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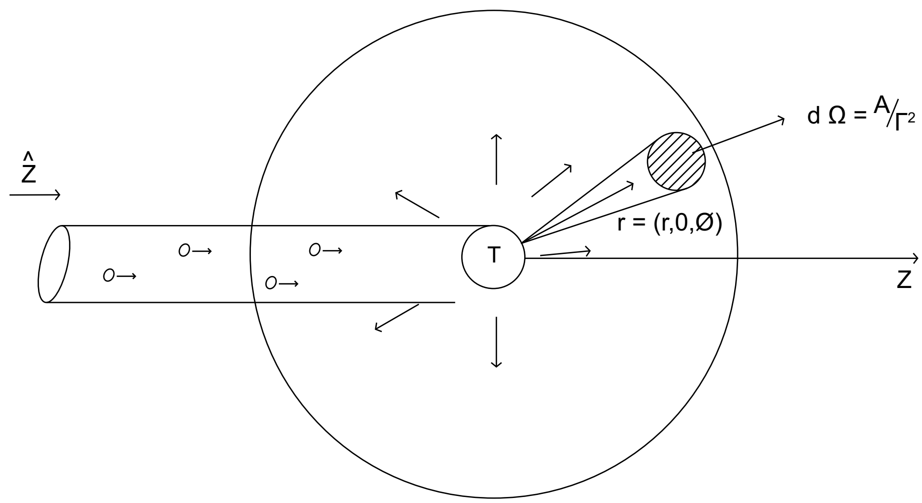
COLLISION THEORY (QUANTUM SCATTERING)

Consider target T
A flux, J_{inc} of particles is incident on T.
$J_{\text{inc}} \equiv$ Number of particles/Time/Unit area arriving at T



** NB typo in figure: should be $\underline{r} = (r, \theta, \phi)$.

$N(\theta, \phi) \equiv$ Number of particles scattered into direction $\hat{r} = (\theta, \phi)$ per unit time.

N_D = Number of particles collected by a detector which subtends solid angle $d\Omega$ (per time)

then

$$N_D = N(\theta, \phi) d\Omega \tag{5.1}$$

Clearly,

$$N(\theta, \phi) d\Omega \propto J_{\text{inc}}, \tag{5.2}$$

$$\Rightarrow N(\theta, \phi) d\Omega = \underbrace{d\sigma(\theta, \phi)}_{\text{the constant of proportionality}} J_{\text{inc}}$$

we write: number of particles scattered into given direction,

$$N(\theta, \phi) = \frac{d\sigma}{d\Omega} J_{\text{inc}} \tag{5.3}$$

We define

$$\frac{d\sigma}{d\Omega}(\theta, \phi) \equiv \frac{d\sigma}{d\Omega} \equiv \text{DIFFERENTIAL CROSS SECTION.}$$

It has units of AREA/STERADIAN.

Then, *total* cross section

$$\sigma_T = \int \frac{d\sigma}{d\Omega} d\Omega = \int_0^{2\pi} d\phi \int_o^{\pi} \sin\theta d\theta \frac{d\sigma}{d\Omega}(\theta, \phi) \tag{5.4}$$

QUANTUM SCATTERING

The flux is obtained from the current flux operator

$$\begin{aligned} \hat{j} &= \frac{\hbar}{2mi}(\psi^* \nabla \psi - \nabla \psi^* \cdot \psi) \\ &= \text{Re}\left(\psi^* \frac{h}{mi} \nabla \psi\right) \end{aligned} \tag{5.5}$$

The *incoming beam* is described by a plane wave $e^{i\underline{k}\cdot\underline{r}} = e^{ikz}$ if the beam lies along $\hat{z}$ axis

$\psi(r) = Ae^{i\underline{k}\cdot\underline{r}}$ is the solution to free particle TISE:

$$(\nabla^2 + k^2)\psi(r) = 0 \tag{5.6}$$

Then,

$$\begin{aligned} j &= \text{Re}\left(A^* e^{-i\underline{k}\cdot\underline{r}} \frac{\hbar}{mi} \nabla A e^{i\underline{k}\cdot\underline{r}}\right) \\ &= |A|^2 \text{Re}\left(e^{-i\underline{k}\cdot\underline{r}} \frac{i\hbar k}{mi} e^{i\underline{k}\cdot\underline{r}}\right) \\ &= |A|^2 \frac{\hbar \underline{k}}{m} \end{aligned} \tag{5.7}$$

In the scattering problem:
$r \sim 0$ implies the collisional region
$r \sim \infty \Rightarrow$ represents the region far from the collision.

Far from the collision, the scattered particles are indicated by a *spherical wave* which implies an outward radial flux of particles.

Quantum cross section: FINITE RANGED POTENTIAL

We assume that $V(r) \to 0$ as $r \to \infty$ (excludes coulomb potential)

In the large r region, $\psi(\underline{r})$ describes both the incident and scattered waves

$$\psi(\underline{r}) \underset{r\to\infty}{\longrightarrow} \psi_{inc}(\underline{r}) + \psi_{sc}(\underline{r}) \tag{5.8}$$

$$\to \underbrace{e^{i\underline{k}\cdot\underline{r}}}_{\text{incoming plane wave}} + \psi_{sc}(\underline{r})$$

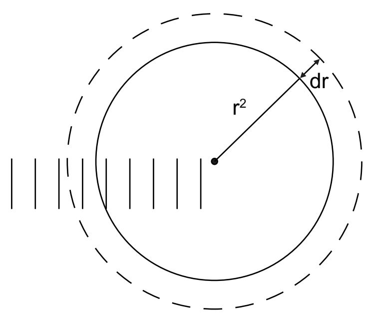
$$e^{i\underline{k}\cdot\underline{r}} = e^{ikz} \tag{5.9}$$

If incident beam lies along z axis.

The scattered wave gives an outward radial flux of particles. For elastic scattering, k is constant (before and after collision)

$$\left.\psi_{sc}(r) = \underset{\substack{\text{probability}\\ \text{amplitude in each}\\ \text{direction}}}{f(\theta,\phi)}\frac{e^{ikr}}{r}\right\} \text{ spherical wave} \tag{5.10}$$

SPHERICAL WAVE: TAKE SPHERICAL SHELL, RADIUS r



Volume = $4\pi r^2\,dr = d\tau$.

Probability of finding particles in shell

$$\left.|\psi(r)|^2\,d\tau = \left|\frac{e^{ikr}}{r}\right|^2 \cdot 4\pi r^2\,dr\right\} \text{ independent of } r$$

An expanding ‘shell’ of particles moves with constant velocity

$$\frac{\hbar k}{m} = \frac{p}{m}$$

k is constant.

We can show (5.9) & (5.10) solve the Schrodinger asymptotically, eq for $r \to \infty$ solve $(\hat{H} - E)\psi = 0$

$$\Rightarrow \left[\nabla^2 + k^2 - \frac{2m}{\hbar^2}V(r)\right]\left\{\underbrace{e^{i\underline{k}\cdot\underline{r}}}_{(1)} + \underbrace{f(\theta,\phi)}_{(2)}\frac{e^{ikr}}{r}\right\} = 0 \tag{5.11}$$

Consider first *Term* (1):

$$\{\nabla^2 + k^2\}e^{ik\cdot r} = 0$$

this leaves only (faster than $\frac{1}{r}$).

$$\frac{-2mV(r)}{\hbar^2}e^{i\underline{k}\cdot\underline{r}}$$

But $V(r) \to 0$ as $r \to \infty$ so this vanishes.

NOW CONSIDER *Term* (2):

Also, as in (1), the

$$\frac{-2mV(r)}{\hbar^2}\,f(\theta,\phi)\frac{e^{ikr}}{r} \to 0 \text{ since } V(r) \to 0$$

This leaves us to show only that:

$$\{\nabla^2 + k^2\}f(\theta,\phi)\frac{e^{ikr}}{r} = 0 \tag{5.12}$$

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{L(\theta,\phi)}{r^2}$$

where $L(\theta,\phi)$ has $\frac{\partial}{\partial\theta}$, $\frac{\partial}{\partial\phi}$ terms, and is function of ϕ, θ only. So,

$$\{L(\theta,\phi)f(\theta,\phi)\}\frac{1}{r^2}\frac{e^{ikr}}{r} \sim O(\frac{1}{r^3}) \to 0 \quad \text{as } r \to \infty$$

The radial part of ∇^2

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)f(\theta,\phi)\cdot\frac{e^{ikr}}{r} = f(\theta,\phi)\cdot\frac{1}{r^2}\frac{\partial}{\partial r}[ikr-1]e^{ikr}$$

$$= \frac{f}{r^2}[ik - k^2r - ik]e^{ikr} = -\frac{k^2e^{ikr}}{r} \tag{5.13}$$

back to (5.12)

$$\{\nabla^2 + k^2\}f(\theta,\phi)\frac{e^{ikr}}{r} = f\left[-\frac{k^2e^{ikr}}{r} + \frac{k^2e^{ikr}}{r}\right] = 0$$

So, $e^{i\underline{k}\cdot\underline{r}} + f\frac{e^{ikr}}{r}$ is asymptotic solution of T·I·S·E·

Now we derive (important) relation between $f(\theta, \phi)$ and the collisional cross section σ.

We calculate the flux for ψ_{inc}, ψ_{sc}

$$\begin{aligned} \hat{j} &= \text{Re}\left(\Psi^* \frac{\hbar}{mi} \nabla \Psi\right) \qquad (5.14) \\ \nabla &= \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial \phi} \end{aligned}$$

so

$$\begin{aligned} \hat{j} &= \text{Re}\left(\psi^*_{inc}\frac{\hbar\nabla}{mi}\psi_{inc}\right) + \text{Re}\left(\psi^*_{sc}\frac{\hbar\nabla}{mi}\psi_{sc}\right) \\ &\quad + \text{interference term between } \psi_{inc},\ \psi_{sc}. \end{aligned}$$

$$\hat{j} = j_{inc} + j_{sc} + j_{int}.$$

$$j_{inc} = \text{Re}\left[e^{-ik\cdot r}\frac{\hbar}{mi} i\underline{k} e^{i\underline{k}\cdot\underline{r}}\right] = \frac{\hbar k}{m} \qquad (5.15)$$

Now

$$\nabla\psi_{sc} = \overset{(1)}{\frac{e^{ikr}}{r}\nabla f(\theta,\phi)} + \overset{(2)}{f(\theta,\phi)e^{ikr}\nabla\left(\frac{1}{r}\right)} + \overset{(3)}{\frac{f(\theta,\phi)}{r}\nabla e^{ikr}}.$$

(1) $\nabla f(\theta, \phi)$ involves only $\hat{\theta}, \hat{\phi}$ terms in (5.14). These are of form $\frac{L(\theta,\phi)}{r}$. Hence as a 'short cut' we can see that

$$\frac{e^{ikr}}{r}\nabla f(\theta,\phi) \sim O\left(\frac{1}{r^2}\right),$$

which, as $r \to \infty$ is small.

(2) $f(\theta, \phi)e^{ikr}\nabla\left(\frac{1}{r}\right) \sim O\left(\frac{1}{r^2}\right)$
since

$$\nabla\left(\frac{1}{r}\right) = -\frac{1}{r^2}\hat{r}.$$

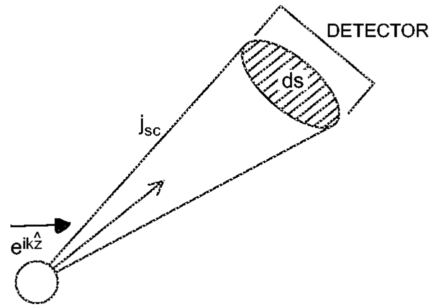
(3) $\frac{f(\theta,\phi)}{r}\nabla e^{ikr} = ik\hat{r}\psi_{sc} \sim O\left(\frac{1}{r}\right)$

HENCE, at large r, (3) is the dominant contribution.

Hence, using term (3) only,

$$j_{sc} = \text{Re}\left(\psi^*_{sc}\frac{\hbar}{mi}ik\hat{r}\psi_{sc}\right) = \frac{\hbar k}{m}\frac{|f(\theta,\phi)|^2}{r^2}\hat{r} \to A \text{ radial fiux.} \qquad (5.16)$$

j_{int}, has a complicated form. Fortunately it is negligible away from the forward direction k. We ignore it for the moment (but return to it later in Eq. 5.46)



j_{sc} represents the number of particles crossing unit area per unit time.
The detector presents area $dS = r^2\,d\Omega$.
The number of particles entering solid angle $d\Omega$ per unit time:

$$N(\theta,\phi)d\Omega = j_{sc}\cdot dS = \frac{\hbar k}{m}|f(\theta,\phi)|^2\,d\Omega \tag{5.17}$$

From (5.3)

$$J_{inc}\,\frac{d\sigma}{d\Omega}(\theta,\phi) = \frac{\hbar k}{m}|f(\theta,\phi)|^2$$

But, since $J_{inc} = \frac{\hbar k}{m}$,

$$\Rightarrow \frac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2 \tag{5.18}$$

The relation between the *differential cross section* and the quantum *scattering amplitude*.

The total cross section,

$$\sigma = \int \frac{d\sigma}{d\Omega}\,d\Omega$$

$$\sigma_{TOT} = \int |f(\theta,\phi)|^2\,d\Omega \quad d\Omega = \sin\theta d\theta d\phi \;\text{ in sphericalpolars.} \tag{5.19}$$

SCATTERING BY A CENTRAL POTENTIAL—METHOD OF PARTIAL WAVES

$$V(r) \equiv V(\underline{r})$$

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(r) \tag{5.20}$$

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{\hat{L}^2}{\hbar^2 r^2}$$

$\hat{L}^2$ has only θ, ϕ dependence of $\hat{H}$.

Recall that for hydrogen atom:

$$[H, \hat{L}^2] = [H, \hat{L}_z] = 0 \tag{5.21}$$

Here, with the central potential, as for the H-atom with $V(r) = -\frac{1}{r}$, we can find simultaneous eigenfunctions of $\hat{H}$, $\hat{L}^2$, $\hat{L}_z$.
We can look for solutions of the form:

$$\psi_{\text{Elm}}(\underline{r}) = R_{\text{Elm}}(r)Y_{\ell m}(\theta, \phi) \tag{5.22}$$

But don't want *BOUND STATES* necessarily: IF $E > 0$, then E is not quantised. By the same procedure we employed in eg (the 2nd year course PH2222 at UCL) we can reduce the full 3-D problem to 1D radial equation (plus another for the spherical harmonics):

$$\left\{-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{l(l+1)\hbar^2}{2mr^2} + V(r)\right\} R_{El}(r) = ER_{El}(r) \tag{5.23}$$

(from $\hat{L}^2 Y_{\ell m} = l(l+1)\hbar^2 Y_{\ell m}$)

$$\frac{l(l+1)h^2}{2mr^2} \equiv \text{repulsive centrifugal barrier term.}$$

multiply by $\frac{2m}{\hbar^2}$, differentiate [ ] becomes:

$$\left\{\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} - U(r) + k^2\right\} R_{El}(r) = 0 \tag{5.24}$$

FREE PARTICLE SOLUTIONS

:

A very useful mathematical property is that spherical waves can be expressed as a superposition of plane waves : the '*PARTIAL WAVES'*.

This forms a useful 'basis' for solutions of atomic scattering problems.

Consider the radial eq with $V(r) = 0$

$$\left\{ \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + k^2 \right\} R_{kl}(r) = 0 \tag{5.25}$$

Change variable to $\rho = kr$

$$= \left\{ \frac{d^2}{d\rho^2} + \frac{2}{\rho}\frac{d}{d\rho} - \frac{l(l+1)}{\rho^2} + 1 \right\} R_l(\rho) = 0 \tag{5.26}$$

This 2nd order differential equation has known solutions:

1) *regular*: Spherical Bessel function $j_l(\rho)$
$j_l(\rho)$ remain finite as $\rho \to 0$.

ASYMPTOTICALLY,

$$\underset{r\to\infty}{j_\ell}(\rho) \to \sin\left(\rho - \frac{l\pi}{2}\right) \Big/ \rho \tag{5.27}$$

2) *irregular*: Spherical Neumann functions $\eta_l(\rho)$

But $\eta_l(\rho) \to \infty$ as $\rho \to 0$.
ASYMPTOTICALLY, (ie for large r ie $\rho \to \infty$):

$$\eta_l(\rho) \to -\frac{1}{\rho}\cos\left(\rho - \frac{l\pi}{2}\right) \tag{5.28}$$

The only physically acceptable solution is $j_\rho(\rho)$.

Hence, $R_{lE}(r) = c j_l(kr)$
The 3D solution

$$\psi_{\mathrm{Elm}}(r) = C j_\ell(kr)\; Y_{\ell m}(\theta, \phi) \tag{5.29}$$

But we know that the solution for a free particle in 3D is also the 3D plane wave

$$e^{i\underline{k}\cdot\underline{r}} = e^{i(k_x\cdot x + k_y\cdot y + k_z\cdot z)}$$

Both spherical AS WELL AS plane waves form a complete set and any solution can be expressed as a superposition of them. eg

The plane wave:

$$e^{i\underline{k}\cdot\underline{r}} = \sum_{l=0}^{\infty}\sum_{m=-\ell}^{+\ell} a_{lm}\ j_\ell(kr)\ Y_{\ell m}(\theta,\phi) \tag{5.30}$$

The a_{lm} are probability amplitudes (constant coeffs) for a given Elm.
If $k \equiv k\hat{z}$, 1D plane wave $\underline{k}\cdot\underline{r} \equiv kr\cos\theta = kz$

$$e^{ikz} = \sum_{l=0}^{\infty} a_\ell j_\ell(kr)\ P_\ell(\cos\theta) \tag{5.31}$$

From orthogonality of the Legendre polynomials, $P_\ell(\cos\theta)$ it can be shown that

$$a_\ell = (2l+1)\ i^\ell. \tag{5.32}$$

$*$ Note that plane wave *along* $\hat{z}$, has no component of L *about* z (ie $m=0, L_z = 0$).

(Note that if $E < 0$ H atom solns at large $r \sim e^{\frac{-r}{n}}$: we have bound states not plane, spherical waves)

For large r,

$$e^{ikz} \underset{r\to\infty}{\longrightarrow} \sum_{l=0}^{\infty}(2l+1)i^l \frac{\sin(kr-\frac{l\pi}{2})}{kr} P_\ell(\cos\theta) \tag{5.33}$$

The plane wave $\frac{\sin(kr-\frac{l\pi}{2})}{kr}$ is a superposition of:

$$\frac{1}{2i}\left[\underbrace{\frac{e^{i(kr-\frac{\ell\pi}{2})}}{kr}}_{\text{outgoing spherical waves}} - \underbrace{\frac{e^{-i(kr-\frac{\ell\pi}{2})}}{kr}}_{\text{incoming spherical waves converging on origin}}\right]$$

Now, we consider the effect of the central potential, $U(r)$ in (5.24). Since $U(r)$ is a central potential, it does not couple different angular momenta (ie does not re-distribute probability amplitudes. This is *elastic scattering*.

Its effect will appear in the outgoing wave, as a scattering coefficient S_ℓ in each 'partial wave'.

ie we write

$$\psi(r) \underset{r\to\infty}{\longrightarrow} \frac{1}{2k}\sum_{l=0}^{\infty}(2l+1)i^{(l+1)}\left[\frac{e^{-i(kr-\frac{\ell\pi}{2})}}{r} - S_\ell\frac{e^{+i(kr-\frac{\ell\pi}{2})}}{r}\right]\cdot P_\ell(\cos\theta) \tag{5.34}$$

Conservation of flux means that incoming radial flux = outgoing radial flux.
It requires: $|S_\ell|^2 = 1$.
Hence S_ℓ represents at most a phase-shift (in the case of *elastic* scattering)

We write

$$S_\ell(k) = e^{2i\delta_e} \tag{5.35}$$

$\delta_e =$ elastic scattering phase shift for l-th partial wave.

The S_ℓ are related to the scattering amplitudes $f(\theta, \phi)$. The *total wave function* is given by (5.34). But compare with (5.10):

$$\psi_{TOT} \to e^{ikz} + f(\theta, \phi)\frac{e^{ikr}}{r}$$

so, for large r,

$$f(\theta, \phi)\frac{e^{ikr}}{r} = \psi_{TOT} - e^{ikz}$$

(where e^{ikz} is given by (5.33).

Subtracting (5.33)–(5.34) gives:

$$\frac{1}{2k}\sum_{l=0}^{\infty}(2l+1)i^{(l+1)}P_\ell(\cos\theta)\left\{\left[\frac{e}{r}^{-i(kr-\frac{\ell\pi}{2})} - S_\ell(k)\frac{e}{r}^{+i(kr-\frac{\ell\pi}{2})}\right] - \left[\frac{e}{r}^{-i(kr-\frac{\ell\pi}{2})} - \frac{e}{r}^{+i(kr-\frac{\ell\pi}{2})}\right]\right\}$$

using $i^l = e^{i\frac{\ell\pi}{2}}$,

$$\Rightarrow f(\theta, \phi)\frac{e^{ikr}}{r} = \frac{1}{2kr}\sum_{l=0}^{\infty}(2l+1)i[1 - S_\ell(k)]e^{ikr}P_\ell(\cos\theta) \tag{5.36a}$$

$$\Rightarrow f(\theta, \phi) = \sum_{l=0}^{\infty}(2\ell+1)\left[\frac{S_\ell(k) - 1}{2ik}\right]P_\ell(\cos\theta) \tag{5.36b}$$

(If $U(r) = 0$ we set all $S_\ell(k) = 1$.
ie if all $\delta_\ell(0)$ then the scattering amplitude $f = 0$.
which we may write:

$$f(\theta, \phi) = \sum_{l=0}^{\infty}(2l+1)f_\ell P_\ell(\cos\theta)$$

where

$$\left.f_\ell = \frac{S_\ell(k) - 1}{2ik}\right\} \text{ l-th partial wave scattering amplitude.} \tag{5.37}$$

From (5.19), $\sigma_{tot} = \int |f(\theta,\phi)|^2 d\Omega$

The total elastic cross section

$$\sigma_{el} = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta \cdot \frac{1}{4k^2} \sum_{l,l'} (2l+1)(2l'+1) \cdot (S_l^* - 1)(S_{l'} - 1) P_l(\cos\theta) P_{l'}(\cos\theta) \tag{5.38}$$

The ϕ integral, $\int_0^{2\pi} d\phi = 2\pi$.

The θ integral$\equiv$

$$\sum_{ll'} \cdots \int_0^{\pi} P_\ell(\cos\theta) P_{\ell'}(\cos\theta) \sin\theta d\theta$$

The Legendre polynomials are orthogonal polynomials and the integral = $\frac{2}{(2l+1)}\delta_{ll'}$

Hence

$$\sigma_{el} = \frac{2\pi}{4k^2} \sum_{l=0}^{\infty} 2(2l+1)|S_l - 1|^2 = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1)|S_l(k) - 1|^2 \tag{5.39}$$

Inelastic cross sections

In (5.33), we saw that a plane wave may be seen as a partial wave expansion of incoming and outgoing spherical waves

$$\frac{e^{\pm ikr}}{2kr}$$

Elastic scattering. de-phases these relative to each other$\Rightarrow$ net scattering wave. But no flux change.

The presence of the scatterer affects the outgoing spherical waves.

$$\frac{e}{r}^{+ikr} \rightarrow S_\ell \frac{e}{r}^{+ikr}$$

+ for elastic scattering $S_\ell = e^{2i\delta_\ell}, \Rightarrow |S_\ell| = 1$

For inelastic scattering

$$S_\ell = \eta_\ell(k)e^{2i\delta_\ell} \tag{5.40}$$

where, $0 < \eta_\ell < 1$

inelastic processes involve a loss of flux between the incoming spherical waves and the corresponding outgoing spherical waves

They can be due to eg

(1) inelastic collisions: internal states of the target are excited $K_{\text{initial}} \neq K_{\text{final}}$;

(2) particle capture

(3) particle decay

A more detailed solution of the schrödinger eg (for (1) or (2) or Q field theory) is needed to calculate precisely how much flux goes into each channel.

For the moment we just want to calculate the total flux loss between incoming/outgoing spherical waves.

We calculate the *integrated radial* flux associated with the incoming part in Eq.5.34:
$\frac{1}{2k}\sum_{l=0}^{\infty}(2l+1)i^{(l+1)}P_\ell(\cos\theta)\frac{e}{r}^{-i(kr-\frac{\ell\pi}{2})}$.

This takes the form:

$f\ \frac{e^{ikr}}{r}$

with:

$f = \sum_{l=0}^{\infty}(2\ell+1)\left[\frac{1}{2ik}\right]P_\ell(\cos\theta)$

We know that for a spherical wave $f\ \frac{e^{ikr}}{r}$ the radial flux is
$\frac{\hbar k}{m}\frac{|f|^2}{r^2}\hat{r}$ (Eq 5.16) and the total integrated flux over all directions is:
$\frac{\hbar k}{m}\int |f|^2 d\Omega$.

We can repeat integration of Eq 5.38 to obtain:

$$F_{inc} = \frac{\hbar k}{m}\frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1) \qquad (5.41)$$

(*Exercise* !). The outgoing part, likewise, gives similar result.

But $|S_l|^2 \neq 1$ for inelastic scattering, we now work out the flux for the *outgoing* scattered spherical waves. Same method, just replace $f_l = S_l$ in (5.36b) then repeat integral.

Outgoing flux is

$$F_{out} = \frac{\hbar k}{m}\frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)|S_l(k)|^2 \qquad (5.42)$$

We subtract (5.40)–(5.42) to obtain the loss of flux in spherical waves. This, divided by the incident flux, $\frac{\hbar k}{m}$, of the original plane wave is the *inelastic cross section*:

$$\sigma_{in} = \frac{F_{in} - F_{out}}{\frac{\hbar k}{m}} = \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)[1 - |S_\ell(k)|^2] \qquad (5.43)$$

Finally, the total cross section is the sum of the elastic (5.39) and inelastic (5.43) cross section

$$\sigma_{el} + \sigma_{in} = \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)[|S_l - 1|^2 + 1 - |S_l|^2]$$

$$\sigma_{TOT} = \frac{2\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)(1 - ReS_l(k)) \qquad (5.44)$$

Now, from (5.36b) $f_{(\theta)} = \sum_l (2l+1)\left[\frac{S_\ell - 1}{2ik}P_\ell(\cos\theta)\right]$.

But if $\theta = 0$ (the forward direction, ie the z axis), $P_l(1) = 1$, and

$$f(\theta = 0) = \sum_l (2l+1)\left(\frac{S_l - 1}{2ik}\right) \qquad (5.45)$$

and

$$Imf(0) = \sum_{l=0}^{\infty}\frac{(2l+1)}{2k}(1 - ReS_\ell)$$

$$\Rightarrow \quad \sigma_T = \frac{4\pi}{k}I_m f(0) \qquad (5.46)$$

This is the *optical theorem*.

The optical theorem relates the forward scattering amplitude to the total cross section.

The interference between the scattered wave and incident wave leads to a decrease in current in the forward direction. The total interference current is proportional to $Im f(0)$. This decrease in fact gives the total cross section.

The optical theorem is a statement of conservation of probability.

More Elastic Scattering

With $S_\ell = e^{2i\delta_\ell}$, the elastic cross section, (5.39) becomes

$$\begin{aligned} \sigma_{el} &= \frac{\pi}{k^2}\sum(2l+1)|e^{2i\delta_l}-1|^2 \\ &= \frac{4\pi}{k^2}\sum(2l+1)\sin^2\delta_\ell \end{aligned} \qquad (5.47)$$

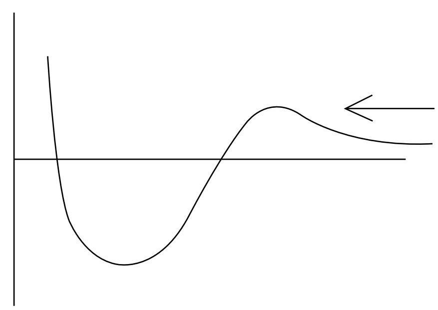
Similarly, from (5.36b) we can write

$$f(\theta,\phi) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_\ell}\sin\delta_\ell P_\ell(\cos\theta) \qquad (5.48)$$

l-dependence of scattering phaseshifts

From (5.24) we see that a particle experiences an effective potential
$V_l(r) = U(r) + \frac{l(l+1)}{r^2}$ including the centrifugal barrier term. This provides a $\Rightarrow$
repulsive barrier for $l > 0$.
$U(r)$ is of finite range; Let $r \sim a$ represent typical length scale.
That is, we take $U(r) \sim 0$ for $r > a$.

If we sketch $V_l(r)$ against r , we see that if E is less than the height of the barrier, the particles cannot sample the small r region (except by tunnelling, a weaker contribution).



The barrier height increases with l, so for large enough l, the centrifugal barrier dominates and a particle does not experience $u(r)\cdot$.

Hence, for high $l, \delta_\ell \to 0$

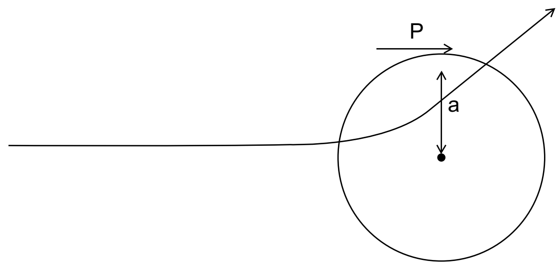
For high energies, the particle can penetrate the barrier and sample the region $r < a$.

The higher l is, the higher the energy needed to penetrate the barrier.

For low energies $\delta_\ell = 0$ if $l > 0$:

Low E scattering $\Rightarrow$ scattering is 's-wave' scattering.

We can also look at this process with a simple classical model.



POTENTIAL HAS FINITE RANGE, a

Trajectories which pass at distance from the nucleus ('impact parameter') larger than a experience no deflection (and continue along Z axis). Figure illustrates deflection of a trajectory which passes through the interaction region.

ie there is no deflection for angular momentum:
$L \stackrel{\sim}{>} pa = \hbar pa$

$L = \sqrt{\ell(\ell+1)}\ \hbar \sim \ell\hbar$

ie no deflection if $\ell \stackrel{\sim}{>} ka$

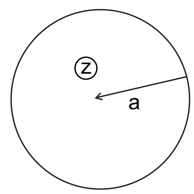
Then, $\Rightarrow \delta_\ell = 0$ in the quantum case.

Solutions of Schrodinger Equation

For most realistic atomic and molecular problems, phaseshifts are calculated by numerical solutions of the Schrodinger equation. A standard way of calculating scattering cross-sections (ie from the δ_ℓ) for a potential with a finite range, is to solve the TISE over 2 regions :

(1) An outer region, $r > a$, where we can use eqs 5.20 – 5.40 and apply large r BCs

(2) An inner region $r < a$, where $U(r)$ is important.



A match of $\psi_{(1)}$, $\psi_{(2)}$ 'Log-derivative' method at the boundary solves the problem. For atomic/molecular collisions, a variant of this is called the "R-matrix" model and is used extensively by the Tennyson group at UCL.

But for the simple 1-D, finite range potential, we show $\delta_\ell \to 0$ as $k \to 0$

In general, one can show that:

$$\delta_\ell \propto k^{2l+1} \tag{5.49}$$

From 5.48

$$f_\ell = \frac{\sin \delta_\ell}{k} \propto k^{2l} \quad (\text{As } \sin \delta_\ell \sim \delta_l \text{ for small } \delta_\ell)$$

and

$$\sigma_\ell \propto \ k^{4l}$$

For small energies ie $(k \to 0)$, $l = 0$ dominates.

Then, from (5.49) as $(k \to 0)$:

$$\delta_0 \to Cak$$

where C is a constant which depends on the potential (and $a =$ is the 'range' of the potential)

$$\sigma_{tot} = \frac{4\pi^2}{k^2} \sin^2 \delta_0 \approx \frac{4\pi^2}{k^2} \delta_0^2 = 4\pi^2 (C_a)^2 \tag{5.50}$$

$-A_0 = Ca$ is called the 'scattering' length, and is a characteristic parameter for different atom pairs; it is very important in BEC theory/ultracold collisions.

There is a general definition for the scattering length in the l-th partial wave:

$$A_l = -\lim_{k\to 0}\left[\frac{\tan\delta_\ell(k)}{k^{2l+1}}\right] \tag{5.51}$$

or

$$-\frac{1}{A_l} = \lim_{k\to 0}[k^{2l+1}\cot\delta_\ell]. \tag{5.52}$$

For a repulsive potential, δ_ℓ is negative, so the scattering length is positive. Conversely, attractive potentials are associated with negative scattering length.

At higher order in k, one can parameterise s-wave scattering by A_0, and an "effective range", r_0:

$$k\cot\delta_0 = \frac{-1}{A\ _0} + \frac{1}{2}r_0k^2\ldots$$

$$\begin{aligned} \Rightarrow \sigma_{\mathrm{TOT}} &= \frac{4\pi^2}{k^2}\sin^2\delta_0 = \frac{4\pi^2}{k^2}\frac{1}{1+\cot^2\delta_0} \quad \text{useful form} \\ &= 4\pi^2\frac{1}{k^2+\left(\frac{-1}{A_0}+\frac{1}{2}r_0k^2\right)^2} \end{aligned} \tag{5.53}$$

$$\sigma_{\text{TOT}} = \sum_l \sigma_l = \sum_l \frac{4\pi}{k^2}(2l+1)\sin^2\delta_\ell \tag{5.54}$$

σ_l has a maximum if $\sin^2\delta_\ell = 1$ ie if $\cot^2\delta_\ell = 0$, giving a 'resonance' .

from (5.52), using

$$\frac{-1}{A_\ell} = k^{2l+1}\cot\delta_\ell \tag{5.55}$$

we expand the l-th wave scattering length about

$$E = E_R \text{ where } E_R = \frac{\hbar k_R^2}{2m}$$

For this k_R then $\cot\delta_\ell = 0$

So $\frac{1}{A_\ell(k_R)} = 0$
We do a Taylor expansion about E_R:

$$\frac{1}{A_\ell(E)} = 0 + (E - E_R)\frac{d}{dE}\left(\frac{1}{A_\ell}\right)_{E=E_e} \cdots$$
$$\Rightarrow \cot\delta_\ell = -(E - E_R)\frac{2}{\Gamma(E)}$$

from Eq(5.55), where

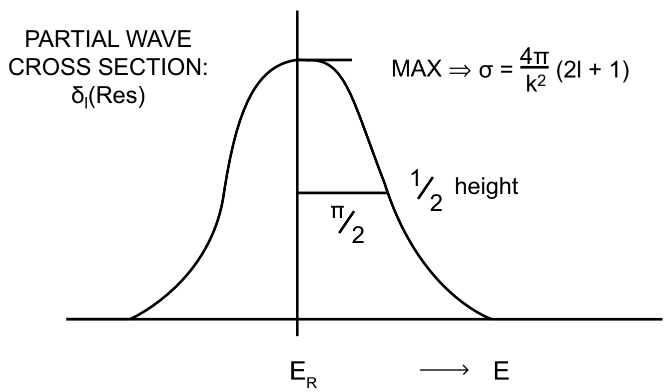
$$\Gamma(E) = \frac{2k^{2l+1}}{\frac{d}{dE}\left(\frac{1}{A_\ell}\right)_{E_R}} \tag{5.56}$$

Now

$$\sigma_\ell = \frac{4\pi}{k^2}(2l+1)\frac{1}{1+\cot^2\delta_\ell}$$
$$\Rightarrow \sigma_e = \frac{4\pi}{k^2}(2l+1)\frac{\frac{\Gamma^2}{4}}{(E-E_R)^2 + \frac{\Gamma^2}{4}} \tag{5.57}$$

NB: typo in figure : half-width is $\Gamma/2$ not $\pi/2$!!! WIDTH of peak (Lorentzian shape) at half-maximum is Γ.

Other partial waves are not resonant so this 'BREIT-WIGNER' resonance is superimposed on a non-resonant background.
READ GASIOROWICZ ch 'Collision Theory'.


PARTIAL WAVE
CROSS SECTION:
δl(Res)
MAX ⇒ σ = 4π/k² (2l + 1)
1/2 height
π/2
ER
⟶ E