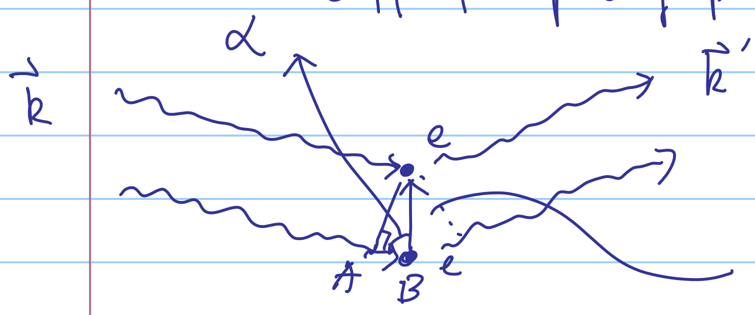
X-ray case

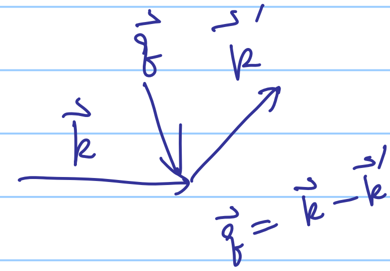
Note Title 31/01/2012

$$\frac{d^2\sigma}{d\Omega} \propto |U(\vec{q})|^2 S(\vec{q})$$

$S(\vec{q}) = S_{nn}(\vec{q}) + \sum_G |\langle n_G \rangle|^2 (2\pi)^2 \delta(\vec{q}-\vec{G})$

$U(\vec{q})$: diff for probing particles





AB: phase difference: $2\pi \frac{AB}{\lambda} = \underbrace{\frac{2\pi}{\lambda}} \cdot |\vec{x}| \cos\alpha$

$= \vec{k} \cdot \vec{x}$

phase difference for $\vec{k}'$: $-\vec{k}' \cdot \vec{x}$

Total phase difference: $(\vec{k} - \vec{k}') \cdot \vec{x} = \vec{q} \cdot \vec{x}$

Total scattering amplitude: $U(\vec{q}) = -r_0 (1 + e^{i\vec{q}\cdot\vec{x}})$

$$r_0 = \frac{e^2}{4\pi\epsilon_0 m c^2} \simeq 2.82 \times 10^{-5} \, \text{Å}$$

Classical Thomson scattering length

① 180° phase shift

② constant ($U(\vec{q})$ is constant)

Total scattering intensity $I(\vec{q}) = |U|^2 = 2r_0^2 (1 + \cos \vec{q}\cdot\vec{x})$

For many electrons

$$U(\vec{q}) = -r_0 \sum_i e^{i\vec{q}\cdot\vec{x}_i} = -r_0 \int d\vec{x} \, \rho_e(\vec{x}) \, e^{i\vec{q}\cdot\vec{x}}$$

(semiclassical picture)

For bound electrons

$$U(\vec{q})\left(= f(\vec{q})\right) = \int \rho_e(\vec{x})\, e^{i\vec{q}\cdot\vec{x}}\, d\vec{x} = \begin{cases} Z & \vec{q} \to 0 \\ 0 & \vec{q} \to \infty \end{cases}$$

$\Rightarrow$ atomic form factor

$\boxed{\text{Example}}$ 1s electron in H

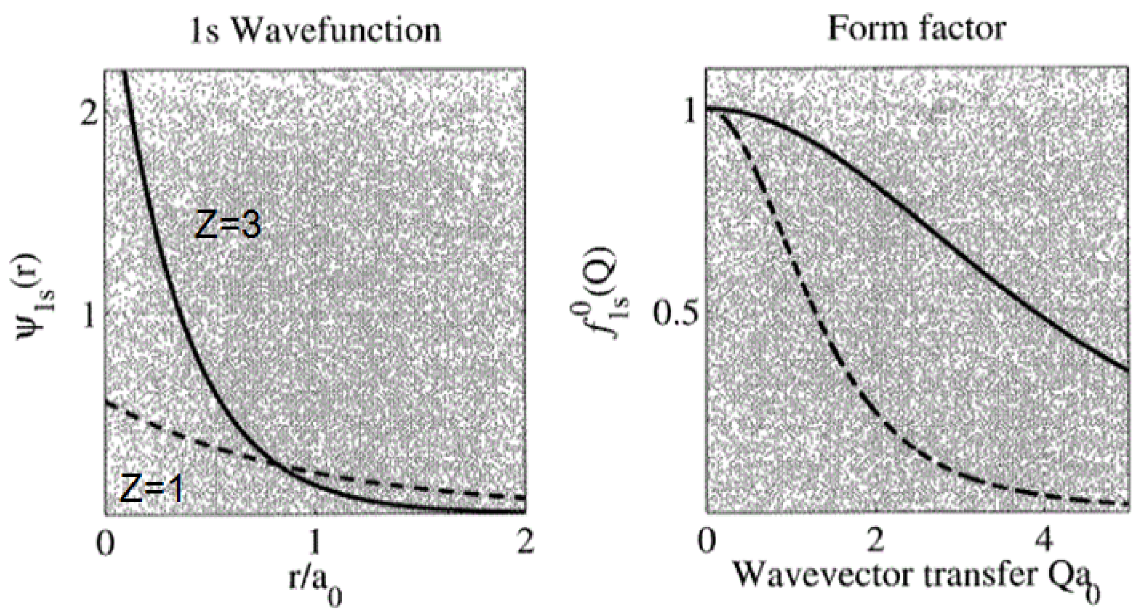
$$\psi_{1s}(r) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a} \qquad a = \frac{a_0}{Z - Z_s}$$

$Z_s \sim 0.3$ (screening)

$$f_{1s}(\vec{q}) = \frac{1}{\pi a^3}\int e^{-2r/a} e^{i\vec{q}\cdot\vec{x}}\, d\vec{x}$$

$$\vdots$$

$$= \frac{1}{\left[1 + \left(qa/2\right)^2\right]^2}$$



Wavefn. localized $\longleftrightarrow$ Form factor falls slowly with Q

Scattering from a molecule.

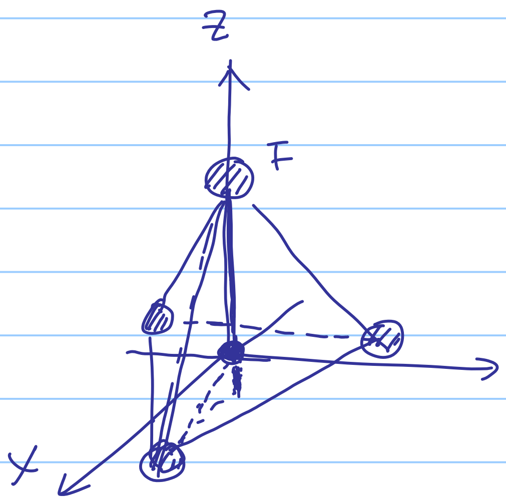
For each electron : $U(\vec{q})$ constant $(-r_0)$

" " atom : $f(\vec{q})$: atomic form factor

" " molecule : $F_{mol}(\vec{q})$: molecular form factor

$$= \sum_j f_j(\vec{q})\, e^{i\vec{q}\cdot\vec{r}_j}$$

$\boxed{\text{Example}}$ CF_4 (perfect tetrahedron)



C: origin, C−F: a

F: $(0, 0, a)$

$\left(\frac{2\sqrt{2}}{3}a, 0, -\frac{a}{3}\right)$

$\left(-\frac{\sqrt{2}}{3}a, \sqrt{\frac{2}{3}}a, -\frac{a}{3}\right)$

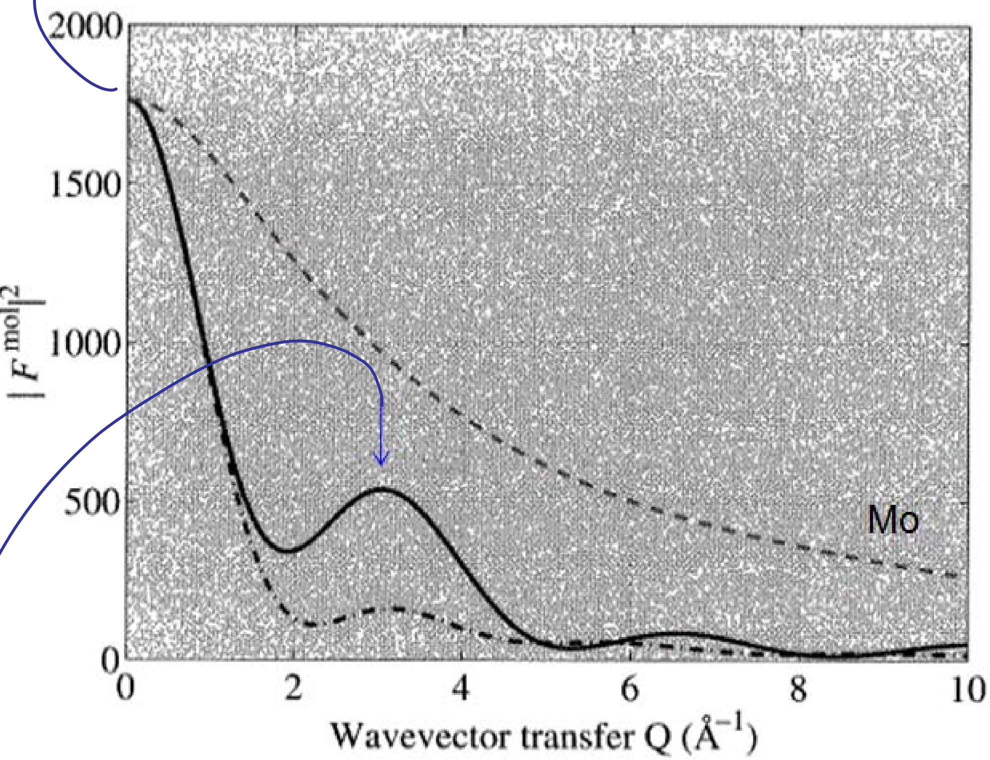
$\left(-\frac{\sqrt{2}}{3}a, -\sqrt{\frac{2}{a}}a, -\frac{a}{3}\right)$

$\vec{q} \parallel \hat{z}$

$$F^{mol}(\vec{q}) = f_C(\vec{q}) + f_F(\vec{q})\left[3e^{-iqa/3} + e^{iqa}\right]$$

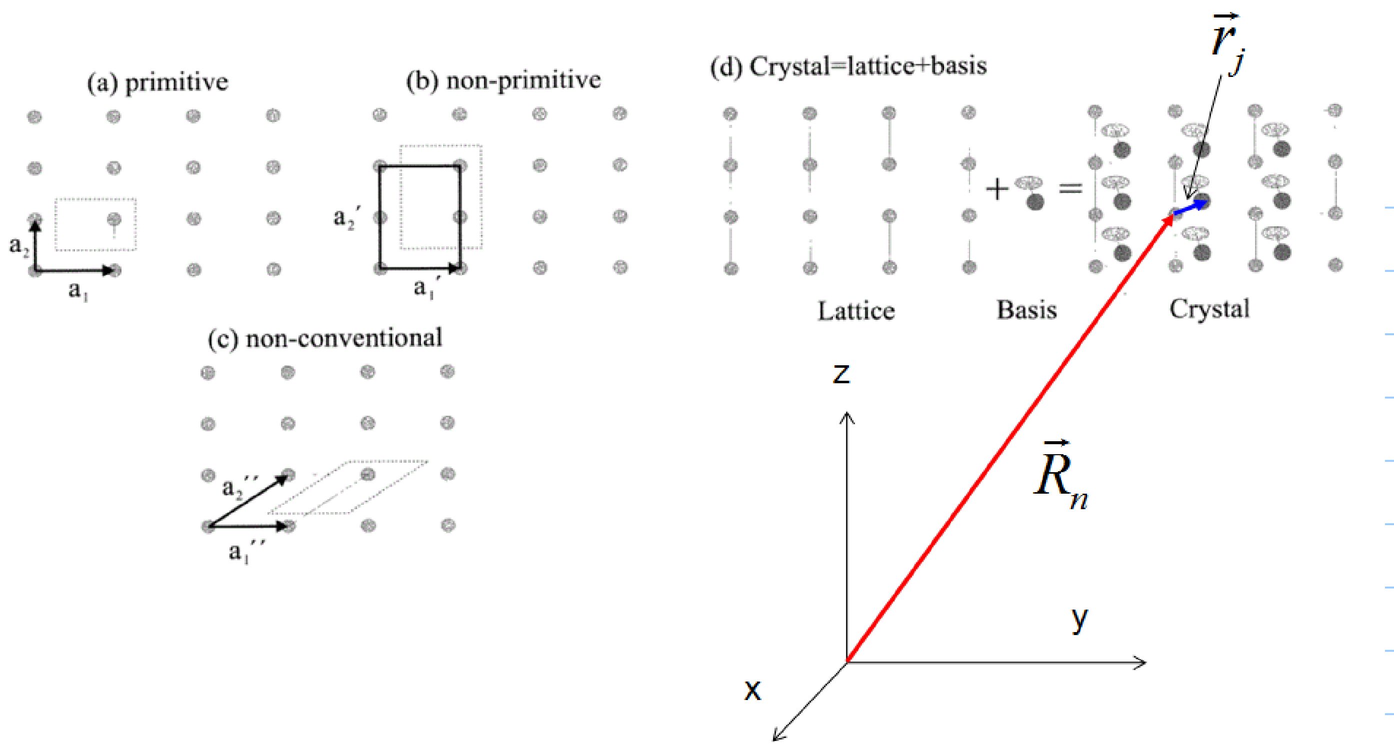
↑ molecular form factor ↑ A.F.F.

$(42)^2$ @ $q=0$



F-F bond length $\sim a \cdot \sqrt{\frac{8}{3}} \sim 1.38\sqrt{\frac{8}{3}}$ Å

$$\frac{2\pi}{(F\text{-}F)} \sim \frac{2\pi}{1.3\sqrt{\frac{8}{3}}} \sim 2.8\,(\mathring{A}^{-1})$$



$$F^{\text{crystal}}(\vec{q}) = \sum_{\vec{r}_j,\,\vec{R}_n} f_j(\vec{q})\, e^{i\vec{q}\cdot(\vec{R}_n+\vec{r}_j)}$$

$$= \underbrace{\left(\sum_{\vec{r}_j} f_j(\vec{q})\, e^{i\vec{q}\cdot\vec{r}_j}\right)}_{\text{basis (molecular) form factor}} \underbrace{\left(\sum_{n} e^{i\vec{q}\cdot\vec{R}_n}\right)}_{\text{lattice sum} \to I(\vec{q})}$$

$\boxed{\text{1D example}}$ $\quad \vec{R}_n = na \qquad n = 0, 1, 2, \ldots$

$$\left|\sum\right|^2 = \sum_{q} N \frac{2\pi}{a}\, \delta\!\left(q - \frac{2\pi}{a} n\right)$$

} exercise