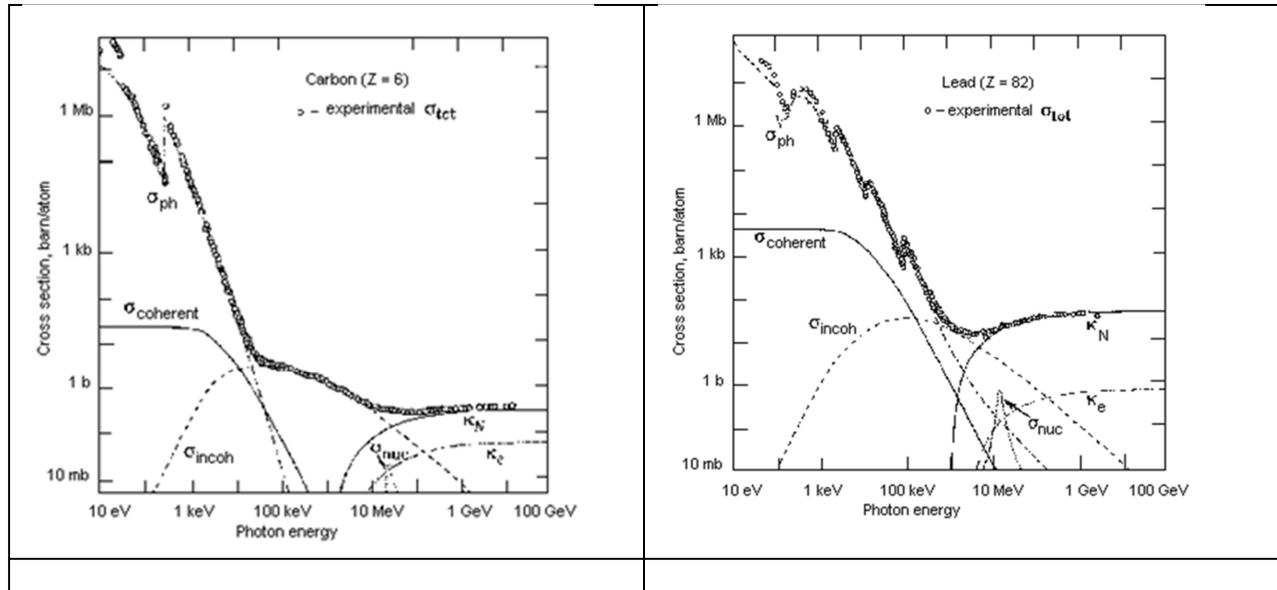


Notes on x-ray scattering - M. Le Tacon, B. Keimer (06/2015)

Interaction of x-ray with matter:



- Photoelectric absorption
- Elastic (coherent) scattering (Thomson Scattering)
- Inelastic (incoherent) scattering (Compton Effect)
- Creation of electron-positron pair ($E > 1.022$ MeV)
-

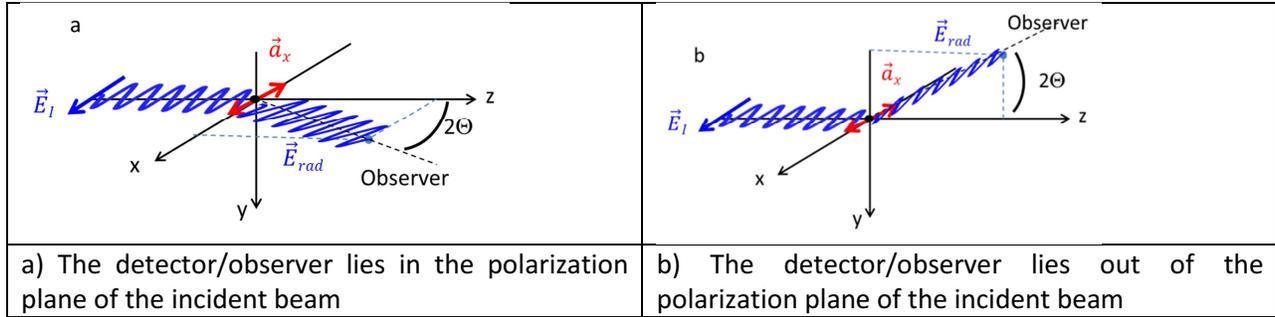
1) Scattering from a single electron – classical description

Here we will deal only with the case of elastic scattering, where an incident photon of momentum \vec{k}_I and polarization $\hat{\epsilon}_I$ will be scattered from a single electron. After the scattering event, the photon has a momentum \vec{k}_F and a polarization $\hat{\epsilon}_F$. In the case of elastic scattering, the final state of the electron is identical to its initial state, and the energy of the photon is therefore unchanged.

$$E_I = \hbar\omega_I = \hbar c|\vec{k}_I| = \hbar c|\vec{k}_F| = \hbar\omega_F = E_F$$

a) Assume the electron is a point charge

The electric field corresponding to the incident x-ray beam can be written as: $\vec{E}_I(\vec{r}, t) = \hat{\epsilon}_I E_0 e^{i(\vec{k}_I \cdot \vec{r} - \omega_I t)}$. The electron (at $\vec{r} = 0$) experiences the Lorentz force from this electric field and gets accelerated: $\vec{a}(t) = \frac{\vec{F}}{m} = \frac{e}{m} \vec{E}_I(\vec{r} = 0, t)$, and therefore radiates.



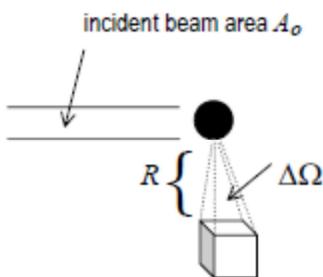
The electric field radiated in X, at distance R from the electron can be written as (cf electromagnetism):

$\vec{E}_{rad}(R, t) = -\frac{e}{4\pi\epsilon_0 c^2 R} \vec{a}_X(t')$, where \vec{a}_X is the apparent acceleration seen by the observer (or the detector) in X at $t' = t - R/c$. If the observer is in the plane of polarization (the (x, z) plane in the figure above): $\vec{a}_X(t') = \vec{a}_x(t') \cos(2\theta) = \frac{e}{m} \vec{E}_I(\vec{r} = 0, t) e^{i\frac{\omega_1 R}{c}} \cos(2\theta)$, and we get:

$$\frac{\vec{E}_{rad}(R, t)}{\vec{E}_I(\vec{r} = 0, t)} = -\frac{e^2}{4\pi\epsilon_0 c^2 m} \frac{e^{ik_1 R}}{R} \cos(2\theta)$$

$r_0 \sim 2.8 \times 10^{-5} \text{Å}$ is the 'classical electron radius'. If the observer does not lie in the plane of polarization of the incident x-ray, the $\cos(2\theta)$ must be dropped. This yields the conventional dipole radiation pattern (valid as long as the electron acceleration remains un-relativistic).

A detector counts the number of photons per unit of time, which can also be expressed as the power [=energy per unit of time] flowing through the area of the detector, divided by the energy of each photons. Because the detector has a finite size, it catches the photons emitted within a solid angle $\Delta\Omega$ (if A_{det} is the area of the detector, then: $\Delta\Omega = A_{det}/R^2$)



$$\frac{I_{det}}{I_{in}} = \frac{|\vec{E}_{rad}(R, t)|^2 R^2 \Delta\Omega}{|\vec{E}_I(\vec{r} = 0, t)|^2 A_0}$$

We introduce a quantity that is independent of the experimental conditions (size and position of the detector, area of the incident beam etc..), the differential cross-section

$$\frac{d\sigma}{d\Omega} = \frac{\# \text{ of photons detected within } \Delta\Omega}{\text{incident flux} \times \Delta\Omega}$$

For a single, point like electron, we therefore get:

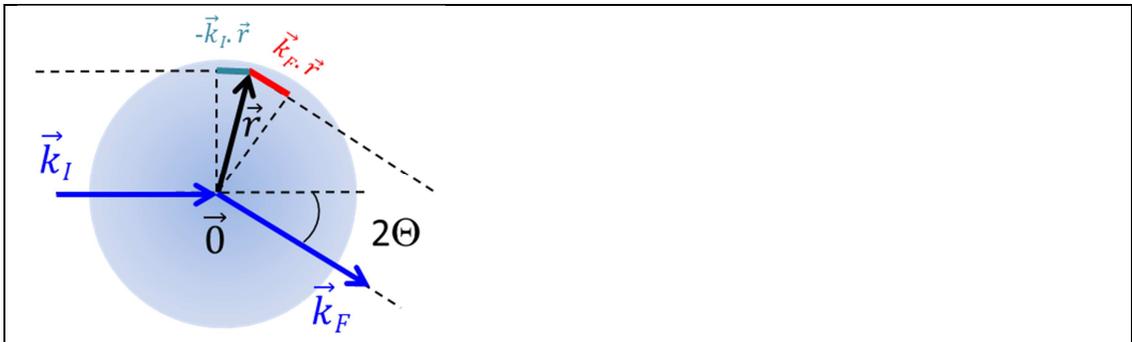
$$\frac{d\sigma}{d\Omega} = \frac{|\vec{E}_{rad}(R, t)|^2 R^2}{|\vec{E}_I(\vec{r} = 0, t)|^2} = r_0^2 \wp$$

with the polarization factor $\wp = \begin{cases} \cos^2(2\Theta) & \text{if the detector lies in the } xz \text{ plane} \\ r_0^2 & \text{if the detector does not lie in the } xz \text{ plane} \\ \frac{1}{2}(1 + \cos^2(2\Theta))r_0^2 & \text{if the incident beam is unpolarized} \end{cases}$

NB: obviously the scattering cross section for the nuclei will be much smaller than for the electron given the mass differences.

b) Atom case

Approximated by a charged sphere. The electron density is given by $\rho(\vec{r})$.



The phase difference between the wave scattered by an infinitesimal point-like charge $\rho(\vec{r}) d\vec{r}$ at the center of the atom ($\vec{r} = \vec{0}$) and \vec{r} is simply given by: $\vec{r} \cdot (\vec{k}_I - \vec{k}_F) \equiv \vec{r} \cdot \vec{Q}$. \vec{Q} is the transferred wave vector, which can be expressed as function of the scattering angle 2Θ : $Q = 2|\vec{k}_I| \sin(\Theta) = \frac{4\pi}{\lambda} \sin(\Theta)$



Volume element $d\vec{r}$ at \vec{r} will contribute to the radiated field as $r_0\rho(\vec{r}) d\vec{r} e^{i\vec{Q}\cdot\vec{r}}$. The total radiated field is obtained by summing up all the waves radiated by each part of the charge cloud, yielding:

$$\frac{d\sigma}{d\Omega} = \left| r_0 \int \underbrace{\rho(\vec{r}) e^{i\vec{Q}\cdot\vec{r}} d\vec{r}}_{f(\vec{Q})} \right|^2 \times \wp$$

The atomic form factor $f(\vec{Q})$ is simply the Fourier transform of the charge density.

2) Scattering from a single electron – Quantum mechanical description

The calculation can also be done in a full quantum mechanical approach. To do so, we use the quantized version of the electromagnetic field, through the vector potential $\vec{A}(\vec{r}, t)$. We recall that the electric and magnetic fields are derived from the scalar (Φ) and vector potential through: $\vec{E} = -\vec{\nabla}\Phi - \frac{\partial\vec{A}}{\partial t}$ and $\vec{B} = \vec{\nabla} \times \vec{A}$.

$$\vec{A}(\vec{r}, t) = \sum_{\hat{e}, \vec{k}} \sqrt{\frac{\hbar}{2\varepsilon_0 V \omega_{\vec{k}, \hat{e}}}} \left[\hat{e} a_{\vec{k}, \hat{e}} e^{i(\vec{k}\cdot\vec{r} - \omega_{\vec{k}, \hat{e}} t)} + \hat{e}^* a_{\vec{k}, \hat{e}}^\dagger e^{-i(\vec{k}\cdot\vec{r} - \omega_{\vec{k}, \hat{e}} t)} \right]$$

The operator $a_{\vec{k}, \hat{e}}$ ($a_{\vec{k}, \hat{e}}^\dagger$) annihilates (create) a photon of momentum \vec{k} and polarization \hat{e} . The total Hamiltonian of the electromagnetic field in free space is simply given by:

$$\hat{H}_{rad} = \sum_{\hat{e}, \vec{k}} \hbar\omega_{\vec{k}} \left(a_{\vec{k}, \hat{e}}^\dagger a_{\vec{k}, \hat{e}} + \frac{1}{2} \right)$$

and the actual electromagnetic field is described by an assembly of $N = \sum_{\hat{e}, \vec{k}} n_{\vec{k}, \hat{e}}$ photons $\{|n_{\vec{k}, \hat{e}}\}$, each characterized by a momentum and polarization state.

We consider the case of a single electron in the electromagnetic field. The Hamiltonian reads:

$$\hat{H} = \frac{(\hat{p} + e\hat{A}(\hat{r}))^2}{2m} + \hat{V} + \hat{H}_{rad} = \hat{H}_e + \hat{H}_{rad} + \hat{H}_{e-photon}$$

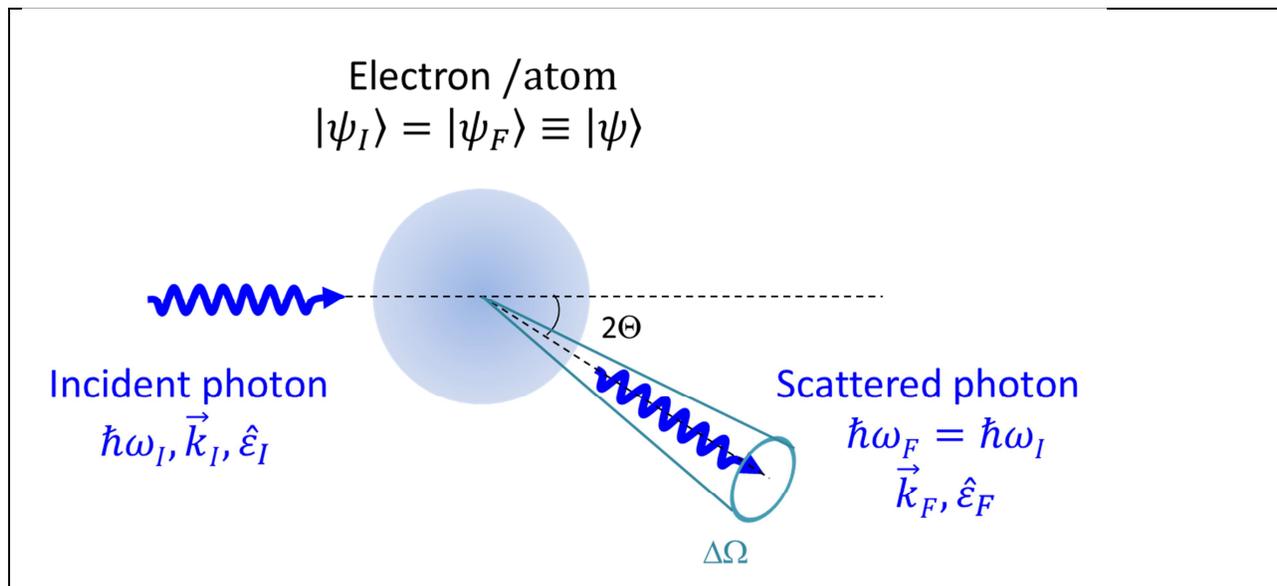
$\hat{H}_e = \frac{\hat{p}^2}{2m} + \hat{V}$ is the Hamiltonian describing the electron in the absence of the field. Remember that we consider only the case of elastic scattering, where the quantum state of the electron is not modified by the scattering event. This state is an eigenstate of \hat{H}_e , labelled $|\psi\rangle$. The corresponding electronic wave function $\psi(\vec{r}) = \langle \vec{r} | \psi \rangle$ is related to the charge density through: $|\psi(\vec{r})|^2 = \psi^*(\vec{r})\psi(\vec{r}) = \rho(\vec{r})$.

(NB it does not have to be a single electron, $|\psi\rangle$ can as well represent the electronic ground state of the entire atom).

In summary, the quantum state of the system {electron + photons} is given by $|\Psi\rangle = |\psi\rangle \{n_{\hat{\epsilon}, \vec{k}}\}$. During the scattering process, we let the system evolve from the initial $|\Psi_I\rangle = |\psi\rangle | \dots n_{\hat{\epsilon}_I, \vec{k}_I} \dots n_{\hat{\epsilon}_F, \vec{k}_F} \dots \rangle$ to the final quantum state $|\Psi_F\rangle = |\psi\rangle | \dots n_{\hat{\epsilon}_I, \vec{k}_I} - 1 \dots n_{\hat{\epsilon}_F, \vec{k}_F} + 1 \dots \rangle$, through the interaction of the electromagnetic field with the electron. This interaction is described by the electron-photon interaction Hamiltonian:

$$\hat{H}_{e-photon} = \frac{e\hat{p} \cdot \hat{A}(\hat{r})}{m} + \frac{e^2 \hat{A}(\hat{r})^2}{2m} = \hat{H}_A + \hat{H}_{AA}$$

That will be treated within the perturbation theory. The important thing to keep in mind is that the scattering process is accounted for the annihilation of a photon with momentum \vec{k}_I and polarization $\hat{\epsilon}_I$, and the creation of a photon with momentum \vec{k}_F and polarization $\hat{\epsilon}_F$. The perturbation term **must therefore contain** a product of the annihilation operator $a_{\hat{\epsilon}_I, \vec{k}_I}$ and the creation $a_{\hat{\epsilon}_F, \vec{k}_F}^\dagger$. Such terms are present in $\hat{H}_{AA} = \frac{e^2 \hat{A}(\hat{r})^2}{2m}$ that can therefore be treated to the first order of perturbation, but not directly in $\hat{H}_A = \frac{e\hat{p} \cdot \hat{A}(\hat{r})}{m}$, that must be treated in the second order (to the first order, this term can only describe absorption or emission of a photon). This yield to 'resonant scattering', that is far beyond the scope of the present lecture. We will only consider the non-resonant case, that dominates the scattering cross-section as long as the incident energy of the incoming photon is far from any absorption edge.



As in the classical calculation, we want to evaluate the number of photons $W_{\Delta\Omega}$ scattered into a solid angle $\Delta\Omega$ around \vec{k}_F . This is given by Fermi golden rule:

$$W_{\Delta\Omega} = \frac{2\pi}{\hbar} \int |M_{IF}|^2 \rho(E_F) \delta(E_F - E_I) dE_F$$

Where the integral runs over all the possible final photon states within $\Delta\Omega$ [the electronic state is not changing], satisfying the conservation of energy, and $M_{IF} = \langle \Psi_F | \hat{H}_{AA} | \Psi_I \rangle$. The density of photon states $\rho(E)$ is given by: $\rho(E) = \frac{v}{(2\pi)^3} \frac{d\vec{k}}{dE}$, that is, in $\Delta\Omega$: $\rho(E_F) = \frac{v\Delta\Omega k_F^2 d\vec{k}_F}{(2\pi)^3 dE_F} = \frac{vE_F^2 \Delta\Omega}{(2\pi \hbar c)^3}$ (using $E_F = \hbar c |\vec{k}_F|$).

On the other hand, as we saw in the classical calculation, the number of photons detected in $\Delta\Omega$ can also be defined using the differential cross section: $W_{\Delta\Omega} = \frac{d\sigma}{d\Omega} \phi_0 \Delta\Omega$. Where ϕ_0 is the incident photon flux. Let us consider that the incident photon beam is perfectly monochromatic and polarized, that is that the initial quantum state of the system reads: $|\Psi_I\rangle = |\psi\rangle | \dots, n_{\hat{\epsilon}_I, \vec{k}_I} = n_I^0, \dots, n_{\hat{\epsilon}_F, \vec{k}_F} = 0, \dots \rangle$ (We simply mean that there are no other photons than the n_I^0 ones with momentum \vec{k}_I and polarization $\hat{\epsilon}_I$!). The incident photon flux is therefore: $\phi_0 = \frac{n_I^0 c}{v}$

This yields:

$$\frac{d\sigma}{d\Omega} = \frac{V^2}{n_I^0 (2\pi \hbar^2 c^2)^2} \int |M_{IF}|^2 E_F^2 \delta(E_F - E_I) dE_F$$

We now have to evaluate $M_{IF} = \frac{e^2}{2m} \langle \Psi_F | \hat{A}(\hat{r})^2 | \Psi_I \rangle$ (we use $\omega \equiv \omega_{\vec{k}, \hat{\epsilon}}$ and $\omega' \equiv \omega_{\vec{k}', \hat{\epsilon}'}$)

$$\begin{aligned} & \hat{A}(\hat{r})^2 \\ &= \frac{\hbar}{2\varepsilon_0 V} \sum_{\hat{\epsilon}, \vec{k}, \hat{\epsilon}', \vec{k}'} \frac{[\hat{\epsilon} a_{\vec{k}, \hat{\epsilon}} e^{i(\vec{k} \cdot \vec{r} - \omega t)} + \hat{\epsilon}^* a_{\vec{k}, \hat{\epsilon}}^\dagger e^{-i(\vec{k} \cdot \vec{r} - \omega t)}] [\hat{\epsilon}' a_{\vec{k}', \hat{\epsilon}'} e^{i(\vec{k}' \cdot \vec{r} - \omega' t)} + \hat{\epsilon}'^* a_{\vec{k}', \hat{\epsilon}'}^\dagger e^{-i(\vec{k}' \cdot \vec{r} - \omega' t)}]}{\sqrt{\omega \omega'}} \\ &= \frac{\hbar}{2\varepsilon_0 V} \sum_{\hat{\epsilon}, \vec{k}, \hat{\epsilon}', \vec{k}'} \frac{\hat{\epsilon} \hat{\epsilon}' a_{\vec{k}, \hat{\epsilon}} a_{\vec{k}', \hat{\epsilon}'} e^{i((\vec{k} + \vec{k}') \cdot \vec{r} - (\omega + \omega') t)}}{\sqrt{\omega \omega'}} + \frac{\hat{\epsilon} \hat{\epsilon}'^* a_{\vec{k}, \hat{\epsilon}} a_{\vec{k}', \hat{\epsilon}'}^\dagger e^{i((\vec{k} - \vec{k}') \cdot \vec{r} - (\omega - \omega') t)}}{\sqrt{\omega \omega'}} \\ &+ \frac{\hat{\epsilon}^* \hat{\epsilon}' a_{\vec{k}, \hat{\epsilon}}^\dagger a_{\vec{k}', \hat{\epsilon}'} e^{-i((\vec{k} - \vec{k}') \cdot \vec{r} - (\omega - \omega') t)}}{\sqrt{\omega \omega'}} + \frac{\hat{\epsilon}^* \hat{\epsilon}'^* a_{\vec{k}, \hat{\epsilon}}^\dagger a_{\vec{k}', \hat{\epsilon}'}^\dagger e^{-i((\vec{k} + \vec{k}') \cdot \vec{r} - (\omega + \omega') t)}}{\sqrt{\omega \omega'}} \end{aligned}$$

Only the second and third term of this sum will contribute to the matrix element $\langle \Psi_F | \hat{A}(\hat{r})^2 | \Psi_I \rangle$ in the case of elastic scattering. Indeed the aa and $a^\dagger a^\dagger$ terms respectively account for the annihilation and the creation of two photons, and do therefore not contribute to scattering.

Mathematically, this comes from the fact that the photon part of the matrix element involving the aa term is:

$$\begin{aligned} & \langle 0, \dots, n_{\hat{\epsilon}_F, \vec{k}_F} = 1, \dots, n_{\hat{\epsilon}_I, \vec{k}_I} = n_I^0 - 1, \dots, 0 | a_{\vec{k}, \hat{\epsilon}} a_{\vec{k}', \hat{\epsilon}'} | 0, \dots, n_{\hat{\epsilon}_I, \vec{k}_I} = n_I^0, \dots, n_{\hat{\epsilon}_F, \vec{k}_F} = 0, \dots, 0 \rangle \\ &= \sqrt{n_I^0} \langle 0, \dots, n_{\hat{\epsilon}_F, \vec{k}_F} = 1, \dots, n_{\hat{\epsilon}_I, \vec{k}_I} = n_I^0 - 1, \dots, 0 | a_{\vec{k}, \hat{\epsilon}} | 0 \dots n_{\hat{\epsilon}_I, \vec{k}_I} = n_I^0 - 1, \dots, n_{\hat{\epsilon}_F, \vec{k}_F} = 0, \dots, 0 \rangle \delta_{\vec{k}_I, \vec{k}'} \delta_{\hat{\epsilon}_I, \hat{\epsilon}'} \end{aligned}$$

As indeed, there are no photons to annihilate in the initial state but those momentum \vec{k}_I and polarization $\hat{\epsilon}_I$. The application of the second annihilation operator gives

$$\sqrt{n_I^0} \sqrt{n_I^0 - 1} \left\langle 0, \dots, n_{\hat{\epsilon}_F, \vec{k}_F} = 1, \dots, n_{\hat{\epsilon}_I, \vec{k}_I} = n_I^0 - 1, \dots, 0 \middle| 0, \dots, n_{\hat{\epsilon}_F, \vec{k}_F} = 0, \dots, n_{\hat{\epsilon}_I, \vec{k}_I} = n_I^0 - 2, \dots, 0 \right\rangle \delta_{\vec{k}_I, \vec{k}'} \delta_{\hat{\epsilon}_I, \hat{\epsilon}'} \delta_{\vec{k}_I, \vec{k}} \delta_{\hat{\epsilon}_I, \hat{\epsilon}}$$

The same reasoning holds for the $a^\dagger a^\dagger$ term (there of course it is possible to create two photons with any momentum and polarization, but the net result is that the photon state in which we arrive is not the one we expect from the scattering process).

In the end, the only two non-vanishing terms in $\langle \Psi_F | \hat{A}(\hat{r})^2 | \Psi_I \rangle$ come from:

$$\begin{aligned} & \left\langle 0, \dots, n_{\hat{\epsilon}_F, \vec{k}_F} = 1, \dots, n_{\hat{\epsilon}_I, \vec{k}_I} = n_I^0 - 1, \dots, 0 \middle| a_{\vec{k}, \hat{\epsilon}}^\dagger a_{\vec{k}', \hat{\epsilon}'}^\dagger \middle| 0, \dots, n_{\hat{\epsilon}_I, \vec{k}_I} = n_I^0, \dots, n_{\hat{\epsilon}_F, \vec{k}_F} = 0, \dots, 0 \right\rangle \\ &= \sqrt{n_I^0} \delta_{\vec{k}_F, \vec{k}'} \delta_{\hat{\epsilon}_F, \hat{\epsilon}'} \delta_{\vec{k}_I, \vec{k}} \delta_{\hat{\epsilon}_I, \hat{\epsilon}} \end{aligned}$$

and

$$\begin{aligned} & \left\langle 0, \dots, n_{\hat{\epsilon}_F, \vec{k}_F} = 1, \dots, n_{\hat{\epsilon}_I, \vec{k}_I} = n_I^0 - 1, \dots, 0 \middle| a_{\vec{k}, \hat{\epsilon}}^\dagger a_{\vec{k}', \hat{\epsilon}'} \middle| 0, \dots, n_{\hat{\epsilon}_I, \vec{k}_I} = n_I^0, \dots, n_{\hat{\epsilon}_F, \vec{k}_F} = 0, \dots, 0 \right\rangle \\ &= \sqrt{n_I^0} \delta_{\vec{k}_F, \vec{k}} \delta_{\hat{\epsilon}_F, \hat{\epsilon}} \delta_{\vec{k}_I, \vec{k}'} \delta_{\hat{\epsilon}_I, \hat{\epsilon}'} \end{aligned}$$

As a result, we find that:

$$\begin{aligned} & \langle \Psi_F | \hat{A}(\hat{r})^2 | \Psi_I \rangle \\ &= \frac{\hbar}{2\epsilon_0 V} \sqrt{n_I^0} \sum_{\hat{\epsilon}, \vec{k}, \vec{k}', \hat{\epsilon}'} \frac{\langle \psi | \hat{\epsilon} \hat{\epsilon}'^* e^{i((\vec{k} - \vec{k}') \cdot \vec{r} - (\omega - \omega')t)} \delta_{\vec{k}_F, \vec{k}'} \delta_{\hat{\epsilon}_F, \hat{\epsilon}'} \delta_{\vec{k}_I, \vec{k}} \delta_{\hat{\epsilon}_I, \hat{\epsilon}} + \hat{\epsilon}' \hat{\epsilon}^* e^{-i((\vec{k} - \vec{k}') \cdot \vec{r} - (\omega - \omega')t)} \delta_{\vec{k}_F, \vec{k}} \delta_{\hat{\epsilon}_F, \hat{\epsilon}} \delta_{\vec{k}_I, \vec{k}'} \delta_{\hat{\epsilon}_I, \hat{\epsilon}'} | \psi \rangle}{\sqrt{\omega \omega'}} \end{aligned}$$

using $\vec{Q} = \vec{k}_I - \vec{k}_F$ and $\omega_I = \omega_F = E_F / \hbar$, we simply obtain:

$$\langle \Psi_F | \hat{A}(\hat{r})^2 | \Psi_I \rangle = \frac{\hbar^2}{\epsilon_0 V E_F} \sqrt{n_I^0} \hat{\epsilon}_I \cdot \hat{\epsilon}_F^* \langle \psi | e^{i\vec{Q} \cdot \vec{r}} | \psi \rangle$$

and thus:

$$M_{IF} = \frac{e^2 \hbar^2}{2m\epsilon_0 V E_F} \sqrt{n_I^0} \hat{\epsilon}_I \cdot \hat{\epsilon}_F^* \langle \psi | e^{i\vec{Q} \cdot \vec{r}} | \psi \rangle$$

Which allows us to write the differential cross-section as:

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= \frac{V^2}{n_I^0 (2\pi \hbar^2 c^2)^2} \left(\frac{e^2 \hbar^2}{2m\epsilon_0 V} \hat{\epsilon}_I \cdot \hat{\epsilon}_F^* \right)^2 n_I^0 \left| \langle \psi | e^{i\vec{Q} \cdot \vec{r}} | \psi \rangle \right|^2 \int \delta(E_F - E_I) dE_F \\ &= \left(\frac{e^2}{4\pi m\epsilon_0 c^2} \right)^2 (\hat{\epsilon}_I \cdot \hat{\epsilon}_F^*)^2 \left| \langle \psi | e^{i\vec{Q} \cdot \vec{r}} | \psi \rangle \right|^2 = r_0^2 \wp \left| \langle \psi | e^{i\vec{Q} \cdot \vec{r}} | \psi \rangle \right|^2 \end{aligned}$$

Finally, inserting the completeness conditions $\int d\vec{r} |\vec{r}\rangle\langle\vec{r}| = 1$ in the above equation and the fact that $\psi^*(\vec{r})\psi(\vec{r}) = \rho(\vec{r})$ we easily get that $\langle\psi|e^{i\vec{Q}\cdot\vec{r}}|\psi\rangle = f(\vec{Q})$ and therefore prove the equivalence of the classical and quantum approaches for the calculation of the Thomson cross section from a charge distribution:

$$\left(\frac{d\sigma}{d\Omega}\right)_{Th} = r_0^2 \wp |f(\vec{Q})|^2$$

3) Physical meaning of $f(\vec{Q})$

As mentioned earlier, $f(\vec{Q}) = \int \rho(\vec{r}) e^{i\vec{Q}\cdot\vec{r}} d\vec{r}$ is the Fourier transform the electronic density. As $\vec{Q} \rightarrow 0$, all parts of the electronic cloud radiate in phase, and we simply get: $f(\vec{Q} \rightarrow 0) = \int \rho(\vec{r}) d\vec{r} = Z$, where Z is the number of electrons in the charge cloud. Not surprisingly, the heavier atoms are the best scatterers. At large \vec{Q} , all parts of the cloud radiate incoherently, yielding $f(\vec{Q} \rightarrow \infty) = 0$.

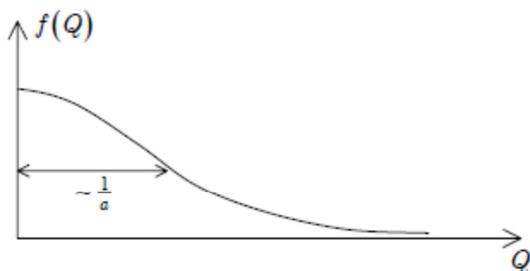
Example: hydrogen atom in its ground state

$\psi(\vec{r}) = \psi_{1s}(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$ where a_0 is the Bohr radius.

$$\begin{aligned} f(\vec{Q}) &= \int \rho(\vec{r}) e^{i\vec{Q}\cdot\vec{r}} d\vec{r} = \frac{1}{\pi a_0^3} \int e^{-2r/a_0} \cdot e^{i\vec{Q}\cdot\vec{r}} d\vec{r} = \frac{2\pi}{\pi a_0^3} \iint e^{-2r/a_0} \cdot e^{iQr \cos\theta} \sin\theta d\theta r^2 dr \\ &= \frac{2}{a_0^3} \int e^{-2r/a_0} \cdot \frac{e^{iQr} - e^{-iQr}}{iQ} r^2 dr \end{aligned}$$

After integration by part, we get:

$$f(\vec{Q}) = \frac{-2}{a_0^3 Q} \int \frac{e^{-\frac{2r}{a_0} + iQr}}{-\frac{2}{a_0} + iQ} + \frac{e^{-\frac{2r}{a_0} - iQr}}{\frac{2}{a_0} + iQ} dr = \frac{-2}{a_0^3 Q} \left[\frac{1}{\left(-\frac{2}{a_0} + iQ\right)^2} - \frac{1}{\left(\frac{2}{a_0} + iQ\right)^2} \right] = \frac{1}{\left(1 + \left(\frac{Qa}{2}\right)^2\right)^2}$$



width of form factor
 $\sim \frac{1}{\text{size of atom}}$

Note that this is only valid far away from any resonance. In this case, the electrons always appear 'free' to the x-ray electric field, and can accelerate and radiate as discussed. On the other hand, if the photon energy matches the energy of an absorption edge, a resonance phenomenon occurs. This can be simply modeled by a damped forced oscillator.

As a result, the atomic form factor becomes $f(\vec{Q}, \omega) = f^0(\vec{Q}) + f_1(\vec{Q}, \omega) + if_2(\vec{Q}, \omega)$. In this expression, $f^0(\vec{Q})$ is the non-resonant form factor that has been discussed so far, corrected by a complex form factor $f_1(\vec{Q}, \omega) + if_2(\vec{Q}, \omega)$, strongly frequency dependent that accounts for the resonant absorption during the scattering process. In the quantum mechanical approach, this correction arises from the H_A term, treated to the second order in perturbation.