PARTIAL WAVES, PHASE SHIFTS, REACTION CROSS-SECTIONS

The general cross-section $\sigma$ 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

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \int |f(\theta)|^2 d\Omega = \sum_l \frac{\pi}{K^2} (2l+1) \left| 1 - S_l \right|^2$$

The summand for each $l$ is called the $l$th partial cross-section, $\sigma_l = \frac{\pi}{K^2} (2l+1) \left| 1 - S_l \right|^2$. Hence $\sigma = \sum_l \sigma_l$ 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 through the relationships

$$L = m_0 v_0 b = \sqrt{2(l+1)} \frac{h}{K}$$

Thus each $l$ corresponds to a "ring" of radius $\pi \sqrt{2(l+1)} / K$ and radius thickness $1 / h$. The geometric area of this ring is

$$A = (2l+1) \pi / K^2 \rightarrow \pi (l+1)^2 - \pi l^2 \frac{2}{3}$$

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

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 $\sigma_l$ defined earlier. The maximum value of $\sigma_l$ occurs when $S_l = -1$ that is $e^{2iS_l} = -1 \Rightarrow S_l = \pi / 2$. In contrast, when $S_l = +1$ or $S_l = 0, \pi$, the cross-section is zero. The value of $K$ has not changed in either of these cases.
When $|S_k| < 1$ we call the scattering as inelastic, since under this condition the amplitude of the outgoing wave is less than unity. (The ingoing wave has amplitude = 1 by definition)  

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

$$\sigma_{\text{react}, \ell} = \frac{\pi}{K^2} (2\ell + 1) (1 - |S_k|^2)$$

Based on this partial wave cross-section, we define the full reaction cross-section as

$$\sigma_{\text{react}} = \sum_{\ell} \sigma_{\text{react}, \ell} = \sum_{\ell} \frac{\pi}{K^2} (2\ell + 1) (1 - |S_k|^2)$$
The differential cross-section for inelastic scattering of an electron from an atom can be written as
\[
\frac{d\sigma}{d\Omega} = \frac{m^2 p'}{4\pi^2 \hbar^4} |\langle n \bar{p}' | U | 0 \bar{p} \rangle|^2
\]
where \( n, \bar{p}' \) are labels for the final state of the atom & electron respectively and \( 0, \bar{p} \) are the initial state labels. Energy conservation implies \( (p^2 - p'^2)/2m = E_n - E_0 \). We now evaluate the matrix element
\[
\langle n \bar{p}' | U | 0 \bar{p} \rangle = \frac{1}{p} \int d\tau_1 d\tau_2 \ldots \int d\tau_2 \psi^*_n \psi_0 e^{i(\mathbf{K} \cdot \mathbf{r})} U(\mathbf{r})
\]
and
\[
U(\mathbf{r}) = \frac{Ze^2}{r} \sum_j \frac{e^2}{|\mathbf{r} - \mathbf{r}_j|} \quad \bar{r}_j : \text{electron in atom} \quad \mathbf{F} : \text{incident electron}
\]
The first integral term containing \( Ze^2/r \) is zero because it involves a product:
\[
\int \psi^*_n \psi_0 d\tau_1 d\tau_2 \ldots d\tau_2 \int (Ze^2/r) e^{i\mathbf{q} \cdot \mathbf{r}} d\tau
\]
in which the first integral is zero due to orthonormality of the \( \psi \)'s. The second integral is non-zero, and can be calculated by the Fourier decomposition technique seen before:
\[
\phi_q(\mathbf{r}_j) = \int \frac{e^{-i\mathbf{q} \cdot \mathbf{r}}}{|\mathbf{r} - \mathbf{r}_j|} d\tau \quad \text{is the potential due to the charge density } \rho = \delta(\mathbf{r} - \mathbf{r}_j)
\]
so
\[
\phi_q(\mathbf{r}_j) = \frac{4\pi}{q^2} e^{-i\mathbf{q} \cdot \mathbf{r}_j}
\]
Hence the matrix element
\[
\langle n \bar{p}' | U | 0 \bar{p} \rangle = \frac{4\pi}{q^2} \langle n | \sum_j e^{-i\mathbf{q} \cdot \mathbf{r}_j} | 0 \rangle
\]
\[
\therefore \frac{d\sigma}{d\Omega} = \frac{m^2 e^2}{2\pi^2 \hbar^4} \frac{4}{p} \langle n | \sum_j e^{-i\mathbf{q} \cdot \mathbf{r}_j} | 0 \rangle
\]
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 \( \Delta E \) gained by the target. To do this we note that
\[
q^2 = K^2 + k'^2 - 2KK'\cos \chi \quad \Rightarrow \quad q \, dq = KK' \sin \chi \, d\chi
\]
\[
q \, dq = KK' \, d\Omega / 2\pi
\]
\[ \frac{d\sigma}{dq} = 8\pi \left( \frac{e^2}{\hbar v} \right)^2 \frac{1}{q^2} \left| \langle n | \sum_{j=1}^{\infty} e^{-iq \cdot r_j} | 0 \rangle \right|^2 \]

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

\[ E_n - E_0 = \hbar^2 (K^2-K'^2)/2m = \hbar^2 K (K-K') \]

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

If \( \chi < 1 \), then \( q = K\chi = (mv/h) \theta \chi \)

If we consider energy transfer, \( E_n - E_0 = \Delta E \) 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 \( [..]^\frac{1}{2} \) (the same assumption gives us \( \chi \approx v_0/v \)).

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 \( \vec{q} \):

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

The first term integrates to zero due to orthornormality of \( \vec{v}_n \) & \( \vec{v}_0 \)

The second term gives

\[ \frac{d\sigma}{dq} = 8\pi \left( \frac{e^2}{\hbar v} \right)^2 \frac{1}{q^2} \left| \langle n | \sum_{j=1}^{\infty} Z_j e^{-iq \cdot r_j} | 0 \rangle \right|^2 \]

\[ \Rightarrow \frac{d\sigma}{dq} = 4 \left( \frac{e^2}{\hbar v} \right)^2 \frac{1}{q^2} \left| \langle n | \sum_{j=1}^{\infty} Z_j e^{-iq \cdot r_j} | 0 \rangle \right|^2 \frac{\chi^2}{\chi^2} \]

\[ \sum_{j=1}^{\infty} Z_j \] is the dipole moment

The third term gives a contribution to the cross-section

\[ \frac{d\sigma}{dq} = 2\pi \left( \frac{e^2}{\hbar v} \right)^2 \langle n | \sum_{j=1}^{\infty} Z_j^2 e^{-iq \cdot r_j} | 0 \rangle \]

(The quadrupole term)