

Thomson Scattering

Let H_{atom} be the hamiltonian for an atom in the absence of radiation. Let H_{ph} be the hamiltonian for photons without matter. The interaction V is

$$V = \sum_{i=1}^N -\frac{q}{m} \vec{p}_i \cdot \vec{A}(x_i, 0) + \frac{q^2}{2m} \vec{A}^2(x_i, 0). \quad (1)$$

in which $N=Z$ is the number of electrons in the atom.

So far we've been ignoring the A^2 term. But it plays a role in the scattering of light by atoms. In fact, it dominates when $\hbar\omega$ is much greater than the kinetic energies of the atom's electrons.

Let's compute the amplitude for a photon of momentum $\hbar\vec{k}$ and polarization $\vec{E}_r(\vec{k})$ and an atom in state A to become a photon of momentum $\hbar\vec{k}'$ and polarization $\vec{E}_r(\vec{k}')$ and an atom in state B .

$$A + \hbar \rightarrow B + \hbar'$$

We'll work first at an energy high enough so that we may ignore the $\vec{p} \cdot \vec{A}$ terms,

The amplitude due to the A^2 term is

$$\begin{aligned}
 \langle k' B | S(t, 0) | k A \rangle &= -\frac{i}{\hbar} \int_0^t dt' \langle k' B | e^{i(H_{0B} + H_{0F})t'/\hbar} \sum_{j=1}^N \frac{q^2}{2m} \vec{A}(\vec{x}_j, 0) \\
 &\quad \times e^{-i(H_{0B} + H_{0F})t'/\hbar} | k A \rangle \\
 &= -\frac{i}{\hbar} \frac{q^2}{2m} \langle k' B | \sum_{j=1}^N \vec{A}(\vec{x}_j, 0)^2 | k A \rangle \int_0^t dt' e^{i(E_B + \hbar\omega' - E_A - \hbar\omega)t'/\hbar} \\
 &= -\frac{q^2}{2m} \langle k' B | \sum_{j=1}^N \vec{A}(\vec{x}_j, 0)^2 | k A \rangle \frac{(e^{i\Delta E t/\hbar} - 1)}{\Delta E} \quad (2)
 \end{aligned}$$

where

$$\Delta E = E_B + \hbar\omega' - E_A - \hbar\omega. \quad (3)$$

The atomic matrix element is

$$\begin{aligned}
 \langle k' B | \sum_{j=1}^N \vec{A}(\vec{x}_j, 0)^2 | k A \rangle &= \frac{\hbar}{2\epsilon_0 V \sqrt{\omega\omega'}} \\
 &\times \langle k' B | \sum_{j=1}^N \left(\vec{\epsilon}(\vec{k}) a(\vec{k}) e^{i\vec{k}\cdot\vec{x}_j} + \vec{\epsilon}(\vec{k}') a^\dagger(\vec{k}') e^{-i\vec{k}'\cdot\vec{x}_j} \right)^2 | k A \rangle, \quad (4)
 \end{aligned}$$

At optical frequencies $|\vec{k}\cdot\vec{x}_j| \sim 10^{-3}$, so the dipole approximation is valid even far above optical frequencies. Once we replace

$$e^{i\vec{k}\cdot\vec{x}_j} \quad \text{by} \quad 1,$$

no atomic variable remains in the matrix element, and so we have

$$\begin{aligned} \langle h' B | \sum_{j=1}^{N \rightarrow 2} A(x_j, 0) | h A \rangle &= \frac{\hbar}{2\epsilon_0 V \sqrt{\omega \omega'}} \langle h' B | N (\epsilon a + \epsilon' a'^{\dagger})^2 | h A \rangle \\ &= \frac{N \hbar S_{AB}}{2\epsilon_0 V \sqrt{\omega \omega'}} \langle h' | (\epsilon a + \epsilon' a'^{\dagger})^2 | h \rangle. \end{aligned} \quad (5)$$

In the continuum limit, $\hbar = \hbar'$ never happens, and so we ignore this possibility here. We find

$$\langle h' B | \sum_{j=1}^N \vec{A}(x_j, 0) | h A \rangle = \frac{N \hbar S_{AB}}{\epsilon_0 V \sqrt{\omega \omega'}} \vec{\epsilon}_h(\hbar) \cdot \vec{\epsilon}_{h'}^*(\hbar'). \quad (6)$$

For $\hbar \omega > 100 \text{ eV}$, the dipole approximation still works and the terms due to $p \cdot A$ in second order are small compared to the \vec{A}^2 term, as we'll see presently. In this case, the probability is

$$\begin{aligned} P(t) &= \left(\frac{q^2}{2m} \right)^2 \left(\frac{N \hbar}{\epsilon_0 V} \right)^2 \frac{S_{AB}}{\omega \omega'} \left| \vec{\epsilon}_h(\hbar) \cdot \vec{\epsilon}_{h'}^*(\hbar') \right|^2 \\ &\times 4 \frac{\sin^2 \Delta E t / 2\hbar}{(\Delta E)^2}. \end{aligned} \quad (7)$$

Using again the δ -function identity

$$\lim_{t \rightarrow \infty} \frac{\sin^2 \Delta E t / \hbar}{(\Delta E)^2} = \frac{\pi t}{2\hbar} \delta(\Delta E) \quad (8)$$

and also the δ -term δ_{AB} , we find $\omega' = \omega$ and

$$P(t) = \frac{\pi t}{2\hbar} \left(\frac{q^2 N \hbar}{m \epsilon_0 V \omega} \right)^2 \delta_{AB} |\vec{E}_A(\omega) \cdot \vec{E}_B^*(\omega')|^2 \times \delta(\hbar\omega' - \hbar\omega). \quad (9)$$

The rate is then

$$\hat{w} = \frac{\pi}{2\hbar} \left(\frac{q^2 N \hbar}{m \epsilon_0 V \omega} \right)^2 \delta_{AB} |\vec{E} \cdot \vec{E}'|^2 \delta(\hbar\omega' - \hbar\omega) \quad (10)$$

which we sum over final states.

$$\begin{aligned} W &= \sum_{n'} V \int \frac{d^3 k}{(2\pi)^3} \hat{w} \\ &= \frac{\pi}{2} \sum_{n'} \frac{1}{(2\pi)^3} \frac{\hbar}{V} \left(\frac{q^2 N}{m \epsilon_0 \omega} \right)^2 \delta_{AB} |\vec{E} \cdot \vec{E}'|^2 \delta(\hbar\omega' - \hbar\omega) d^3 k \quad (11) \end{aligned}$$

Now $\hbar\omega = \hbar kc$, so $d^3 k = \frac{k^2}{\hbar c} d\hbar\omega d\Omega$, so

$$W = \sum_{n'} \frac{\pi \hbar}{2} \frac{1}{(2\pi)^3} \frac{1}{V} \left(\frac{q^2 N}{m \epsilon_0 \omega} \right)^2 \delta_{AB} |\vec{E} \cdot \vec{E}'|^2 \frac{k^2}{\hbar c} d\Omega. \quad (12)$$

So dividing by the incident flux $F = c/V$ we get

$$\frac{d\sigma}{d\Omega} = \frac{v}{c} \sum_{\omega'} \frac{\pi \hbar}{2} \frac{1}{(2\pi)^3} \frac{1}{V} \left(\frac{q^2 N}{m\omega} \right)^2 S_{AB} |\mathbf{E} \cdot \mathbf{E}'|^2 \frac{k^2}{\hbar c}$$

$$= \sum_{\omega'} \frac{k^2}{16 \pi^2 c^2} \left(\frac{q^2 N}{m\omega} \right)^2 S_{AB} |\mathbf{E} \cdot \mathbf{E}'|^2 \quad (13)$$

Now $q^2 = 4\pi\epsilon_0 \alpha \hbar c$, so

$$\frac{d\sigma}{d\Omega} = \sum_{\omega'} \frac{k^2 N^2}{16 \pi^2 c^2} \left(\frac{4\pi \alpha \hbar c}{m\omega} \right)^2 S_{AB} |\mathbf{E} \cdot \mathbf{E}'|^2$$

$$= \sum_{\omega'} N^2 \left(\frac{\alpha \hbar c}{cm \omega} \right)^2 S_{AB} |\mathbf{E} \cdot \mathbf{E}'|^2$$

$$= \sum_{\omega'} N^2 \left(\frac{\alpha \hbar}{cm} \right)^2 S_{AB} |\mathbf{E} \cdot \mathbf{E}'|^2 \quad (14)$$

The classical radius of the electron r_0 is

$$r_0 = \frac{\alpha \hbar}{mc} \approx 2.82 \times 10^{-13} \text{ cm} \quad (15)$$

So the Thomson-scattering σ -section is

$$\frac{d\sigma}{d\Omega} = \sum_{\omega'} (Nr_0)^2 |\vec{E}_\omega(\mathbf{h}) \cdot \vec{E}_{\omega'}^*(\mathbf{h}')|^2 \quad (16)$$

Actually, Thomson's result is for scattering off a single free electron.

Note the factor of $N = Z^2$ in the formula (16) for the x-section.

So an oxygen atom with $Z=8$ - scatters 64 times more than a hydrogen atom.

This is why H-atoms do not show up in x-ray crystallographs of proteins and other molecules. The locations of the hydrogen atoms must be inferred theoretically.

Now

$$\begin{aligned} \sum_{r'} | \epsilon_r(\mathbf{k}) \cdot \epsilon_r^*(\mathbf{h}') |^2 \\ &= \epsilon_r^*(\mathbf{h}) (1 - \hat{\mathbf{h}}' \hat{\mathbf{h}}'^T) \epsilon_r(\mathbf{h}) \\ &= 1 - (\hat{\mathbf{h}}' \cdot \epsilon_r(\mathbf{k}))^2 \end{aligned} \quad (17)$$

So

$$\frac{d\sigma}{d\Omega} = (N r_0)^2 \left[1 - \left[\hat{\mathbf{h}}' \cdot \epsilon_r(\mathbf{k}) \right]^2 \right]. \quad (18)$$

If the initial beam of photons is unpolarized, then we average over $\epsilon_r(\mathbf{h})$:

$$\begin{aligned} \frac{1}{2} \sum_V [\hat{h}' \cdot \epsilon_r(\hat{h})]^2 &= \frac{1}{2} \hat{h}' (1 - \hat{h} \cdot \hat{h}^T) \hat{h}' \\ &= \frac{1}{2} (1 - (\hat{h} \cdot \hat{h}')^2). \end{aligned} \quad (19)$$

In this case,

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= (Nv_0)^2 \left[1 - \frac{1}{2} (1 - (\hat{h} \cdot \hat{h}')^2) \right] \\ &= (Nv_0)^2 \left[\frac{1}{2} + \frac{1}{2} (\hat{h} \cdot \hat{h}')^2 \right] \\ &= (Nv_0)^2 \frac{1}{2} (1 + \cos^2 \theta) \end{aligned} \quad (20)$$

where θ is the angle between \hat{h} and \hat{h}' , which is the angle of scattering.

Forward and backward scattering are enhanced by a factor of 2 due to $\epsilon_r(\hat{h})$ and $\epsilon_r(\hat{h}')$.

The total x-section is

$$\begin{aligned} \sigma &= \int \frac{d\sigma}{d\Omega} d\Omega = 2\pi \int_{-1}^1 dx (Nv_0)^2 \frac{1}{2} (1 + x^2) \\ &= 2\pi (Nv_0)^2 \left(1 + \frac{1}{3}\right) = \frac{8\pi}{3} (Nv_0)^2. \end{aligned} \quad (21)$$