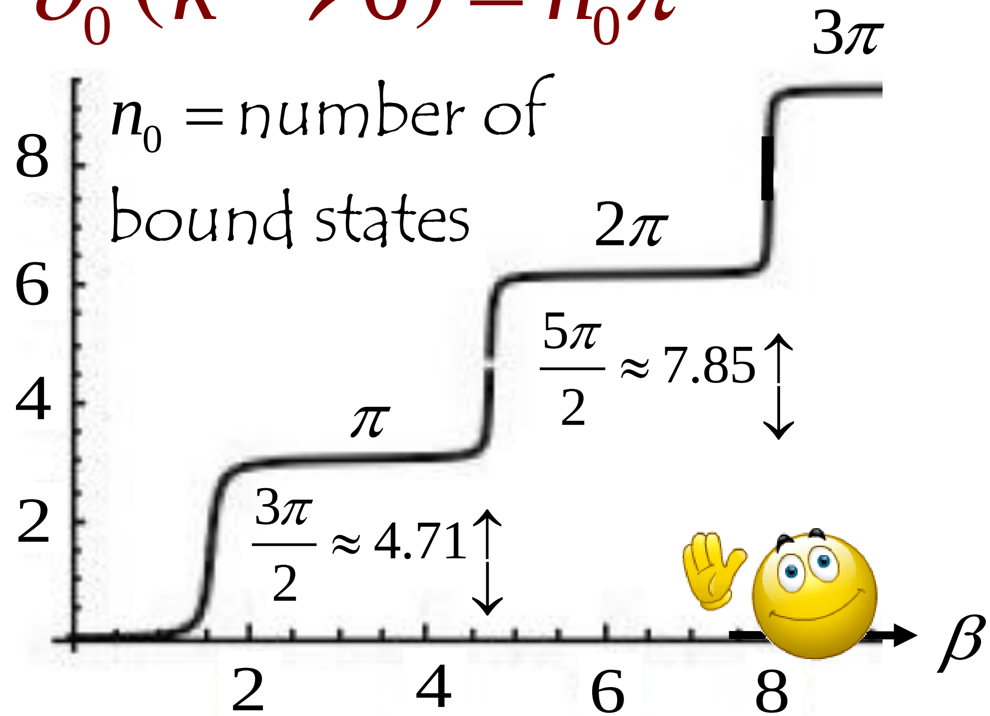
$$\delta_0(k \to 0) = n_0 \pi$$





$\frac{\pi}{2} \approx 1.57 \uparrow$ $\quad \delta_0(k \to 0) = n_0 \pi$

or $\delta_0(k \to 0) = \left(n_0 + \frac{1}{2}\right)$

$$k \cot(\delta_0(k)) \underset{k \to 0}{=} -\frac{1}{\alpha} + \frac{r_0}{2} k^2 + O(k^4)$$

$l \geq 1$:

$\delta_l(k \to 0) = n_l \pi$

QUESTIONS ? Write to: pcd@physics.iitm.ac.in