EPFL

Inelastic scattering formalism (ionisation)

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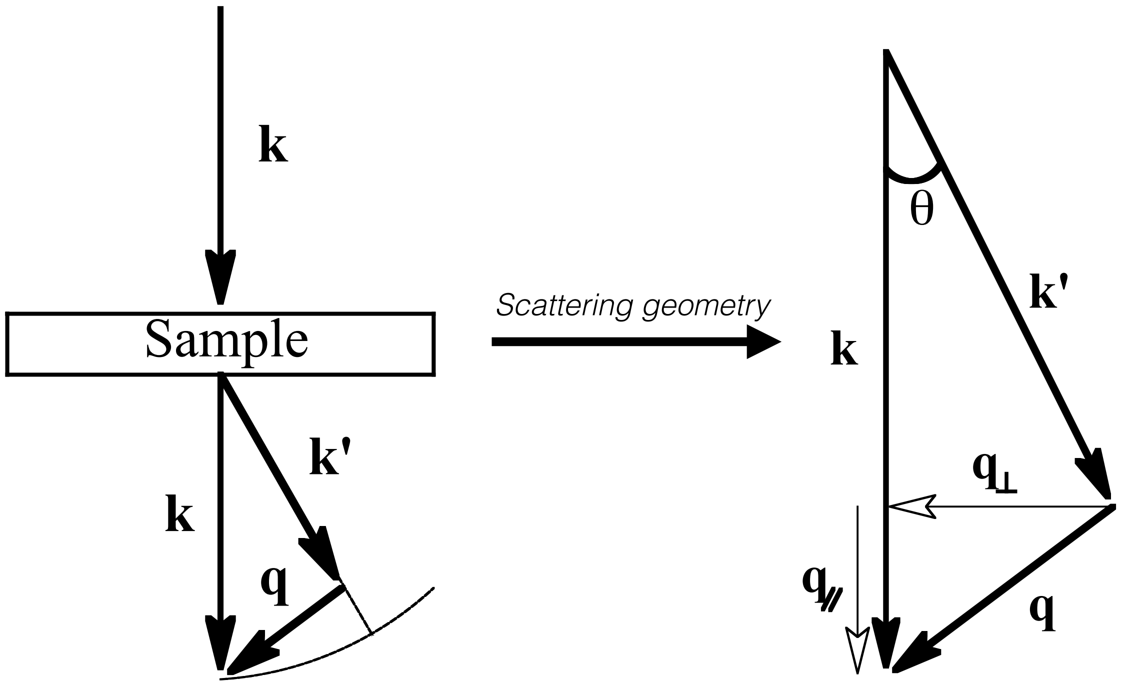
Scattering geometry

$\vec{k}$ – incident wave-vector

$\vec{k'}$ – scattered wave-vector



$\vec{q}$ – wave-vector transfer/momentum transfer for inelastic scattering from an atom

θ_E – describes shortening of wave-vector from scattering i.e. $|\vec{k}| = k = |\vec{k'}| + k\theta_E$

For energy loss E: $\theta_E = \dfrac{Em\gamma}{\hbar^2 k^2}$

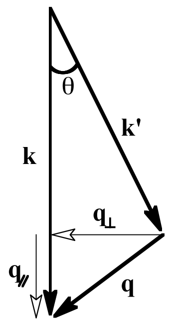
$$q^2 = k^2 + (k')^2 - 2kk'\cos\theta$$

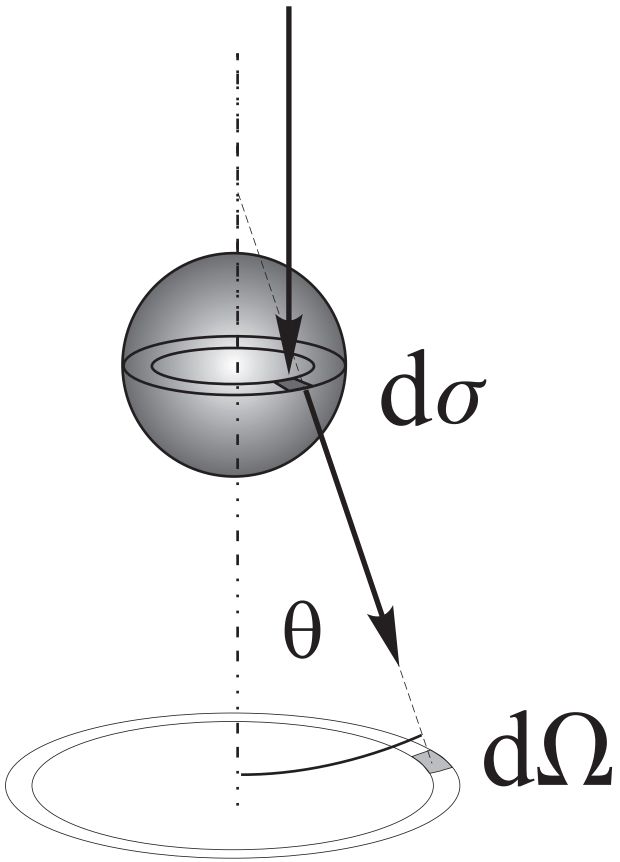
$q_\perp = k\vartheta$ (geometry)

$q_\parallel = k\vartheta_E$ (definition of ϑ_E)

$\vartheta \ll 1$ therefore $q^2 = k^2(\vartheta_E^2 + \vartheta^2)$

Scattering cross section





Want to know the probability of energy-loss scattering from one atom.

Relevant quantity: *scattering cross-section* as a function of angle θ and energy loss *E*.

This is a differential for:
Solid angle dΩ
Interval of energy loss d*E*

We consider a transition from initial state | I > to final state | F > for the core electron of the atom

Theory of core losses

Transition from core (occupied) to unoccupied state
Cannot be treated classically – we need quantum mechanics!
System = fast incoming electron + target electron
Target electron transitions from | I > to final state | F
Incoming electron changes momentum from $\vec{k}$ to $\vec{k'}$

Use:
First order perturbation theory
First Born approximation
Perturbation potential is Coulomb potential

H.A.Bethe: 1930:

Zur Theorie des Durchgangs schneller Korpuskularstrahlen durch Materie

Annalen der Physik, vol. 397, Issue 3, pp.325-400

Theory of core loss

Transition probability per unit time dP_{if} from an initial state $|i\rangle$ to a final state $|f\rangle$ situated between ν_f and $\nu_f + d\nu_f$.

$$dP_{if} = \frac{2\pi}{\hbar} |\langle f|V|i\rangle|^2 d\nu_f \, \delta(E_i - E_f)$$

Initial and final state of the system :

$$|i\rangle = |\vec{k}_a\rangle \otimes |I\rangle$$

and

$$|f\rangle = |\vec{k}_b\rangle \otimes |F\rangle$$

$|I\rangle$ and $|F\rangle$ Initial and final states of the target electron.

Theory of core loss

$\vec{k}_a$ before the interaction $\vec{k}_b$ after.

$\vec{q} = \vec{k}_a - \vec{k}_b$

$$dP_{if} = \frac{2\pi}{\hbar} \left| \langle F| \otimes \langle \vec{k}_b | V | \vec{k}_a \rangle \otimes |I\rangle \right|^2 d\nu_f \delta(E_I - E_F + E)$$

$\langle \vec{k}_b | V | \vec{k}_a \rangle$? ?

$$\langle \vec{k}_b | V | \vec{k}_a \rangle = \frac{1}{4\pi\epsilon_0} \int (2\pi)^{-3} d^3r \frac{e^2}{|\vec{r} - \vec{R}|} e^{i(\vec{k}_a - \vec{k}_b)\vec{R}}$$

$\vec{r}$ position vector of the fast electron $\vec{R}$ of the target electron

Theory of core loss

$$\langle \vec{k}_b | V | \vec{k}_a \rangle = \frac{e^2}{(2\pi)^3 \epsilon_0 q^2} e^{i\vec{q}.\vec{R}}$$

$$dP_{if} = \frac{e^4}{(2\pi)^5 \hbar \epsilon_0^2 q^4} |\langle F | e^{i\vec{q}.\vec{R}} | I \rangle|^2 d\nu_f \, \delta(E_I - E_F + E)$$

Theory of core loss

$$d\sigma = \sum_{i,f} \frac{dP_{if}}{j_0}$$

j_0 current density of the plane wave

$\psi_{\vec{k}_a}(\vec{R}) = (2\pi)^{-3/2} e^{i\vec{k}_a.\vec{R}}$ $\qquad$ $j_0 = (\hbar k_a)/((2\pi)^3 m)$

$$d\sigma = \sum_{I,F} \frac{me^4}{(\hbar 2\pi\varepsilon_0)^2 q^4 k_a} |\langle F| e^{i\vec{q}.\vec{R}} |I\rangle|^2 d\nu_f \delta(E_I - E_F + E)$$

$d\nu_f = d\nu_t \, d\nu_e$ ($d\nu_t$: target electron, $d\nu_e$: fast electron)

$d\nu_e = (k_b m)/\hbar^2 dE d\Omega$

Theory of core loss

If the final state is expressed in an orthogonal basis set :
$d\nu_t = 1$

$$d\nu_f = k_b \frac{m}{\hbar^2} dE d\Omega$$

$$\frac{\partial^2 \sigma}{\partial E \partial \Omega} = \sum_{I,F} 4 \frac{m^2 e^4}{\hbar^4 (4\pi)^2 \varepsilon_0^2 q^4} \frac{k}{k'} |\langle F | e^{i\vec{q}.\vec{R}} | I \rangle|^2 \delta(E_I - E_F + E)$$

Relativistic effects : $m \rightarrow \gamma m$

Theory of core loss

Arrive at an expression for the **double differential scattering cross-section (DDSCS)**:

$$\frac{\partial^2\sigma}{\partial E\partial\Omega} = \sum_{I,F}\frac{4\gamma^2}{a_0^2q^4}\frac{k_b}{k_a}|\langle F|e^{i\vec{q}.\vec{R}}|I\rangle|^2\delta(E_I - E_F + E) = \frac{4\gamma^2}{a_0^2q^4}\frac{k_b}{k_a}S(\vec{q},E)$$

Use **Bohr's radius**: $a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2}$

$$\vec{q} = \vec{k}_a - \vec{k}_b$$

$$\gamma = (1 - v^2/c^2)^{-1/2}$$

Assign the following term as the **dynamic structure factor** $S(\vec{q},E)$:

$$S(\vec{q},E) = \sum_F|\langle F|e^{i\vec{q}.\vec{R}}|I\rangle|^2\delta(E_I - E_F + E)$$

Theory of core losses

$S(\vec{q}, E)$ is a matrix element between initial and final states

Dipole approximation

$$S(\vec{q}, E) = \sum_F |\langle F|e^{i\vec{q}.\vec{R}}|I\rangle|^2 \delta(E_I - E_F + E)$$

If $\vec{q}.\vec{R} \ll 1$ we can write $e^{i\vec{q}.\vec{R}} \simeq 1 + i\vec{q}.\vec{R}$

$$S(\vec{q}, E) = \sum_F |\langle F|i\vec{q}.\vec{R}|I\rangle|^2 \delta(E_I - E_F + E)$$

In conclusion, we have: $S(\vec{q}, E) \propto q^2$ and $\frac{\partial^2\sigma}{\partial E \partial \Omega} \propto \frac{1}{q^4} S(\vec{q}, E)$

Therefore, the DDSCS for inelastic events varies as $\frac{1}{q^2}$

Theory of core losses

Since: $q^2 = k^2(\theta^2 + {\theta_E}^2)$

DDSCS has an angular dependence: $\text{DDSCS}(\theta) = \frac{\partial^2\sigma}{\partial\Omega\partial E} \propto \frac{1}{\theta^2 + {\theta_E}^2}$

Therefore the ionisation edge has an angular distribution of intensity that is **Lorentzian**

θ_E is the scattering angle for the half width at half maximum (HWHM) of this Lorentzian

θ_E is therefore considered as the *characteristic angle of scattering*, because most of the ionisation edge intensity will fall within a collection aperture of this angle

Inelastic scattering angular range

- Inelastic scattering concentrated into much smaller angles than elastic scattering
- Characteristic angle for scattering: $\theta_E = \frac{Em\gamma}{\hbar^2 k^2} = \frac{E}{\gamma m v^2} \left(\approx \frac{E}{2E_0} \right)$ E_0: incident beam energy