~~28 March~~ 2 April - 2018

PARTIAL WAVES, PHASE SHIFTS, REACTION CROSS-SECTIONS

The general cross-section σ is written in terms of the scattering amplitudes f as $d\sigma/d\Omega = |f(\theta)|^2$, where $f(\theta)$ is a sum over partial waves corresponding to different ℓ values.
Using the orthonormality of the Legendre Polynomials appearing in the series expansion of f, we can write

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \int |f(\theta)|^2 d\Omega = \sum_\ell \frac{\pi}{K^2}(2\ell+1)|1-S_\ell|^2$$

The summand for each ℓ is called the ℓ^{th} partial cross-section, $\sigma_\ell = \frac{\pi}{K^2}(2\ell+1)|1-S_\ell|^2$. Hence $\sigma = \sum_\ell \sigma_\ell$ and this can be interpreted semi-classically. Each partial wave corresponds to a definite angular momentum, which can be interpreted to correspond to a definite classical impact parameter ~~or~~ through the relationships

$$L = mv_0 b = \sqrt{\ell(\ell+1)}\,\hbar^2$$ where v_0 is the initial velocity.

Thus each 'ℓ' corresponds to a "ring" of radius $\hbar\sqrt{\ell(\ell+1)}/K$ and ~~radius~~ thickness $1/K$. The geometric area of this ring is ~~[illegible]~~ $(2\ell+1)\pi/K^2$ $\{$i.e. $\pi(\ell+1)^2 - \pi\ell^2\}$

Since ℓ is quantised we take the ring to have inner & outer radii as ℓ and $\ell+1$.

If we interpret the area of this ring as the cross-section for scattering, then there must be a one-to-one correspondence between this area and the "maximal efficient, or 100% scattering" value of σ_ℓ defined earlier. The maximum value of σ_ℓ occurs when $S_\ell = -1$ that is $e^{2i\delta_\ell} = -1 \Rightarrow \delta_\ell = \pi/2$. In contrast, when $S_\ell = +1$ or $\delta_\ell = 0, \pi$, the cross section is zero. The value of K has not changed in either of these cases.

2 April
~~28 March~~ - 2018

When $|S_\ell| < 1$ we call the scattering as inelastic, since under this condition the ~~amplitude~~ intensity of the outgoing wave is less than unity. (The ingoing wave has ~~amplitude~~ intensity $= 1$ by definition) {NOTE amplitude is in general a complex number}

The inelastic, or reaction cross-section, is defined for each partial wave as that part which is missing from the elastic cross-section:

$$\sigma_{reac,\,\ell} = \frac{\pi}{k^2}(2\ell+1)\left(1 - |S_\ell|^2\right)$$

intensity of elastically scattered outgoing wave.

Based on this partial wave cross-sec we define the ~~compl~~ full reaction cross-sec as

$$\sigma_{reac} = \sum_\ell \sigma_{reac,\,\ell} = \sum_\ell \frac{\pi}{k^2}(2\ell+1)\left(1 - |S_\ell|^2\right)$$

2Apr 2018

The differential cross-sec for inelastic scattering of an electron from an atom can be written as

$$\frac{d\sigma_n}{d\Omega} = \frac{m p'}{4\pi^2\hbar^4} \, |\langle n \vec{p}' | U | 0 \vec{p} \rangle|^2$$

where $n, \vec{p}'$ are labels for the final state of the atom & electron respectively and $0, \vec{p}$ are the initial state labels. Energy conservation implies $(p^2 - p'^2)/2m = E_n - E_0$. We now evaluate the matrix element

$$\langle np' | U | 0p \rangle = \frac{1}{p} \int d\tau \, d\tau_1 \ldots d\tau_Z \, \psi_n^* \psi_0 \, e^{i(\vec{k}-\vec{k}')\cdot\vec{r}} \, U(\vec{r})$$

and $$U(\vec{r}) = \frac{Ze^2}{r} - \sum_1^Z \frac{e^2}{|\vec{r}-\vec{r}_j|}$$

$\vec{r}_j$: electron in atom

$\vec{r}$: incident electron

The first integral term containing Ze^2/r is zero because it involves a product: $\int \psi_n^* \psi_0 \, d\tau_1 \, d\tau_2 \ldots d\tau_Z \int (Ze^2/r) \, e^{-i\vec{q}\cdot\vec{r}} d\tau$ in which the first integral is zero due to orthonormality of the ψ's.

The second integral is non-zero, and can be calculated by the Fourier decomposition technique seen before

$$\phi_q(\vec{r}_j) = \int \frac{e^{-i\vec{q}\cdot\vec{r}} \, d\tau}{|\vec{r}-\vec{r}_j|}$$

is the potential due to the charge density $\rho = \delta(\vec{r}-\vec{r}_j)$

so $$\phi_q(\vec{r}_j) = \frac{4\pi}{q^2} e^{-i\vec{q}\cdot\vec{r}_j}$$

Hence the matrix element

$$\langle n\vec{p}' | U | 0\vec{p} \rangle = \frac{4\pi}{q^2} \langle n | \sum_j e^{-i\vec{q}\cdot\vec{r}_j} | 0 \rangle$$

$$\therefore \quad \frac{d\sigma}{d\Omega} = \frac{me^2}{\hbar^2} \, \frac{4}{q^4} \, \frac{p'}{p} \, \langle n | \sum_j e^{-i\vec{q}\cdot\vec{r}} | 0 \rangle$$

It is instructive to write the differential cross-section not in terms of the solid angle, but in terms of the momentum transfer q, since it is this quantity that can be directly related to the energy ~~to~~ gained by the target. To do this we note that

$$q^2 = k^2 + k'^2 - 2kk'\cos\chi \Rightarrow q\,dq = kk' \sin\chi \, d\chi$$
$$= kk' \, d\Omega / 2\pi$$

2 Apr 2018

$$\therefore \quad \frac{d\sigma}{dq} = 8\pi\left(\frac{e^2}{\hbar v}\right)^2 \frac{1\,dq}{q^3}\left|\langle n|\sum_{j=1}^{Z} e^{-i\vec{q}\cdot\vec{r}_j}|0\rangle\right|^2$$

If q is small, i.e. $(K-K') << K$, then χ is small also.
so we have two approximate relationships in this case

$$E_n - E_0 = \hbar^2 (K^2 - K'^2)/2m \simeq \hbar^2 K (K-K')$$

$$q^2 \simeq (K-K')^2 + (K\chi)^2 \Rightarrow q = \left[\{(E_n-E_0)/\hbar v\}^2 + K\chi^2\right]^{1/2}$$

if $\chi << 1$, Then $q \simeq K\chi = (mv/\hbar)\,\chi$

If we consider energy transfer, $E_n - E_0 \equiv \epsilon$ to be small compared with the kinetic energy of the incident particle then the first term can be neglected w.r.t. the second one in $[\quad]^{1/2}$
(The same assumption gives us $\chi \sim v_0/v$)

For small q the exponent appearing in the matrix element can be expanded as a power series taking the $\vec{z}$ axis in the atomic coordinates to be along $\vec{q}$:

$$e^{-i\vec{q}\cdot\vec{r}_j} = 1 - i\vec{q}\cdot\vec{r}_j - q^2 r_j^2$$

The first term integrates to zero due to orthonormality of ψ_n & ψ_0
the second term gives

$$\frac{d\sigma}{dq} = 8\pi\left(\frac{e^2}{\hbar v}\right)^2 \frac{1}{q}\left|\langle n|\Sigma z_j e|0\rangle\right|^2$$

$$\Rightarrow \frac{d\sigma}{d\Omega} \equiv 4\left(\frac{e^2}{\hbar v}\right)^2 \left|\langle n|\Sigma z_j e|0\rangle\right|^2 \frac{1}{\chi^2}$$

NOTE
$\sum_j e z_j$ is the dipole moment

The third term gives a contribution to the cross-section

$$\frac{d\sigma}{dq} = 2\pi\left(\frac{e^2}{\hbar v}\right)^2 \langle n|\Sigma z_j^2 e|0\rangle\, q$$

(The quadrupole term)