Elastic scattering from atoms

- Structural probes: X-rays, neutron, electrons
- Basics of scattering
- X-ray Thomson scattering
- Interference
- Deviations from classical treatment
  - ✓ electronic distribution
  - ✓ Compton effect
  - ✓ electron binding
- Neutron and electron scattering

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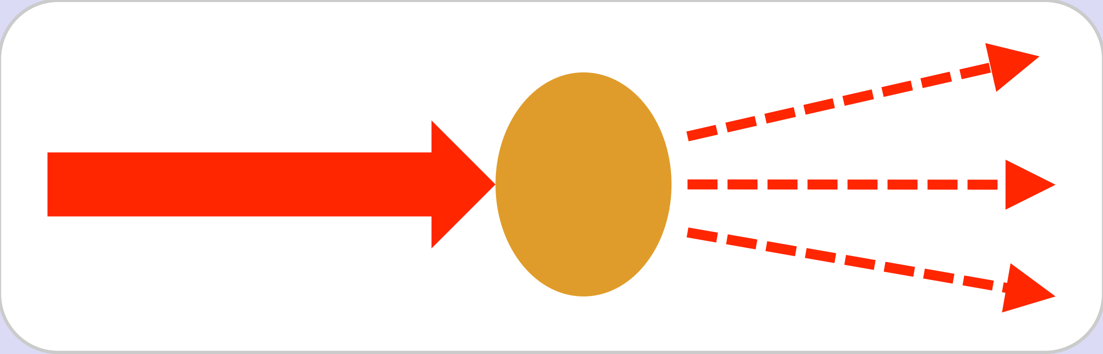
April 2017

Structural probes



Probes

Electromagnetic radiation
- microwaves
- infrared
- visible
- UV
- X-rays

Electrons
Positrons
Neutrons
Ions
....

Wave-particle duality

Info on:

Structural properties
- macroscopic
- ......
- atomic level

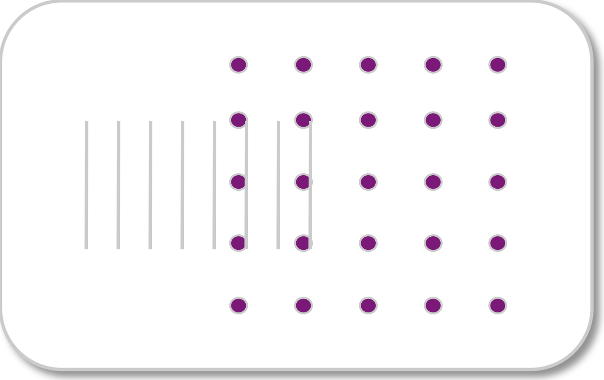
Electronic properties

Vibrational properties

Atomic-level structural probes

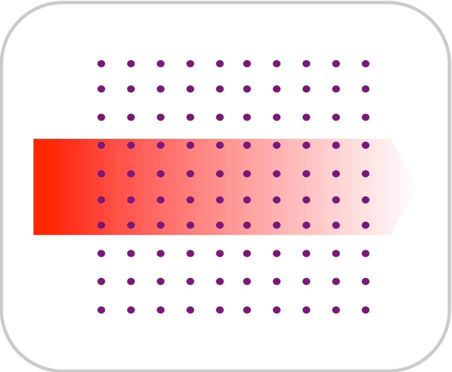
Basic requirement:

Wavelength ≤ inter-atomic distances



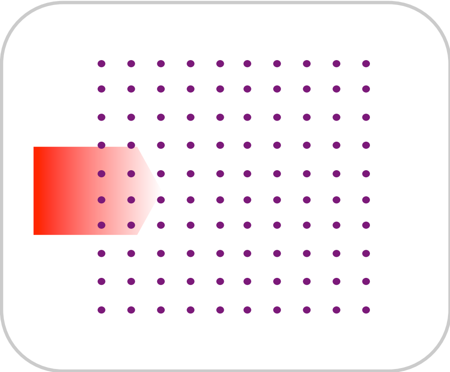
- X-rays
- Thermal neutrons
- Low-energy electrons

Weak interaction
High penetration depth



Bulk probes

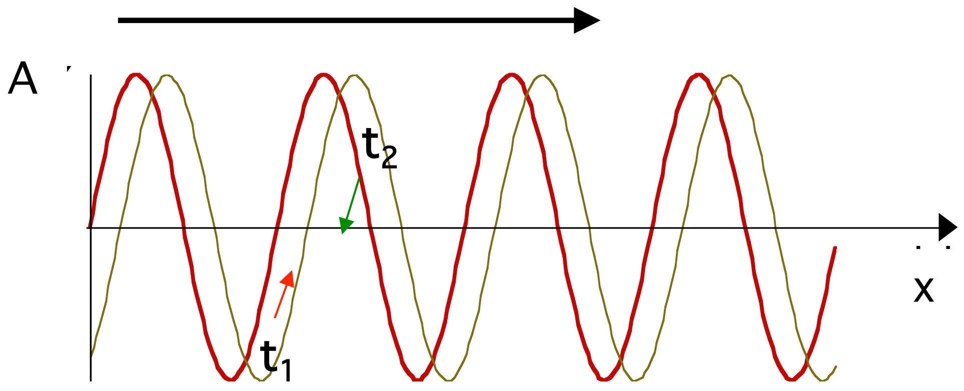
Strong interaction
Low penetration depth



Surface probes

> Properties X-rays, neutrons, electrons

Plane waves equation – 1 dimension



Sinusoidal wave

Electromagnetic fields

$$A(x,t) = \mathrm{Re}\left\{A_0 \exp\left[i(kx - \omega t)\right]\right\}$$

$$= \mathrm{Re}\left\{A_0 \exp\left[i\,2\pi\left(\frac{x}{\lambda} - \frac{t}{T}\right)\right]\right\}$$

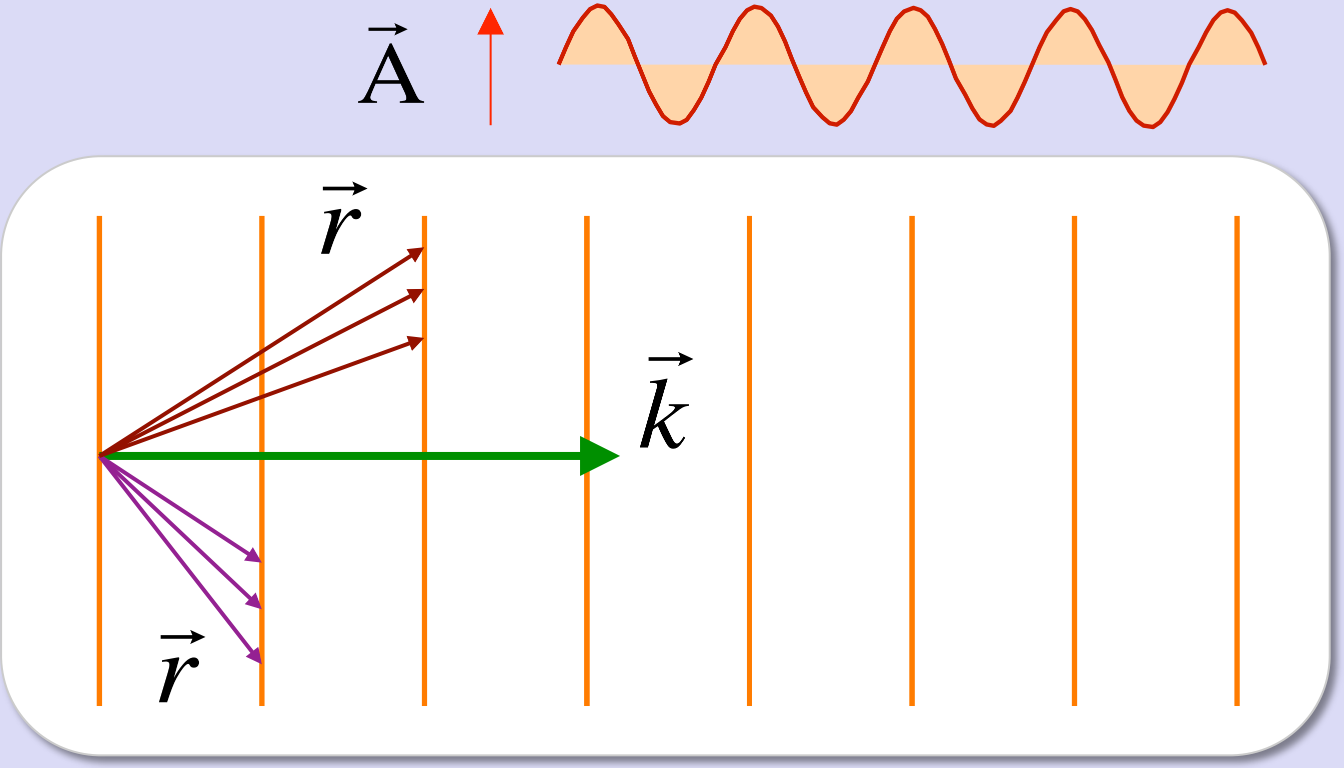
$$= A_0 \cos(kx - \omega t)$$

Matter wavefunctions

$$\Psi(x,t) = \Psi_0 \exp\left[i(kx - \omega t)\right]$$

$$= \Psi_0 \exp\left[i\,2\pi\left(\frac{x}{\lambda} - \frac{t}{T}\right)\right]$$

Plane waves – 3 dimensions



$$\vec{k} = \frac{2\pi}{\lambda}\,\hat{s}$$

Wavevector

Electromagnetic fields

$$\begin{aligned}\vec{A}(\vec{r},t) &= \mathrm{Re}\left\{A_0 \exp\left[i\left(\vec{k}\cdot\vec{r}-\omega t\right)\right]\right\}\\ &= \mathrm{Re}\left\{A_0 \exp\left[i2\pi\left(\frac{\hat{s}\cdot\vec{r}}{\lambda}-\frac{t}{T}\right)\right]\right\}\end{aligned}$$

Matter wavefunctions

$$\begin{aligned}\Psi(\vec{r},t) &= \Psi_0 \exp\left[i\left(\vec{k}\cdot\vec{r}-\omega t\right)\right]\\ &= \Psi_0 \exp\left[i2\pi\left(\frac{\hat{s}\cdot\vec{r}}{\lambda}-\frac{t}{T}\right)\right]\end{aligned}$$

Particle properties

$$\boxed{E^2 = \left(m_0 c^2\right)^2 + (pc)^2}$$

E

energy

$1\,\mathrm{eV} \cong 1.6 \times 10^{-19}\ \mathrm{J}$

$c \cong 3 \times 10^8\ \mathrm{m/s}$

m_0 rest mass

$\vec{p}$

linear momentum

Connection particle – wave properties

$$\boxed{E = \hbar\omega = h\nu}$$

$$\boxed{\vec{p} = \hbar\vec{k} = (h/\lambda)\,\hat{s}}$$

Particle and wave properties

Electromagnetic fields

$$E = pc = \hbar kc$$

(non-relativistic)

Matter

$$E_k = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

$$\omega = kc \Leftarrow E = \hbar\omega \Rightarrow \omega = \frac{\hbar k^2}{2m}$$

Phase velocity

in vacuum $v_\phi = \frac{\lambda}{T} = \frac{\omega}{k} = c$

$$v_\phi = \frac{\lambda}{T} = \frac{\omega}{k} = \frac{\hbar k}{2m} = \frac{p}{2m}$$

Group velocity

in vacuum $v_g = \frac{d\omega}{dk} = c$

$$v_g = \frac{d\omega}{dk} = \frac{\hbar k}{m} = \frac{p}{m} = v$$

Wave – particle properties

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$$\boxed{E_{\text{tot}}^2 = (pc)^2 + \left(m_0 c^2\right)^2}$$

$$m = 0$$

$$\boxed{E = pc}$$

$$m_0 c^2 >> E_k$$

$$\boxed{E_k = \frac{p^2}{2m}}$$

X-ray Photons

$$E[\text{keV}] = \frac{12.4}{\lambda\left[\text{Å}\right]}$$

$$\boxed{E = 12.4 \text{ keV}}$$

Electrons

$$E[\text{eV}] = \frac{150}{\lambda^2\left[\text{Å}^2\right]}$$

$$\boxed{E = 150 \text{ eV}}$$

Thermal neutrons

$$E[\text{meV}] = \frac{81.7}{\lambda^2\left[\text{Å}^2\right]}$$

$$\boxed{E = 81.7 \text{ meV}}$$

$$\lambda = 1\text{Å}$$

Energy – wavelength relation

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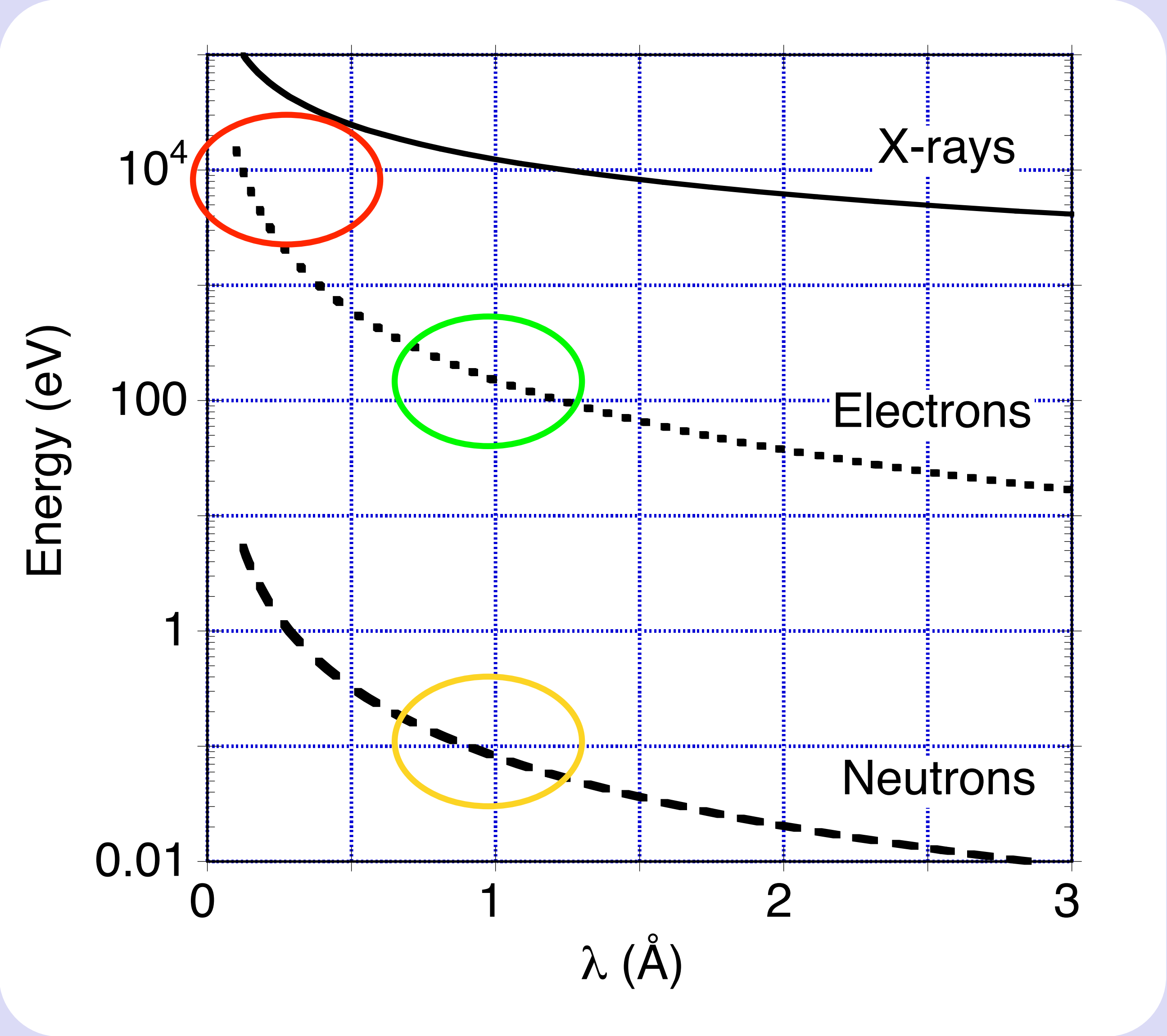
High-energy electrons

Low-energy electrons

Thermal neutrons



X-ray penetration

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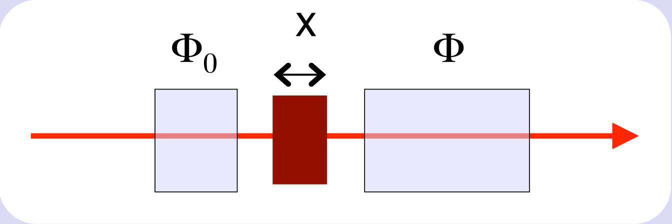

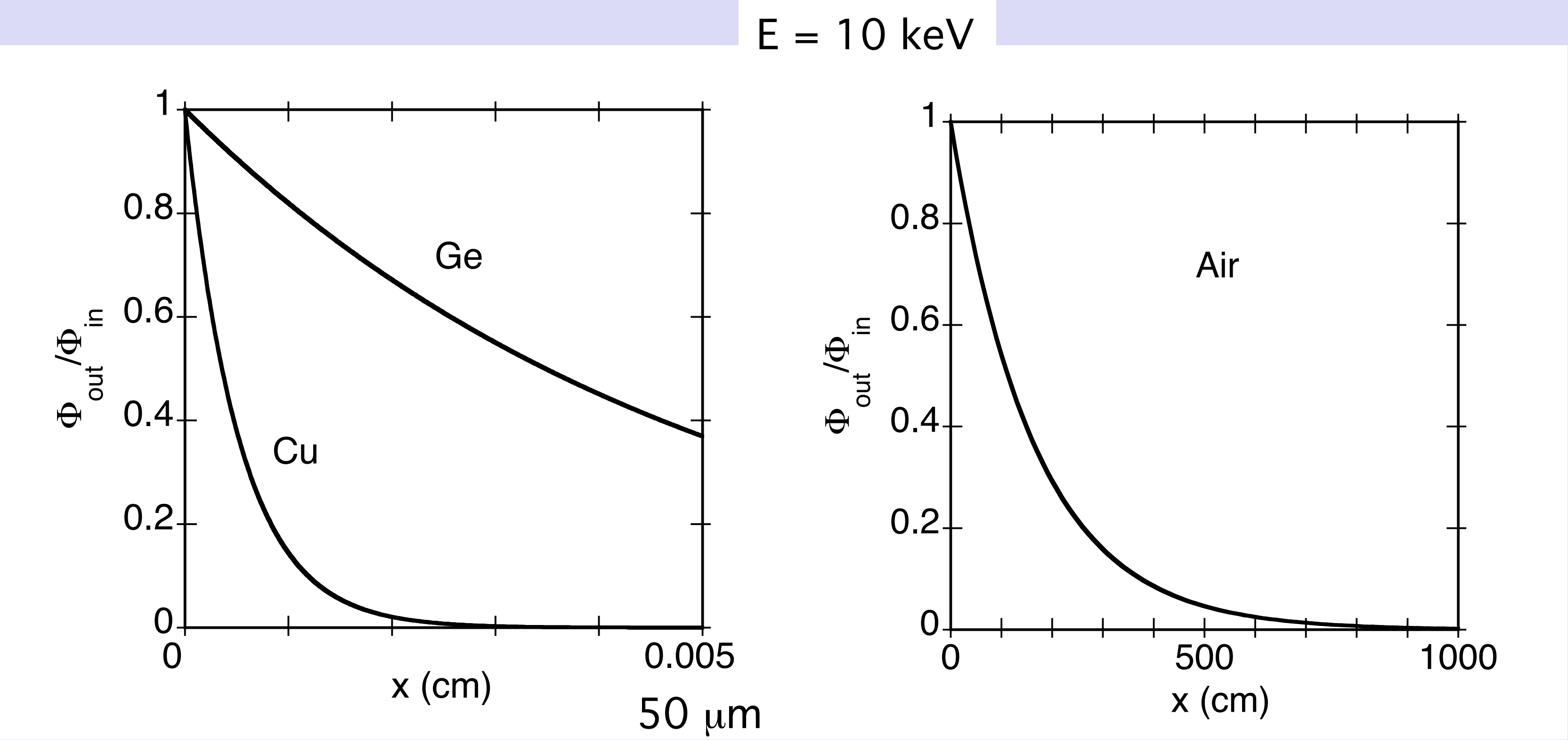

Interaction of x-rays with matter

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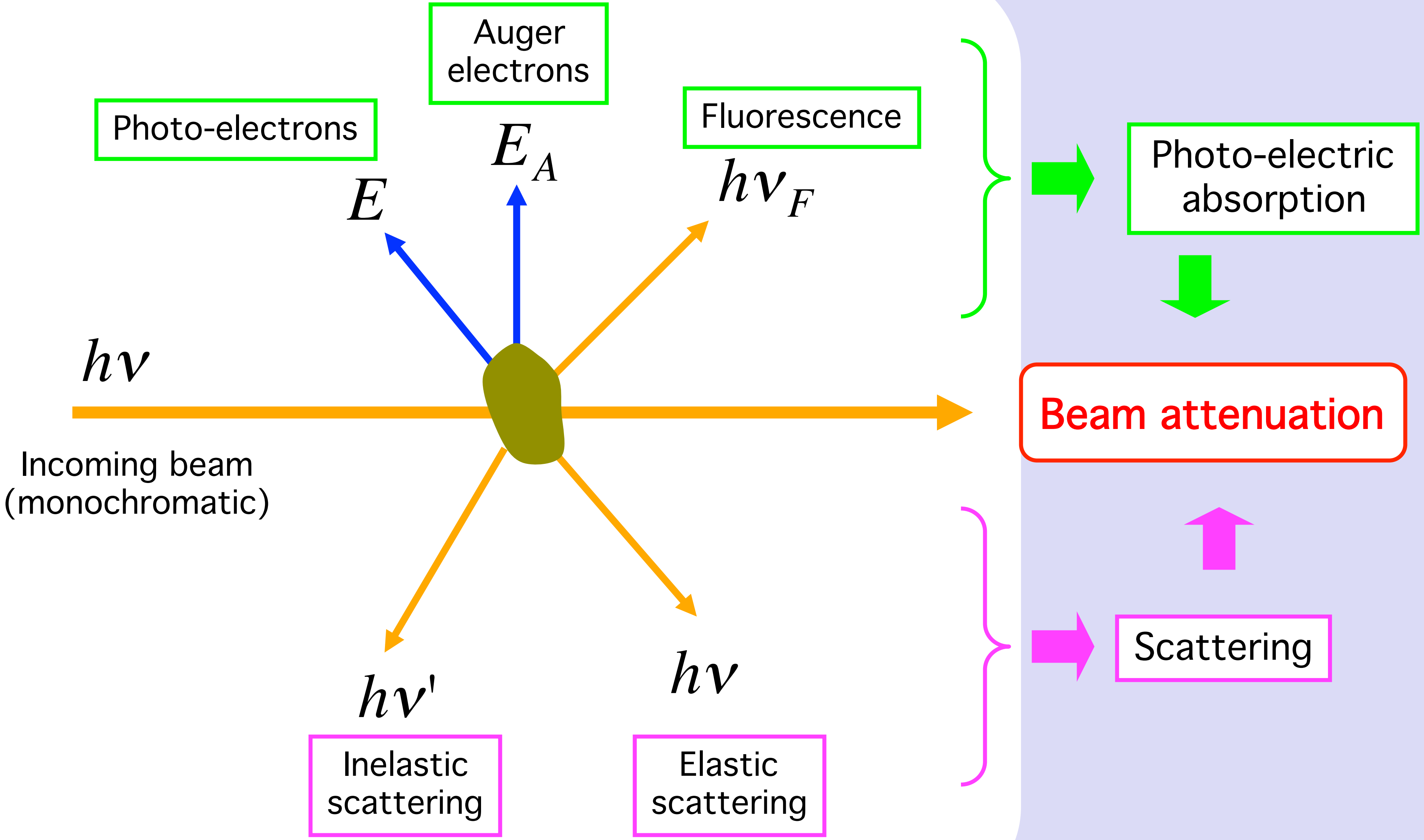
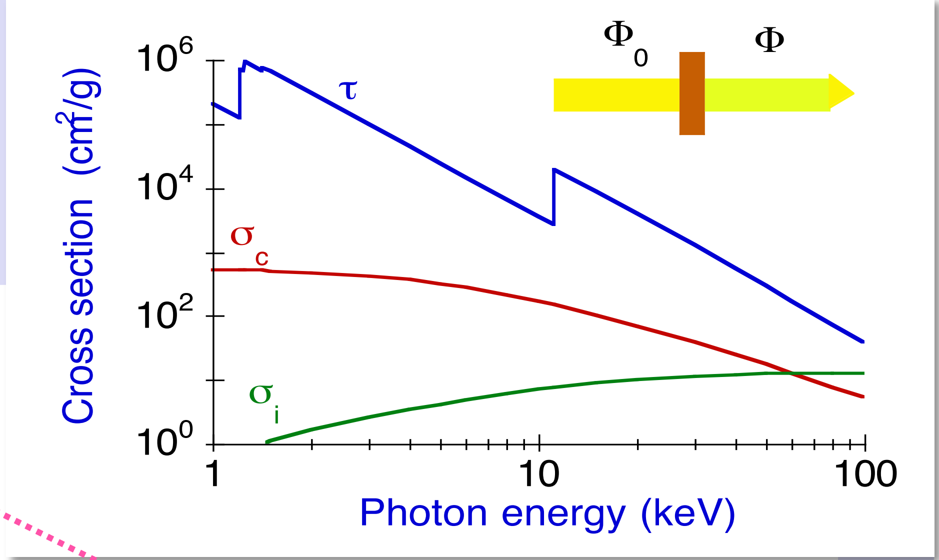


Photo-electric absorption

Beam attenuation

Scattering

Attenuation of X-Rays



Total cross section

τ Photoelectric absorption

Spectroscopy

Scattering

σ_c Coherent

σ_i Incoherent (Compton)

Pair production (hν>1000keV)

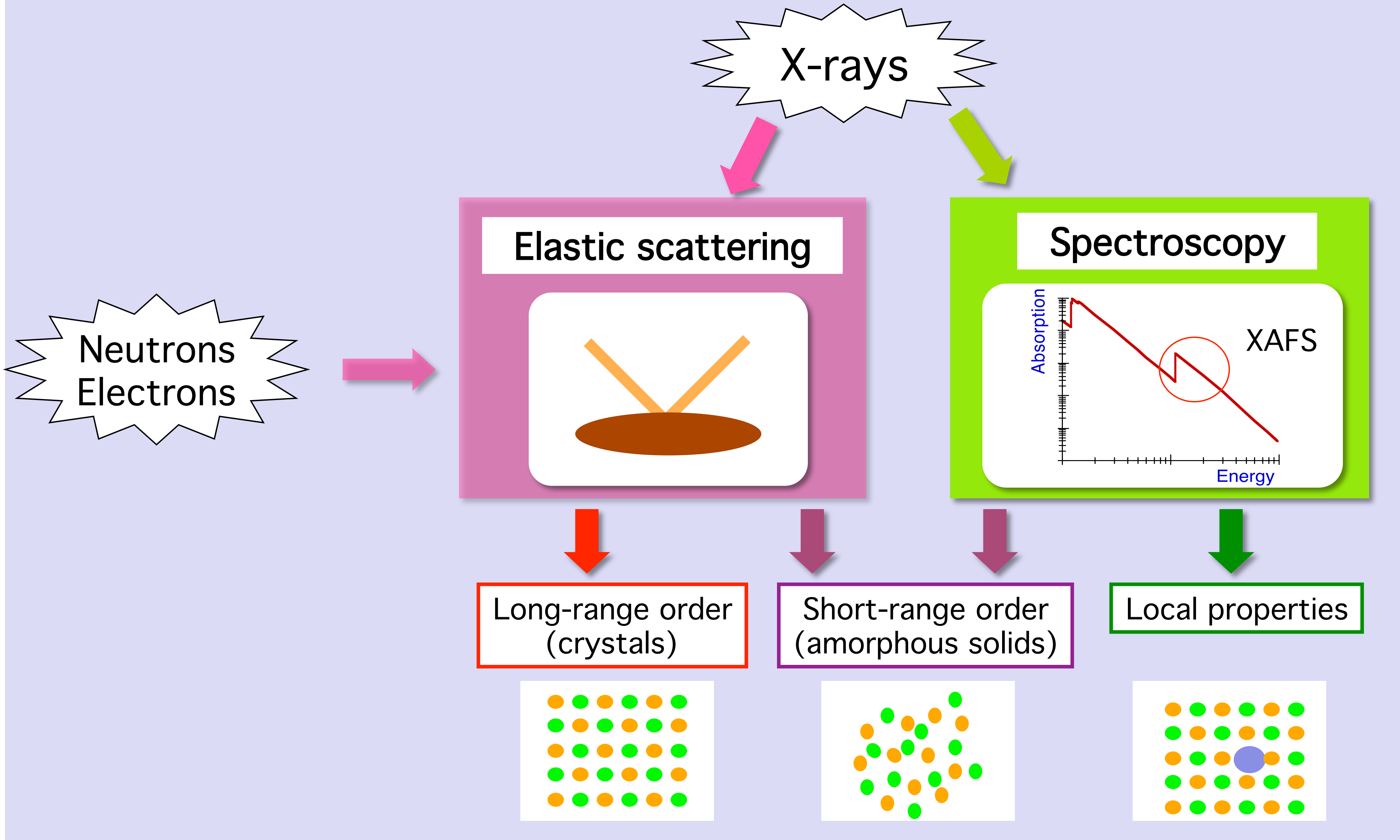
Diffraction
Diffusion

Elastic

Inelastic

Inelastic scattering

Structural techniques



X-rays

Neutrons
Electrons

Elastic scattering

Spectroscopy

Long-range order
(crystals)

Short-range order
(amorphous solids)

Local properties

> Basics of scattering

Scattering angles

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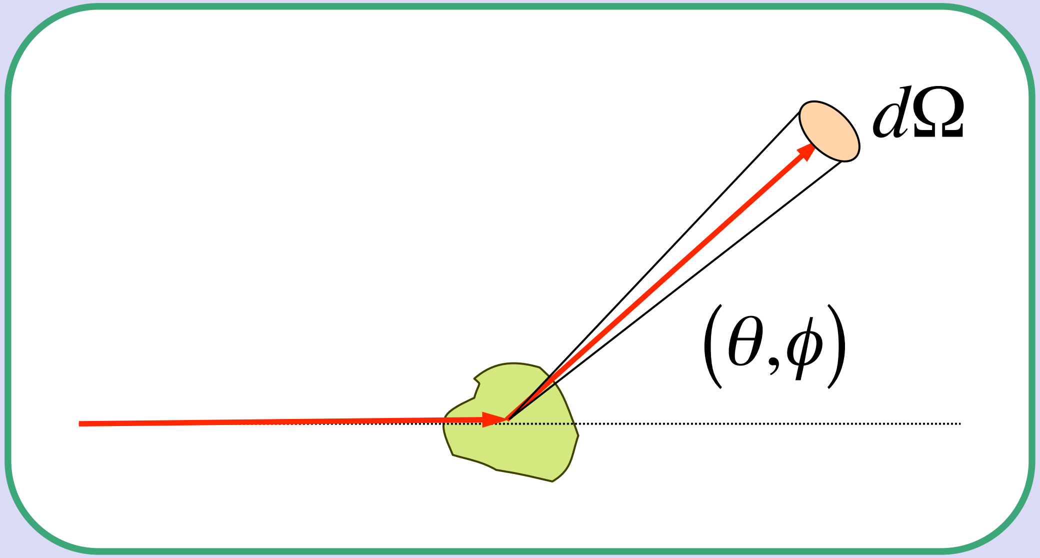
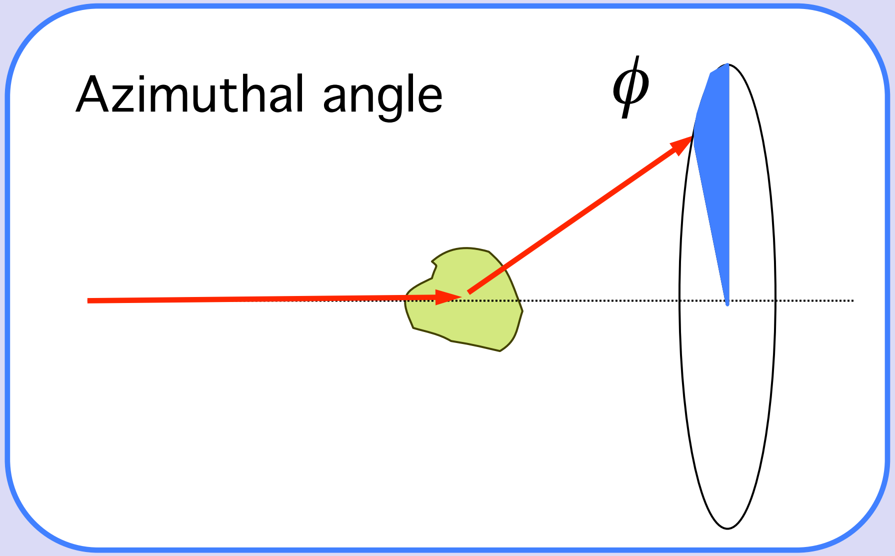
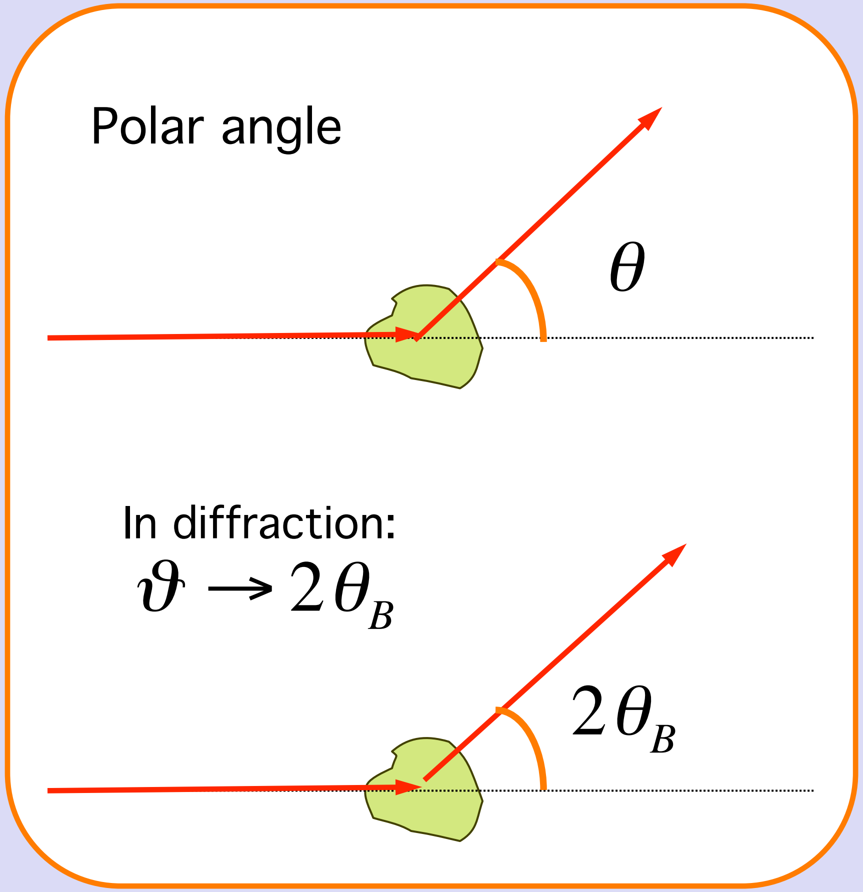


Azimuthal angle





Polar angle

In diffraction:

$$\vartheta \rightarrow 2\theta_B$$

θ_B = Bragg angle

Nomenclature of scattering

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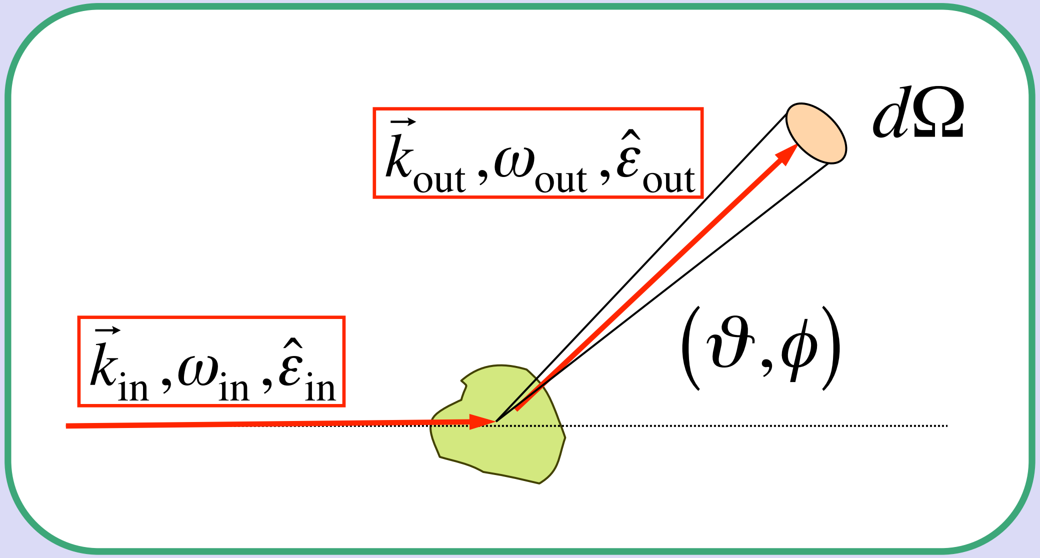

$$\vec{k} = \frac{2\pi}{\lambda}\,\hat{s}$$

$$E = \begin{cases} pc = \hbar kc = \hbar\omega & \text{X-rays photons} \\ \dfrac{p^2}{2m} = \dfrac{(\hbar k)^2}{2m} & \text{electrons, neutrons} \end{cases}$$

Exchanged energy $E = E_{\text{out}} - E_{\text{in}}$

Exchanged momentum $\hbar\vec{K} = \hbar\left(\vec{k}_{\text{out}} - \vec{k}_{\text{in}}\right)$

Elastic scattering

$$E = 0, \quad E_{\text{out}} = E_{\text{in}}, \quad \left|\vec{k}_{\text{out}}\right| = \left|\vec{k}_{\text{in}}\right|$$

Inelastic scattering

$$E \neq 0, \quad E_{\text{out}} \neq E_{\text{in}}, \quad \left|\vec{k}_{\text{out}}\right| \neq \left|\vec{k}_{\text{in}}\right|$$

Scattering cross-sections

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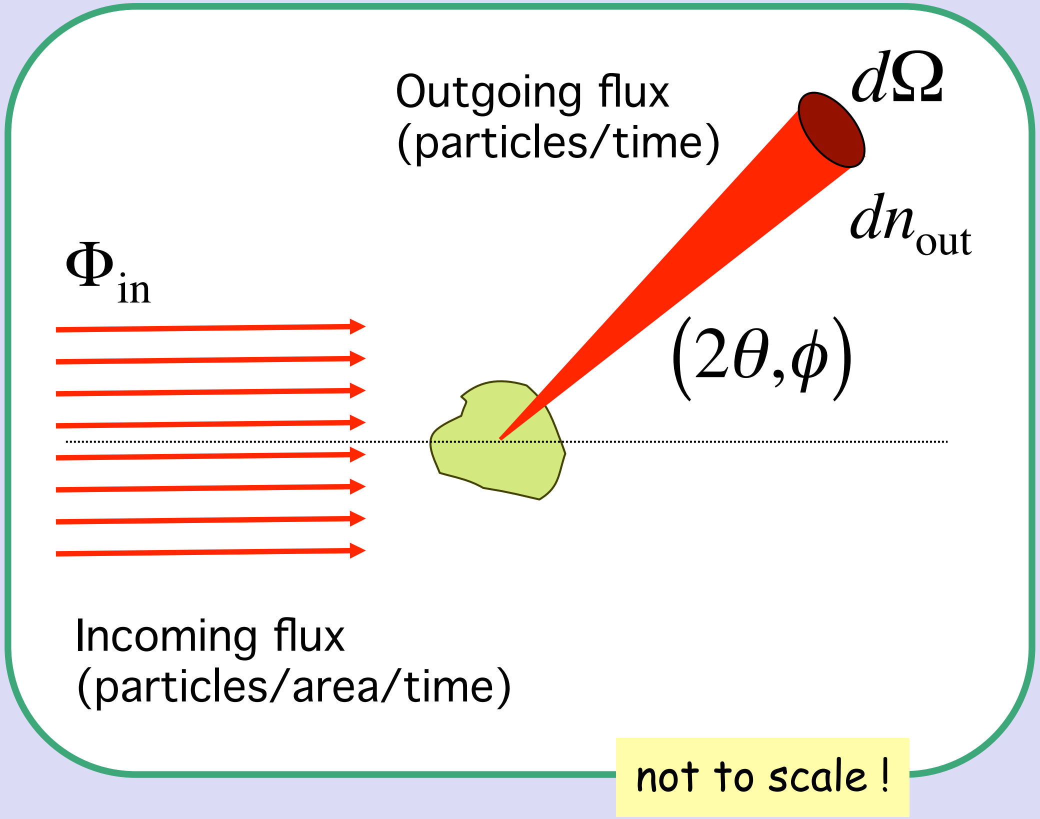


Elastic scattering

$$dn_{\text{out}} = \begin{cases} \Phi_{\text{in}}\ \sigma(2\theta,\phi)\ d\Omega \\ \Phi_{\text{in}} \left(\dfrac{d\sigma}{d\Omega}\right) d\Omega \end{cases}$$

differential cross-section

Inelastic scattering

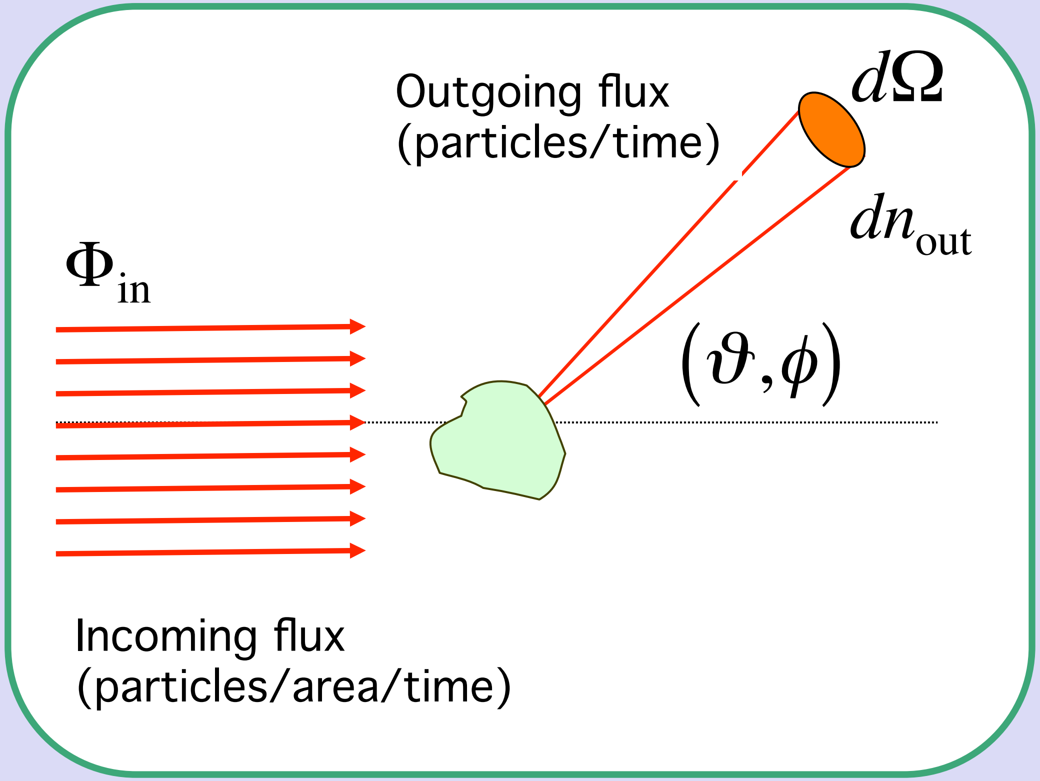
$$dn_{\text{out}} = \begin{cases} \Phi_{\text{in}}\ \sigma(2\theta,\phi,E)\ d\Omega\, dE \\ \Phi_{\text{in}} \left(\dfrac{d^2\sigma}{d\Omega\, dE}\right) d\Omega\, dE \end{cases}$$

double differential cross-section

Total cross-section: $\sigma_{\text{tot}} = \int \sigma(2\theta,\phi)\ d\Omega$

σ depends on incoming energy

Elastic scattering cross-section



Differential cross-section

$$dn_{\mathrm{out}} = \begin{cases} \Phi_{\mathrm{in}}\, \sigma(\vartheta,\phi)\, d\Omega \\ \Phi_{\mathrm{in}} \left(\dfrac{d\sigma}{d\Omega}\right) d\Omega \end{cases}$$

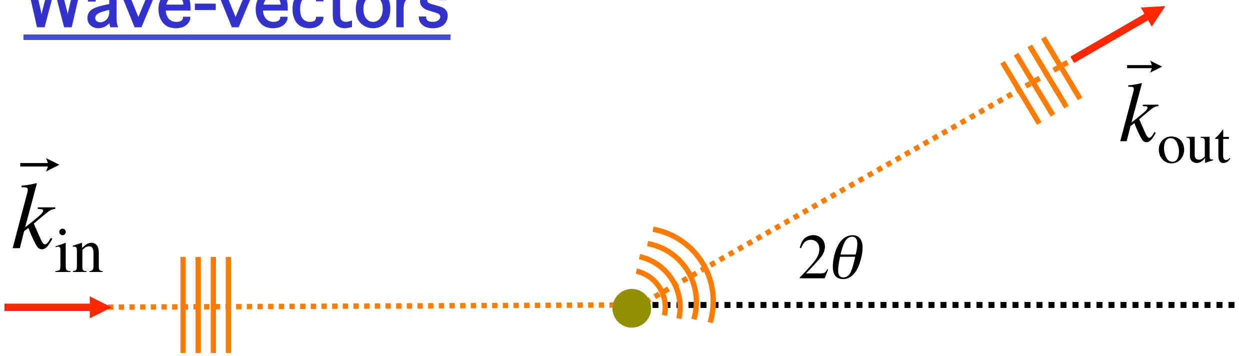
Total cross-section

$$\sigma_{\mathrm{tot}} = \int \sigma(\vartheta,\phi)\, d\Omega$$

The cross section can depend on the energy of incoming particles (say on wavelength).

Scattering vector

Wave-vectors



$$\vec{k}_{\text{in}} = \frac{2\pi}{\lambda}\vec{s}_{\text{in}}$$

$$\vec{k}_{\text{out}} = \frac{2\pi}{\lambda}\vec{s}_{\text{out}}$$

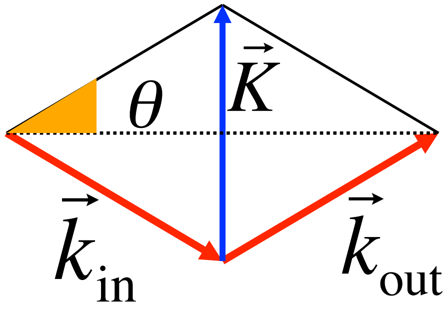
Elasting scattering

$$\left|\vec{k}_{\text{in}}\right| = \left|\vec{k}_{\text{out}}\right| = \frac{2\pi}{\lambda}$$

Scattering vector

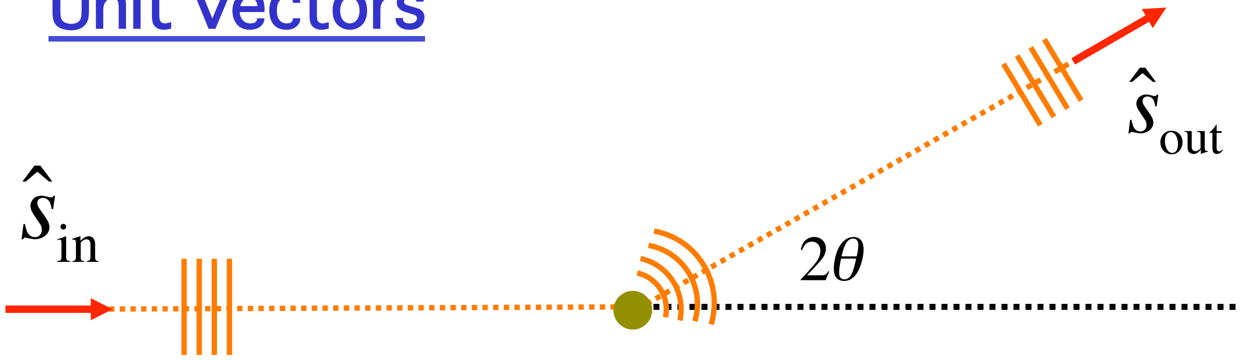
$$\vec{K} = \vec{k}_{\text{out}} - \vec{k}_{\text{in}}$$

$$\left|\vec{K}\right| = 4\pi\frac{\sin\theta}{\lambda}$$



Scattering vector (alternative convention)

Unit vectors



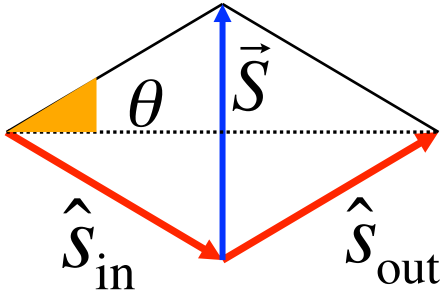
Elastic scattering

$$\lambda_{\text{in}} = \lambda_{\text{out}} = \lambda$$

Scattering vector

$$\vec{S} = \frac{\hat{s}_{\text{out}} - \hat{s}_{\text{in}}}{\lambda}$$

$$S = 2\,\frac{\sin\theta}{\lambda}$$



Connection

$$\boxed{\vec{K} = 2\pi\,\vec{S}}$$

Stationary states of elastic scattering

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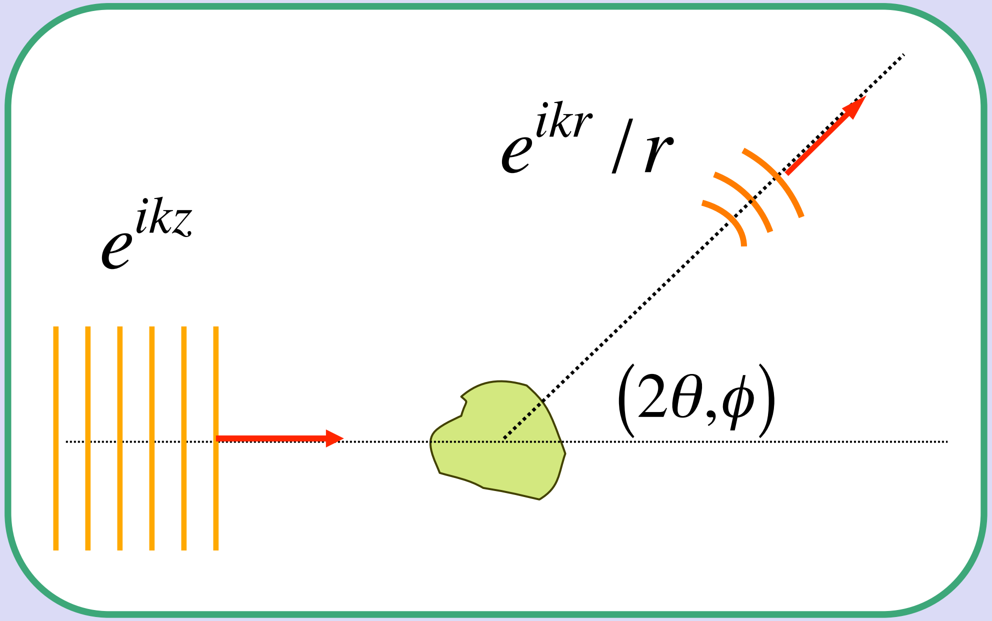


Elastic scattering

scattering amplitude

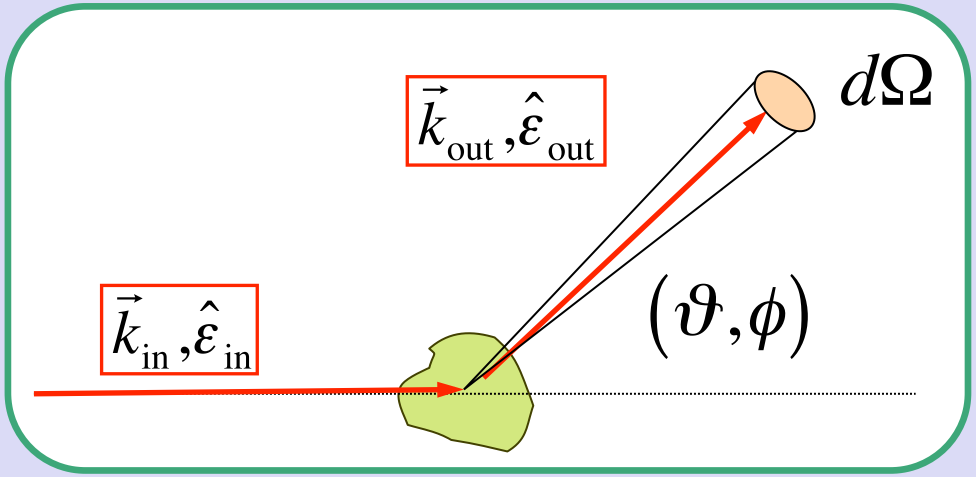
$$\Psi_k^{(\text{scatt})}(\vec{r}) \underset{r\to\infty}{\approx} e^{ikz} + \boxed{f_k(2\theta,\phi)}\,\frac{e^{ikr}}{r}$$

Differential cross-section:

$$\left.\begin{array}{l} \sigma(2\theta,\phi) \\ \left(\dfrac{d\sigma}{d\Omega}\right) \end{array}\right\} = \left|f_k(2\theta,\phi)\right|^2$$

$$? \left\{ \begin{array}{l} \text{X-rays} \\ \text{electrons} \\ \text{neutrons} \end{array} \right.$$

Elastic scattering, intrinsic cross-section



Static scattering function

Sample properties

$$\frac{d\sigma}{d\Omega} = \left(\frac{d\sigma}{d\Omega}\right)_0 S(\vec{K})$$

Differential
scattering cross-section

Intrinsic cross-section

Beam - sample coupling

?

- X-rays
- electrons
- neutrons

Scattering mechanisms

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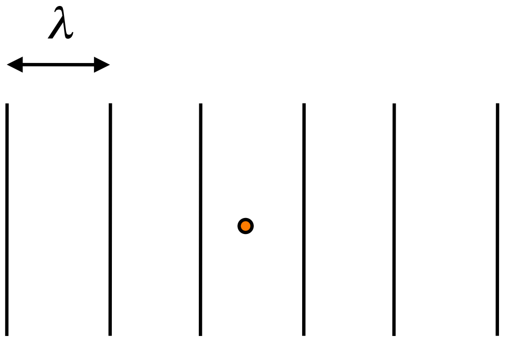
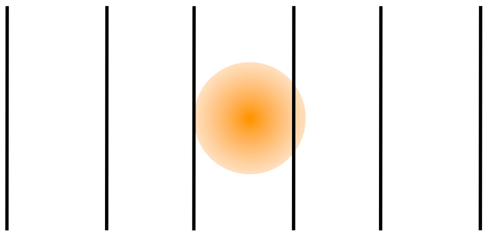
X-rays



Electrons, classical picture

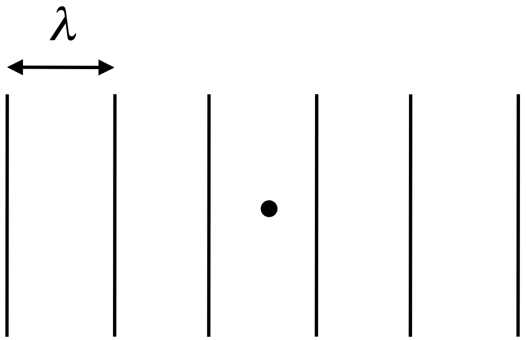
$\lambda >> r$



Electrons, quantum picture:

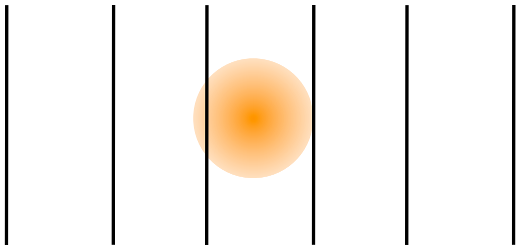
$\lambda \cong R$

Thermal neutrons



Nuclear potential

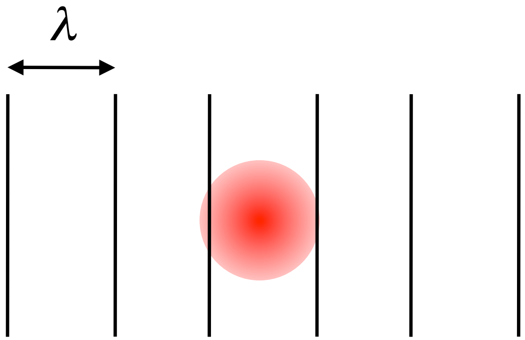
$\lambda >> r$



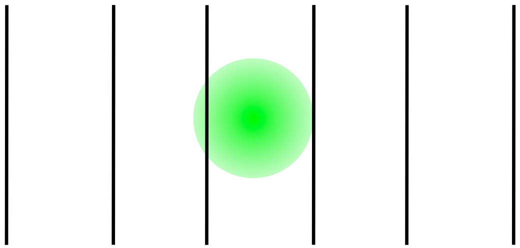
Electrons (magnetic atoms)

$\lambda \cong R$

Electrons



Coulomb potential
from nucleus



Coulomb potential
from electrons

Elastic scattering of X-rays

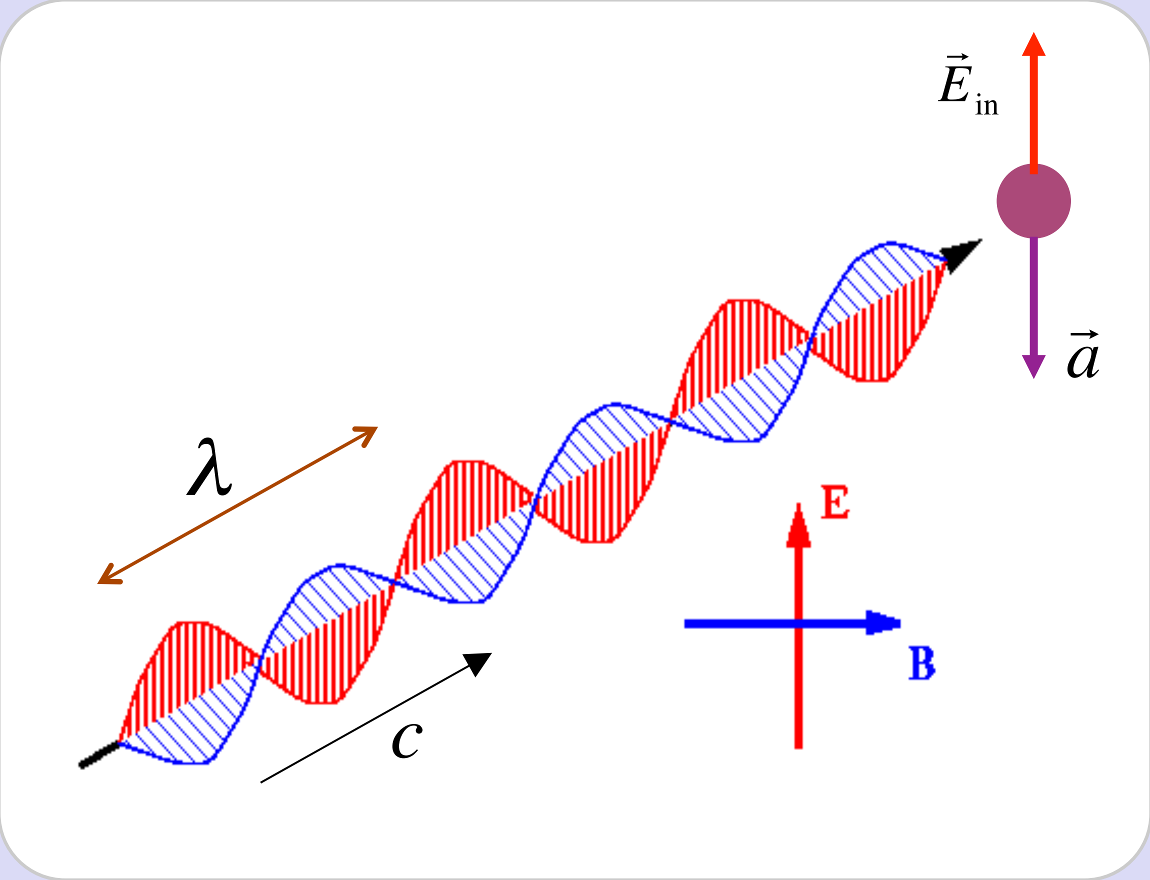
1 Classical theory of scattering from a free electron (Thomson scattering)

2 Basic interference effects

3 Correction for quantum effects:
    1. Probabilistic distribution of the electronic charge
    2. Compton effect for free electrons
    3. Effects of binding

> Thomson scattering

Electromagnetic wave impinging on a free electron



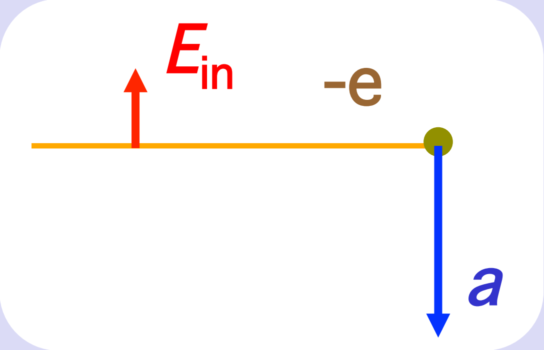
Incoming electric field

$$\vec{E}_{\text{in}}(t) = \vec{E}_0 \cos(\omega t)$$

Electron acceleration

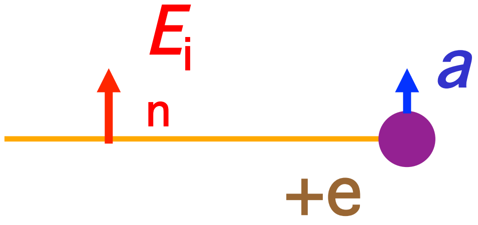
$$\vec{a}(t) = \frac{-e}{m} \vec{E}_0 \cos(\omega t)$$

π phase-shift



Negligible:

- magnetic effects
- proton acceleration



Dipole emission of radiation

Accelerating charge ⇒ electromagnetic field

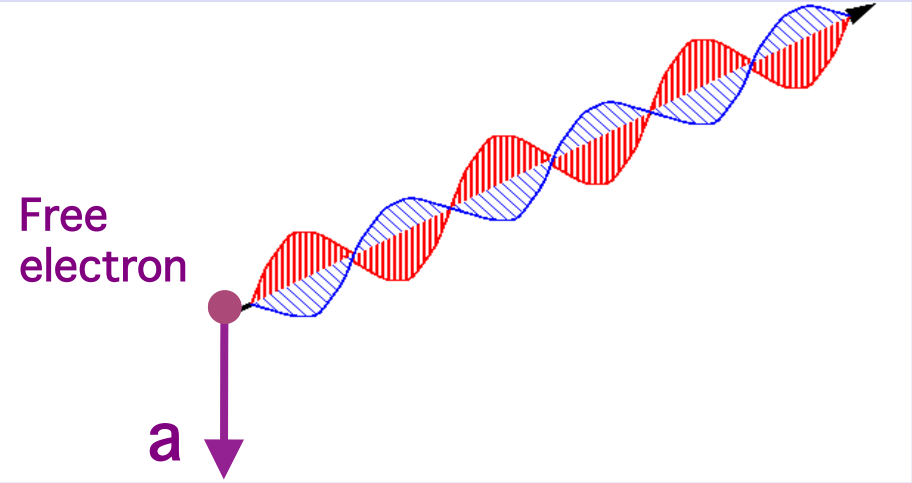
Dipole approximation:

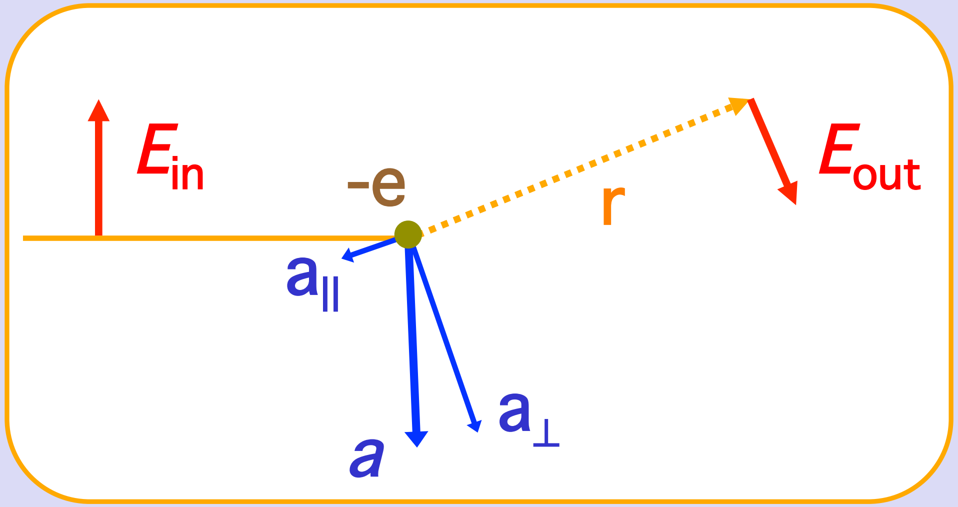
- charge velocity: v << c
- charge distribution: d << λ
- observer distance: r >> λ

$$\vec{a}(t) = \frac{-e}{m} \vec{E}_0 \cos(\omega t)$$

Electron: $q = -e$

$$\vec{E}_{\text{out}}(\vec{r},t) = \frac{e\,\vec{a}_{\perp}(t')}{4\pi\varepsilon_0\, r\, c^2}$$





Electric field polarization

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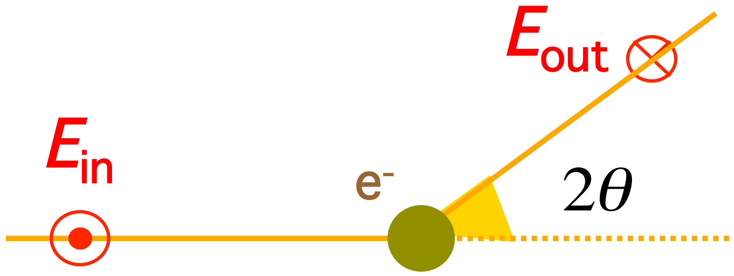
π polarisation

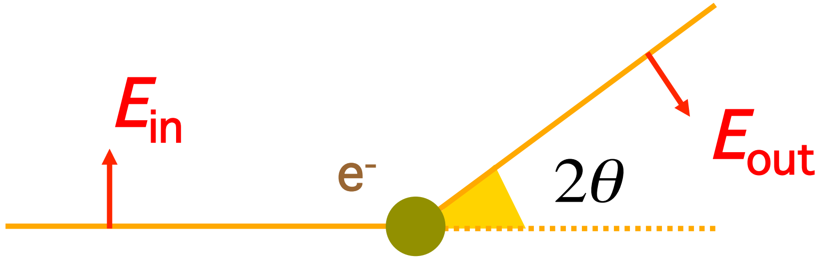
$$a_\perp = a$$



$$E_{\text{out}}(\vec{r},t) = -\frac{r_e}{r} E_0(t')$$

σ polarisation

$$a_\perp = a\cos(2\theta)$$



$$E_{\text{out}}(\vec{r},t) = -\frac{r_e}{r} E_0(t') \cos(2\theta)$$

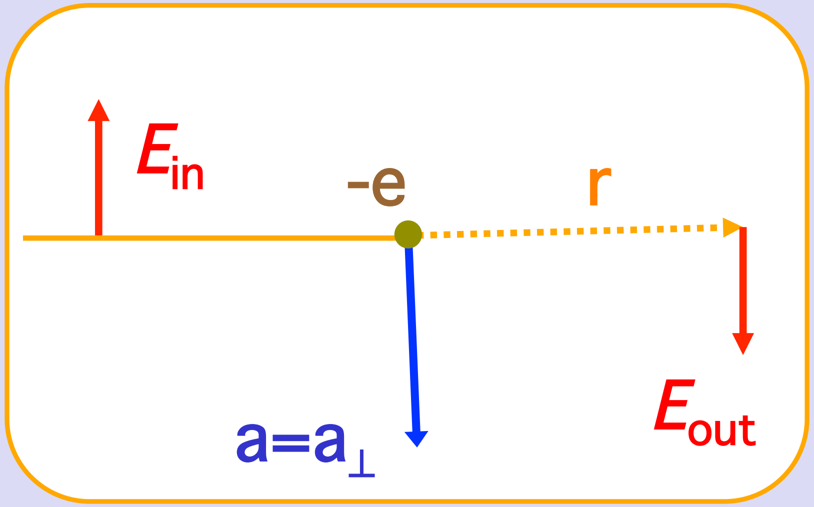
$$r_e = \frac{e^2}{4\pi\varepsilon_0 c^2 m} = 2.8\text{x}10^{-5}\,\text{Å}$$

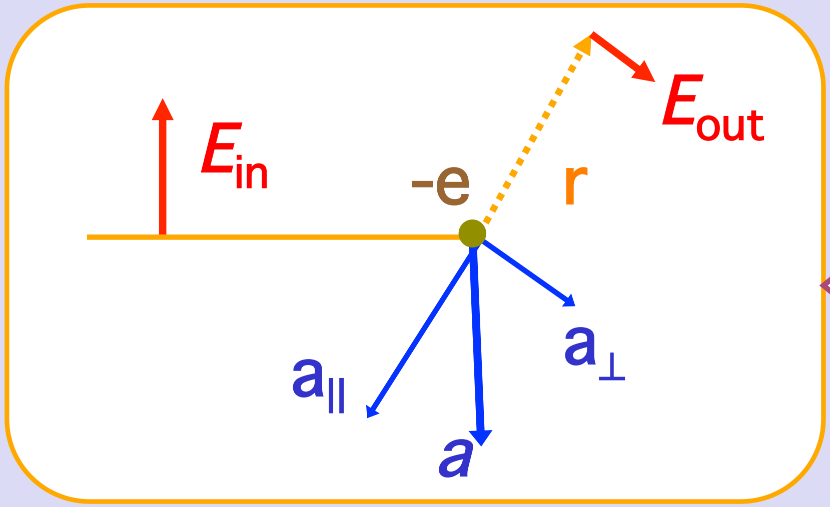
Thomson scattering length

Classical electron radius

More on σ polarization

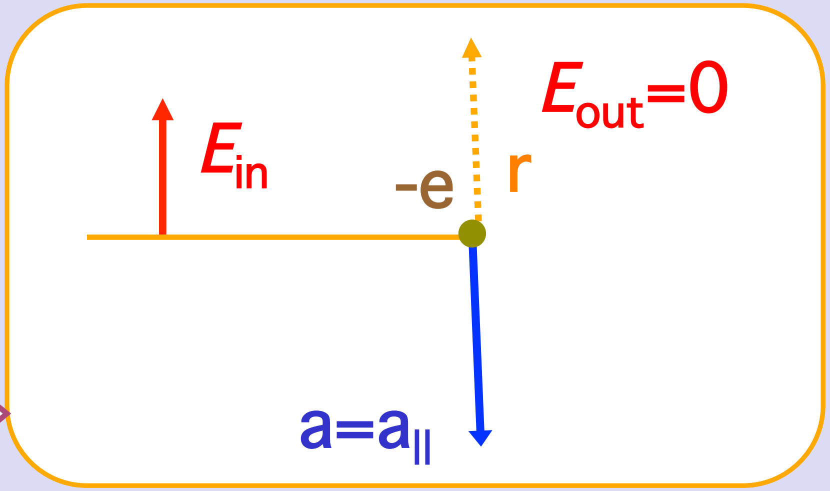
Forward scattering





General case

Normal scattering



Classical electron radius

Energy of a uniformly charged:

- spherical shell

$$U = \frac{1}{2}\left(\frac{1}{4\pi\varepsilon_0}\frac{q^2}{r_e}\right)$$

- spherical volume

$$U = \frac{3}{5}\left(\frac{1}{4\pi\varepsilon_0}\frac{q^2}{r_e}\right)$$

Electron

$$U \approx \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r_e} = \boxed{mc^2}$$

Relativistic rest energy

$$r_e = \frac{e^2}{4\pi\varepsilon_0 c^2 m} = 2.8\mathrm{x}10^{-15}\,\mathrm{m} = 2.8\mathrm{x}10^{-5}\,\mathrm{Å}$$

= Thomson scattering length

Incoming wave: input amplitude

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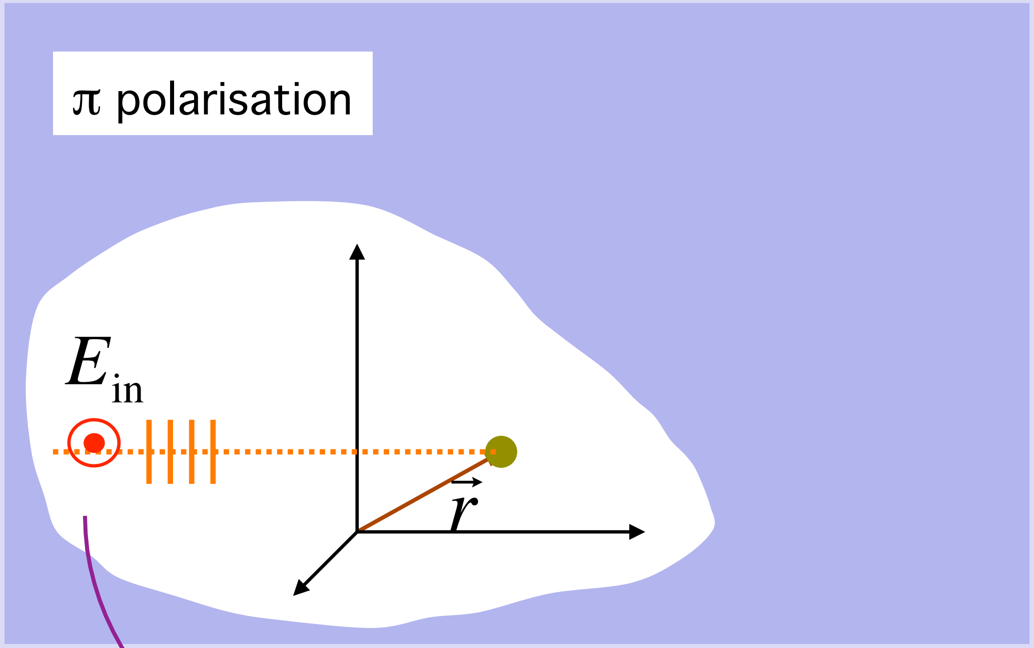


Mathematical machinery useful for treating interference phenomena.

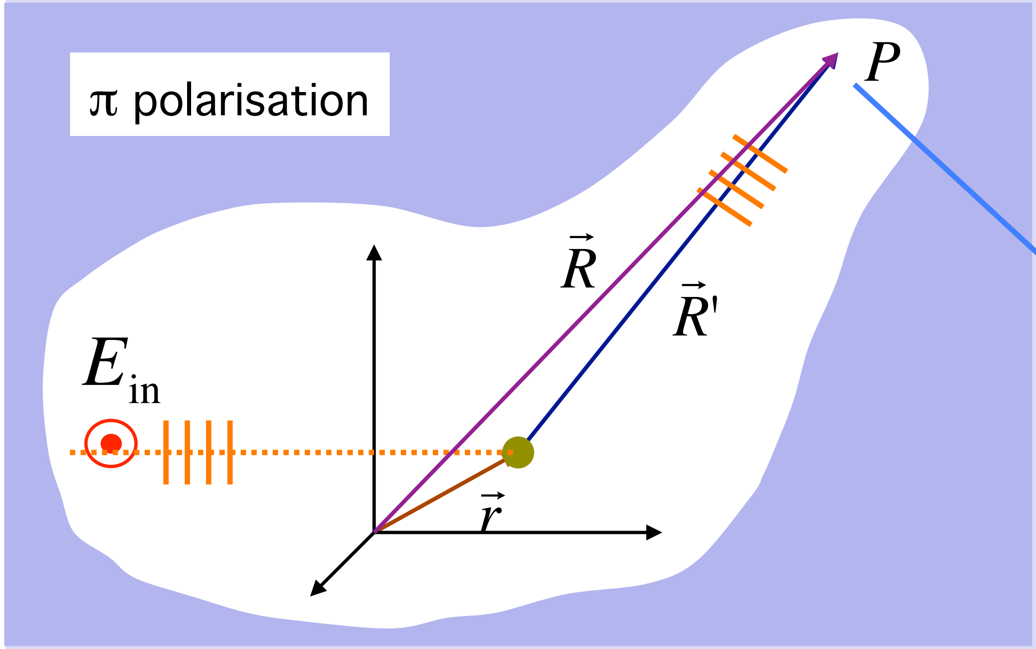
$$E_{\text{in}} = E_0 \cos\left(\omega\, t - \vec{k}_{\text{in}} \cdot \vec{r}\right)$$

$$= \text{Re}\left\{ \underbrace{E_0 e^{i\left(\omega t - \vec{k}_{\text{in}} \cdot \vec{r}\right)}}_{A_{\text{in}}} \right\}$$

Complex notation

$\boxed{A_{\text{in}}}$ **Input amplitude**

Outgoing wave: scattered amplitude

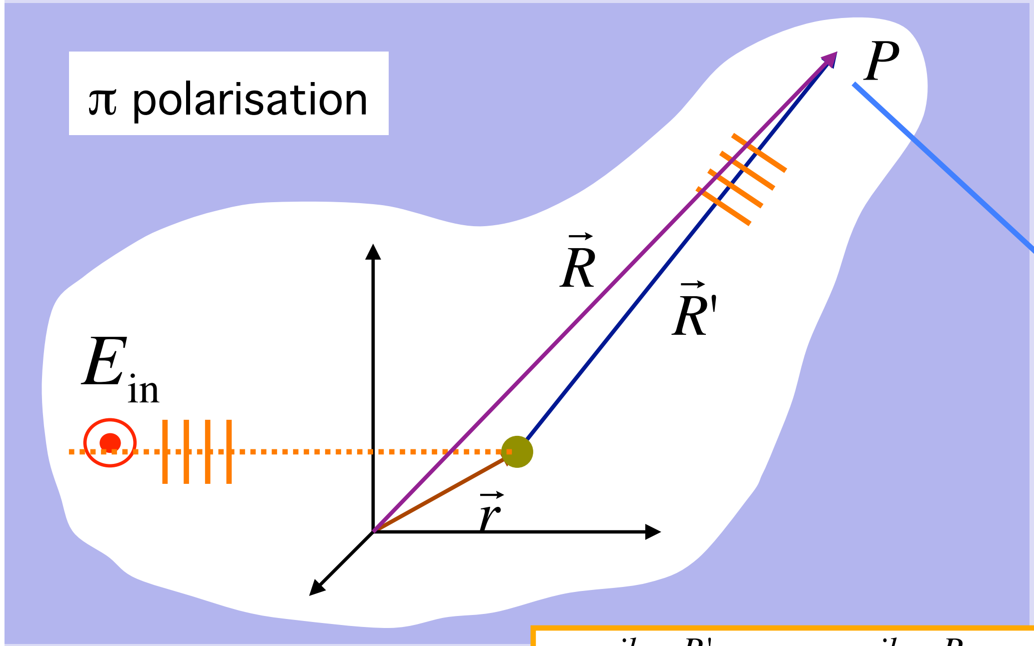


$$\boxed{E_{\text{out}} = \text{Re}\left\{\underbrace{\overbrace{E_0 e^{i\left(\omega t - \vec{k}_{\text{in}} \cdot \vec{r}\right)}}^{A_{\text{in}}} \left(-r_e\right) \frac{e^{-ik_{\text{out}} R'}}{R'}}_{A}\right\}}$$

Scattered amplitude

Scattering from one electron.
Far-field limit, outgoing wave approximate as a plane wave.

Scattered amplitude



$$E_{\text{out}} = \text{Re}\left\{ E_0 e^{i\left(\omega t - \vec{k}_{\text{in}} \cdot \vec{r}\right)} \left(-r_e\right) \frac{e^{-ik_{\text{out}} R'}}{R'} \right\}$$

$$\frac{e^{-ik_{\text{out}} R'}}{R'} \approx \frac{e^{-ik_{\text{out}} R}}{R} e^{ik_{\text{out}} r \left(\vec{k}_{\text{out}} \cdot \vec{r}\right)} = \frac{e^{-ik_{\text{out}} R}}{R} e^{i\vec{k}_{\text{out}} \cdot \vec{r}}$$

Scattered amplitude

$$A(\vec{K}) = -E_0 \, r_e \frac{e^{-ik_{\text{out}} R}}{R} e^{i\omega t} e^{i\left(\vec{k}_{\text{out}} - \vec{k}_{\text{in}}\right) \cdot \vec{r}} \longrightarrow e^{i\vec{K} \cdot \vec{r}}$$

Phase factor

Amplitude and intensity (1 electron)

Amplitude (π polarisation)

$$A(\vec{K}) = \boxed{-E_0\, r_e \frac{e^{-ik_{\text{out}}R}}{R}\, e^{i\omega t}}\, e^{i\vec{K}\cdot\vec{r}} = A_{\text{el}}\, e^{i\vec{K}\cdot\vec{r}}$$

$$E_{\text{out}} = \text{Re}\left\{A\left(\vec{K}\right)\right\}$$

Cannot be measured !

Intensity

$$I = \left|A(\vec{K})\right|^2 = \left|A_{\text{el}}\right|^2$$

$$E_0^2\, r_e^2 \frac{1}{R^2}$$

(π polarisation)

$$E_0^2\, r_e^2 \frac{1}{R^2}\left[\frac{1+\cos^2(2\theta_B)}{2}\right]$$

un-polarized beam

Is actually measured

Polarisation factor

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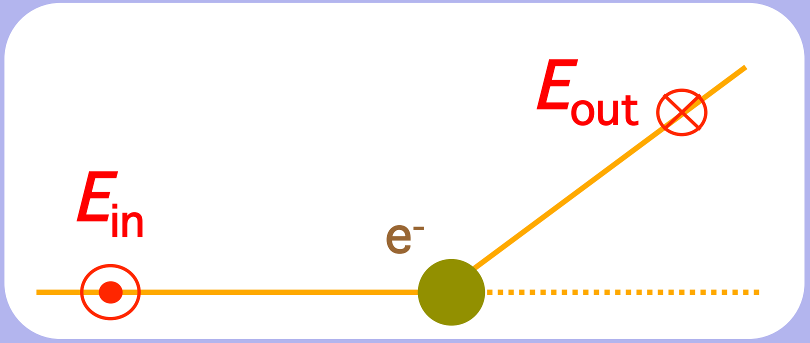
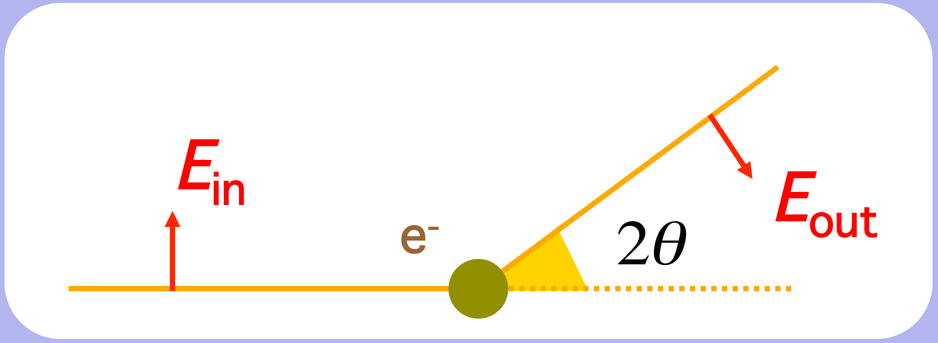
π polarisation



σ polarisation



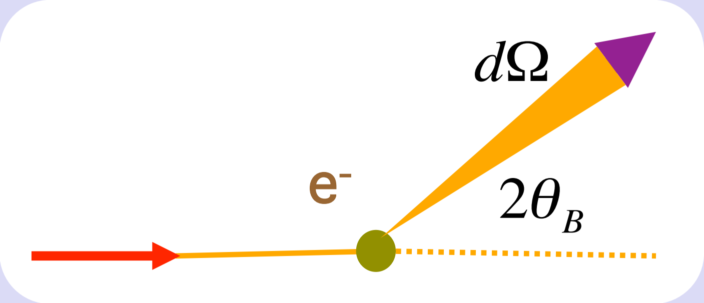
$$E_{out}^2$$

Un-polarised beam

$$\left[\frac{1}{2} + \frac{\cos^2(2\theta)}{2}\right]$$

Laboratory x-ray sources produce unpolarized beams.

Radiated power, unpolarized beam



Incoming power flux

$$\Phi_{\text{in}} = \frac{1}{2}\varepsilon_0 E_0^2 c = \frac{1}{2}\varepsilon_0 \left|A_0^2\right| c \quad \left[\text{W/m}^2\right]$$

$$= \frac{\varepsilon_0 E_0^2 c}{2\hbar\omega} \quad \left[\text{photons/s/m}^2\right]$$

Emitted power

$$P\left(\vec{K}\right) d\Omega \;=\; \Phi_{\text{in}} \; \underbrace{r_e^2 \left[\frac{1+\cos^2(2\theta)}{2}\right]}_{\sigma(2\theta_B,\phi) = \left|f(2\theta_B,\phi)\right|^2} \; d\Omega$$

Differential cross-section

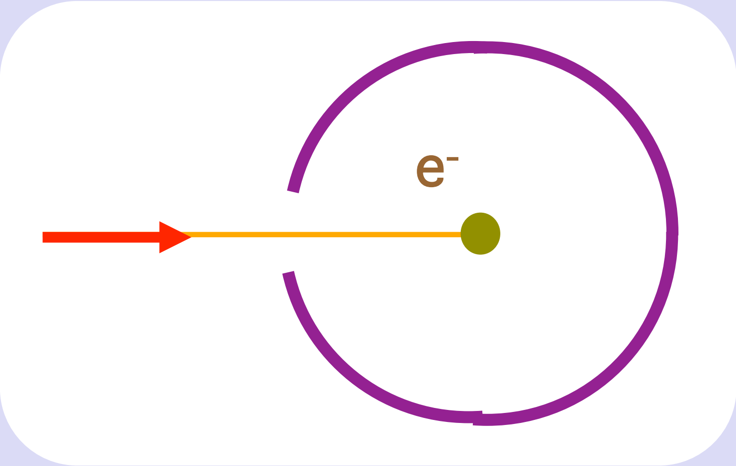
Independent of radiation wavelength

$$r_e \;=\; \frac{e^2}{4\pi\varepsilon_0 c^2 m} \;=\; 2.8\text{x}10^{-15}\,\text{m}$$

Total electron cross-section (1)

Un-polarized beam

$$\sigma_{\mathrm{Th}} = \int \sigma(2\theta_B, \phi)\, d\Omega = \frac{8}{3}\pi\, r_e^2 = 6.66\mathrm{x}10^{-29}\mathrm{m}^2$$



Total radiated power

$$P_{\mathrm{rad}} = \frac{8}{3}\pi\, r_e^2\, P_{\mathrm{in}}$$

Independent of radiation wavelength

Total electron cross-section (2)

Un-polarized beam

$$\sigma_e = \int_{\Omega} \sigma(2\theta,\phi)\, d\Omega = r_e^2 \int_0^{2\pi} d\phi \int_0^{\pi} \sin(2\theta) \frac{1+\cos^2(2\theta)}{2}\, d(2\theta)$$

$$= 2\pi\, r_e^2 \left[\frac{1}{2} \int_0^{\pi} \sin(2\theta)\, d(2\theta) + \frac{1}{2} \int_0^{\pi} \sin(2\theta) \cos^2(2\theta)\, d(2\theta) \right]$$

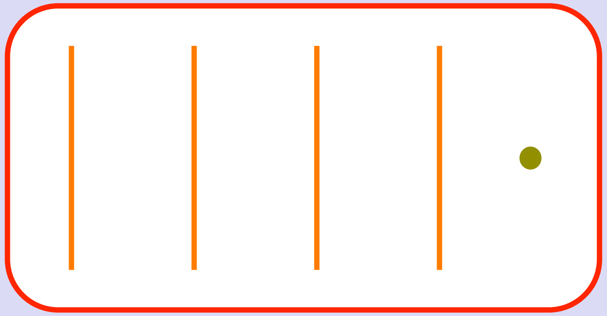
$$= \frac{8}{3} \pi\, r_e^2$$

$$= 66.6 \times 10^{-30}\,\mathrm{m}^2 = 66.6 \times 10^{-10}\,\text{Å}^2 = 66.6\ \mathrm{fm}^2 = 0.66\ \mathrm{barn}$$

Independent of radiation wavelength

Beyond classical treatment

Thomson scattering:



Free electron

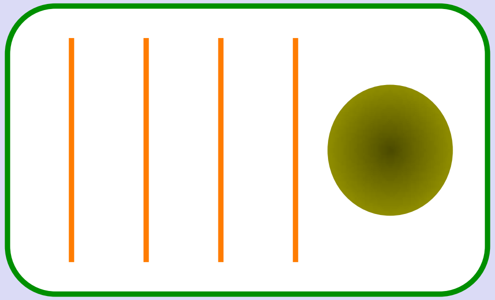
Elastic scattering ☹

$r_e << \lambda$

Free electron ⇒ Inelastic scattering (Compton)

Electrons are bound in atoms

Probabilistic distribution of e^- charge



Interference

> Interference

Scattering from many electrons

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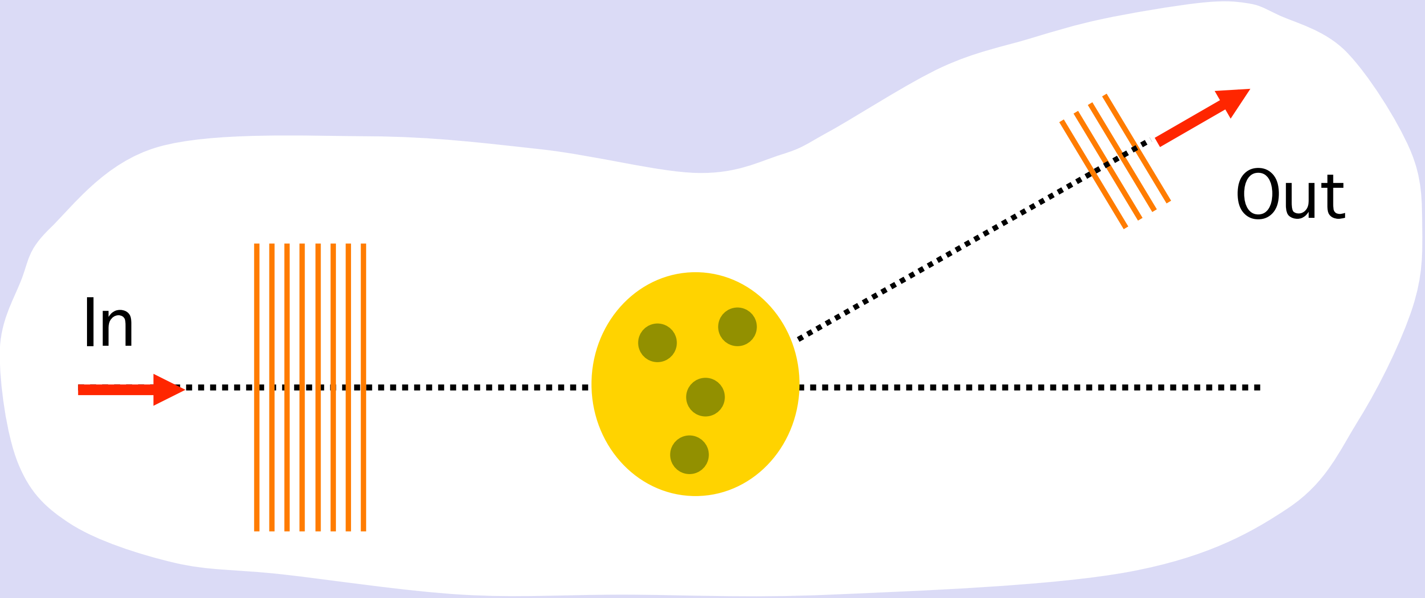


Waves scattered by different electrons → **Interference**

Depending on radiation wavelength

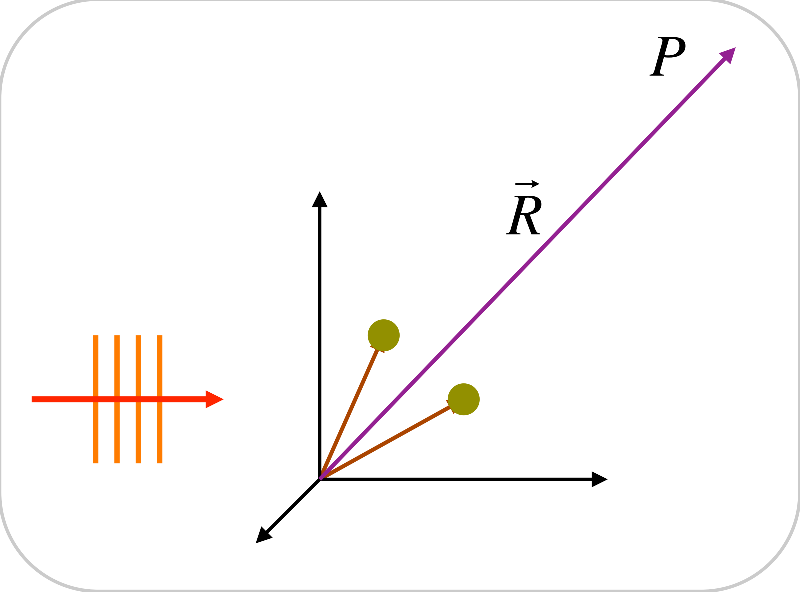
Interference: scattering from 2 electrons

1 electron

$$A(\vec{K}) = A_{\mathrm{el}}\, e^{i\vec{K}\cdot\vec{r}}$$

$$I = \left|A(\vec{K})\right|^2 = \left|A_{\mathrm{el}}\right|^2$$

2 electrons



$$A(\vec{K}) = A_1(\vec{K}) + A_2(\vec{K})$$

$$= A_{\mathrm{el}} \left[e^{i\vec{K}\cdot\vec{r}_1} + e^{i\vec{K}\cdot\vec{r}_2} \right]$$

$$I(\vec{K}) = \left|A(\vec{K})\right|^2$$

$$= A_{\mathrm{el}}^2 \left[\underbrace{2}_{\text{Independent}} + \underbrace{2\cos\left(\vec{K}\cdot\vec{r}_{12}\right)}_{\text{Interference}} \right]$$

Independent

Interference

$\vec{r}_{12} = \vec{r}_2 - \vec{r}_1$

Thomson scattering by 2 electrons (a)

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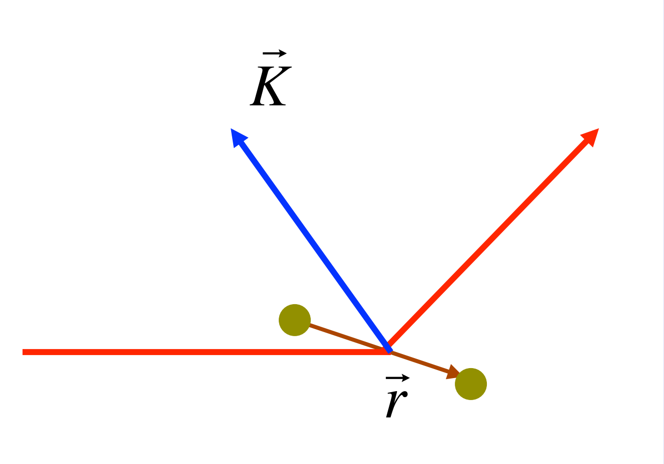
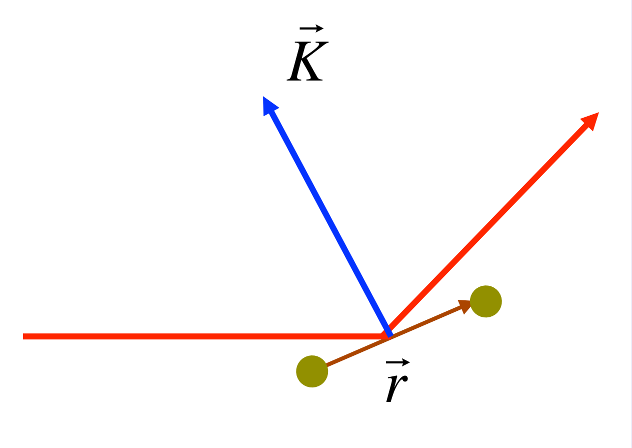
$$I(\vec{K}) = \left|A(\vec{K})\right|^2 = \left(A_1(\vec{K}) + A_2(\vec{K})\right)\left(A_1^*(\vec{K}) + A_2^*(\vec{K})\right)$$

$$= A_{\mathrm{el}}^2 \left(e^{i\vec{K}\cdot\vec{r}_1} + e^{i\vec{K}\cdot\vec{r}_2}\right)\left(e^{-i\vec{K}\cdot\vec{r}_1} + e^{-i\vec{K}\cdot\vec{r}_2}\right)$$

$$= A_{\mathrm{el}}^2 \left[\underbrace{2}_{\text{Independent}} + \underbrace{2\cos\left(\vec{K}\cdot\vec{r}\right)}_{\text{Interference}}\right] \qquad \vec{r} = \vec{r}_2 - \vec{r}_1$$





Particular case:

$\vec{K} \perp \vec{r}$

$I(\vec{K}) = 4\,A_{\mathrm{el}}^2$

Thomson scattering by 2 electrons (b)

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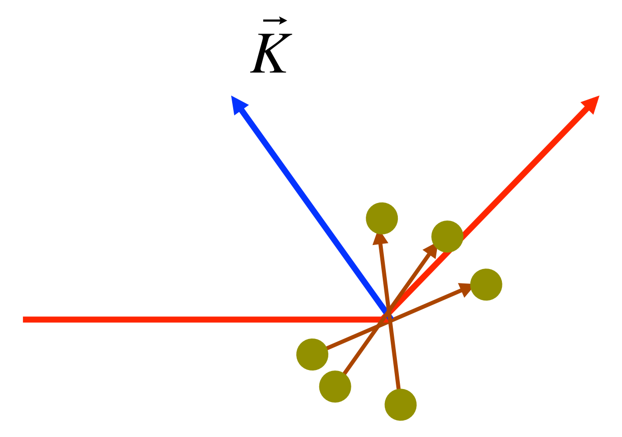
$$I(\vec{K}) = A_{\text{el}}^2 \left[2 \;+\; 2\cos\left(\vec{K}\cdot\vec{r}\right)\right]$$

Independent

Interference

Random orientation of $\vec{r}$ $\left(r \text{ fixed}\right)$



Average over the orientations of r

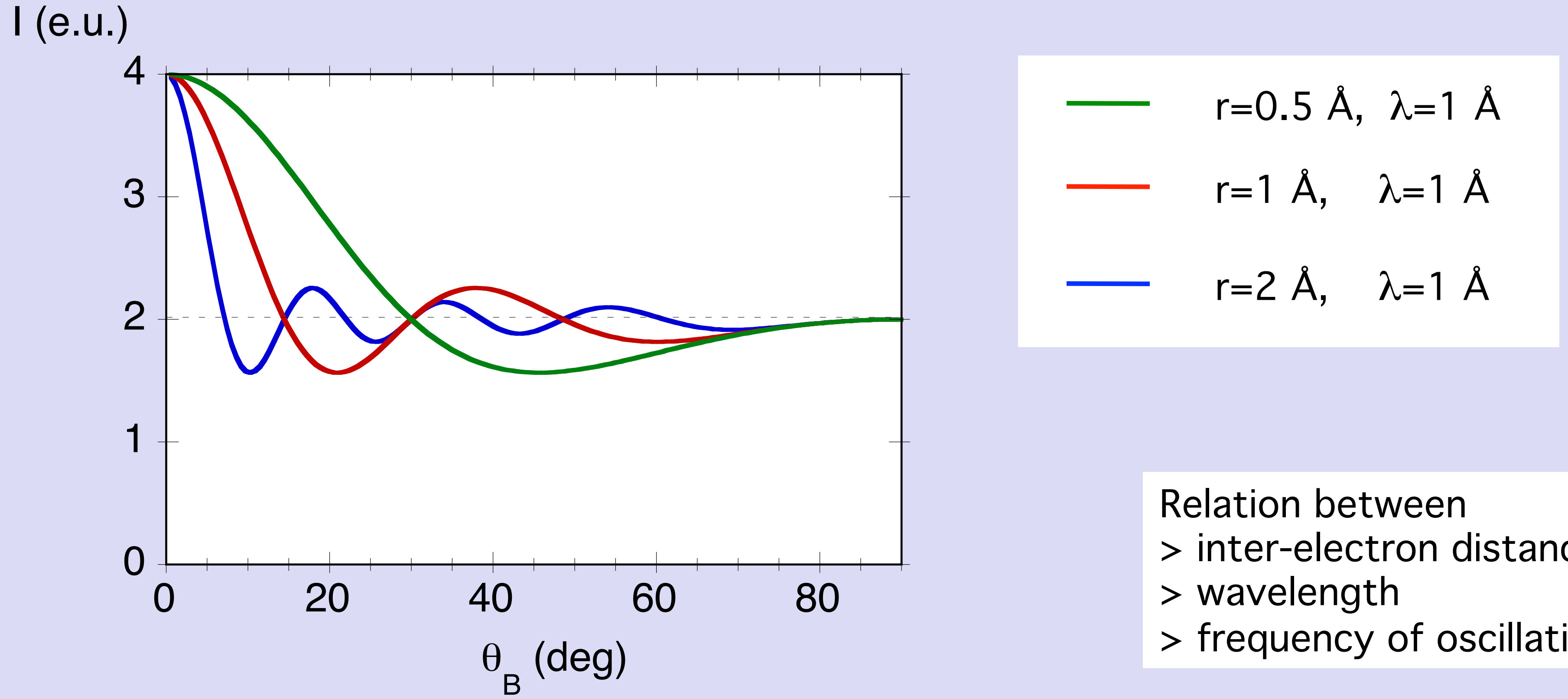
$$I(\vec{K}) = A_{\text{el}}^2 \left[2 \;+\; 2\left\langle\cos\left(\vec{K}\cdot\vec{r}\right)\right\rangle\right]$$

$$= A_{\text{el}}^2 \left[2 \;+\; 2\frac{\sin Kr}{Kr}\right]$$

Thomson scattering by 2 electrons (c)

$$I(\vec{K}) = A_{\mathrm{el}}^2 \left[\underbrace{2}_{\text{Independent}} + \underbrace{2\frac{\sin Kr}{Kr}}_{\text{Interference}} \right]$$

2 electrons: at fixed distance r
random orientation



Relation between
> inter-electron distance,
> wavelength
> frequency of oscillations

Thomson scattering by Z electrons

$$I(\vec{K}) = \left|A(\vec{K})\right|^2 = \left(\sum_i A_i(\vec{K})\right)\left(\sum_j A_j^*(\vec{K})\right)$$

$$= A_{\mathrm{el}}^2 \left(\sum_i e^{i\vec{K}\cdot\vec{r}_i}\right)\left(\sum_j e^{-i\vec{K}\cdot\vec{r}_j}\right)$$

$$= A_{\mathrm{el}}^2 \left[\underset{\downarrow}{Z} + \underbrace{\sum_i \sum_{j\neq i} \cos\left(\vec{K}\cdot\vec{r}_{ij}\right)}\right]$$

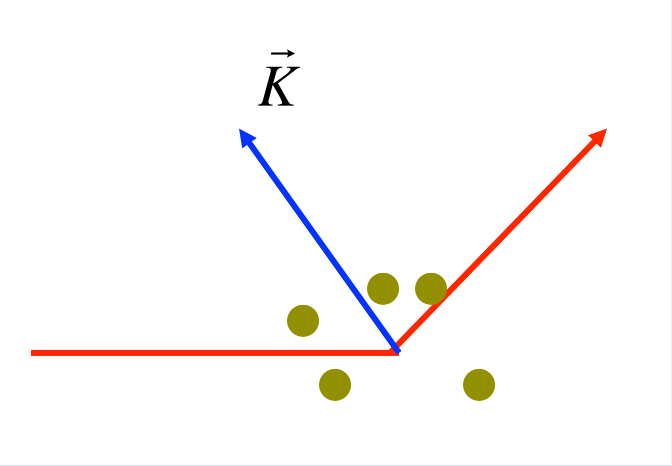
$j = i$

Independent scattering
by single electrons

$j \neq i$

Interference:
Z(Z-1) terms

$\vec{r}_{ij} = \vec{r}_j - \vec{r}_i$



Planar distribution of Z electrons

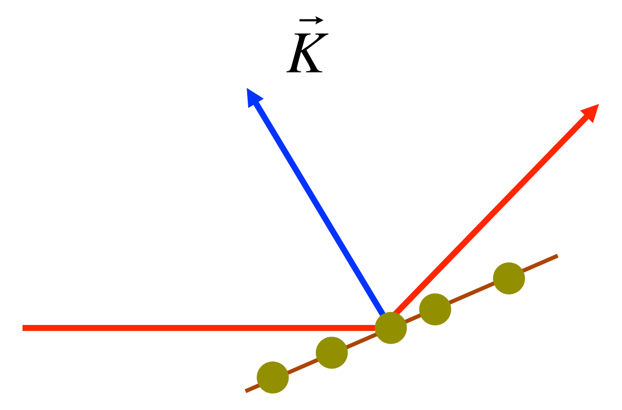
Maximum intensity for $\vec{K} \perp \vec{r}_i$

$$I(\vec{K}) = A_{\mathrm{el}}^2 \left[Z + \sum_i \sum_{j \neq i} \cos\left(\vec{K} \cdot \vec{r}_{ij}\right) \right]$$

$\vec{K} \perp \vec{r}_i$

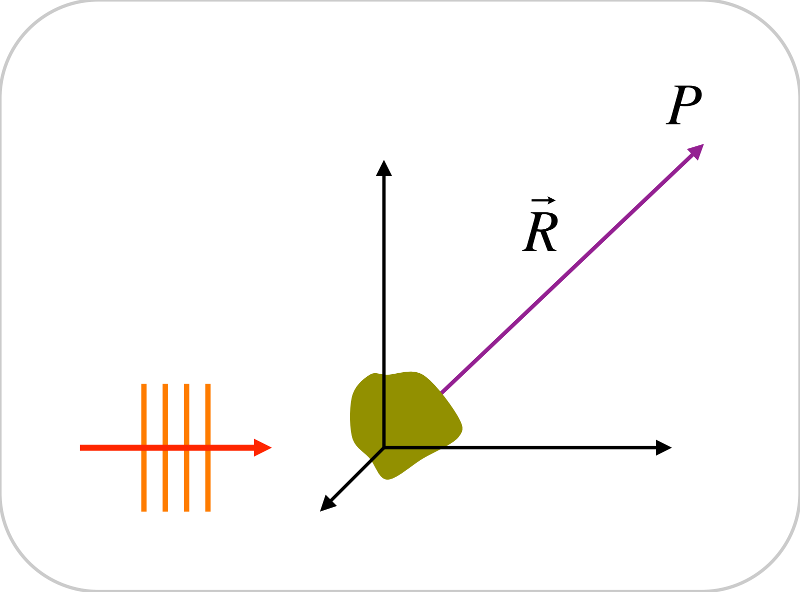
$$\cos\left(\vec{K} \cdot \vec{r}_{ij}\right) = 1$$

$$I(\vec{K}) = A_{\mathrm{el}}^2 \left[Z + Z(Z-1) \right] = A_{\mathrm{el}}^2 \, Z^2$$



Interference: continuous distribution

ρ = number density



$$\boxed{A(\vec{K}) = A_{\mathrm{el}} \int \rho_e(\vec{r})\, e^{i\vec{K}\cdot\vec{r}}\, dV}$$

$$A(\vec{K}) = \text{Fourier Tr. of } \rho(\vec{r})$$

$$\boxed{\begin{aligned} I(\vec{K}) &= \left|A(\vec{K})\right|^2 \\ &= \left|A_{\mathrm{el}}\right|^2 \left|\int \rho_e(\vec{r})\, e^{i\vec{K}\cdot\vec{r}}\, dV\right|^2 \end{aligned}}$$

Continuous distribution of charge - Fourier transform (a)

The **scattered amplitude**

is the Fourier transform

of the **electron density**

$$A(\vec{K}) = A_{\mathrm{el}} \int \rho_e(\vec{r})\, e^{i\vec{K}\cdot\vec{r}}\, dV$$

(number density)

Continuous distribution of charge - Fourier transform (b)

The **scattered intensity**

is the Fourier transform

of the **density-density autocorrelation function**

$$I(\vec{K}) = \left|A_{\mathrm{el}}\right|^2 \int \left\langle \rho_e(\vec{r})\,\rho_e(\vec{r}+\vec{r}\,') \right\rangle e^{-i\vec{K}\cdot\vec{r}\,'}\, dV$$

(number density)

Amplitude and intensity (b)

Amplitude

$$A(\vec{K}) = A_{\mathrm{el}} \int \rho_e(\vec{r})\, e^{i\vec{K}\cdot\vec{r}}\, dV$$

Cannot be measured !

Intensity

$$I(\vec{K}) = \left|A(\vec{K})\right|^2 = \underbrace{\left|A_{\mathrm{el}}\right|^2}\, \underbrace{\left|\int \rho_e(\vec{r})\, e^{i\vec{K}\cdot\vec{r}}\, dV\right|^2}$$

Is measured,
but
phase information
is lost !

Structural info

$$\left|A_{\mathrm{el}}\right|^2 = r_e^2\; E_0^2\; \frac{1}{R^2} \boxed{\left[\frac{1+\cos^2(2\theta)}{2}\right]}$$

Polarisation factor
for unpolarised beam

Z randomly distributed point-like electrons

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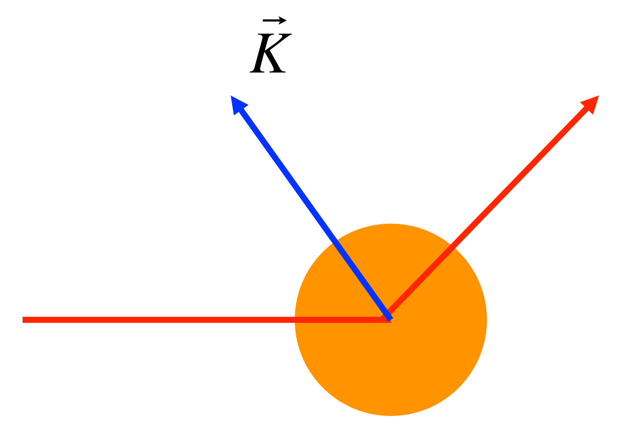
$$I(\vec{K}) = A_{\mathrm{el}}^2 \left[Z + \sum_i \sum_{j \neq i} \cos\left(\vec{K} \cdot \vec{r}_{ij}\right) \right]$$



$$f_e\left(\vec{K}\right) = \int \rho_e(\vec{r})\, e^{i\vec{K}\cdot\vec{r}}\, dV$$

$$= 4\pi \int_0^\infty r^2 \rho_e(r) \frac{\sin Kr}{Kr}\, dr$$

Spherical random distribution of each point-like electron

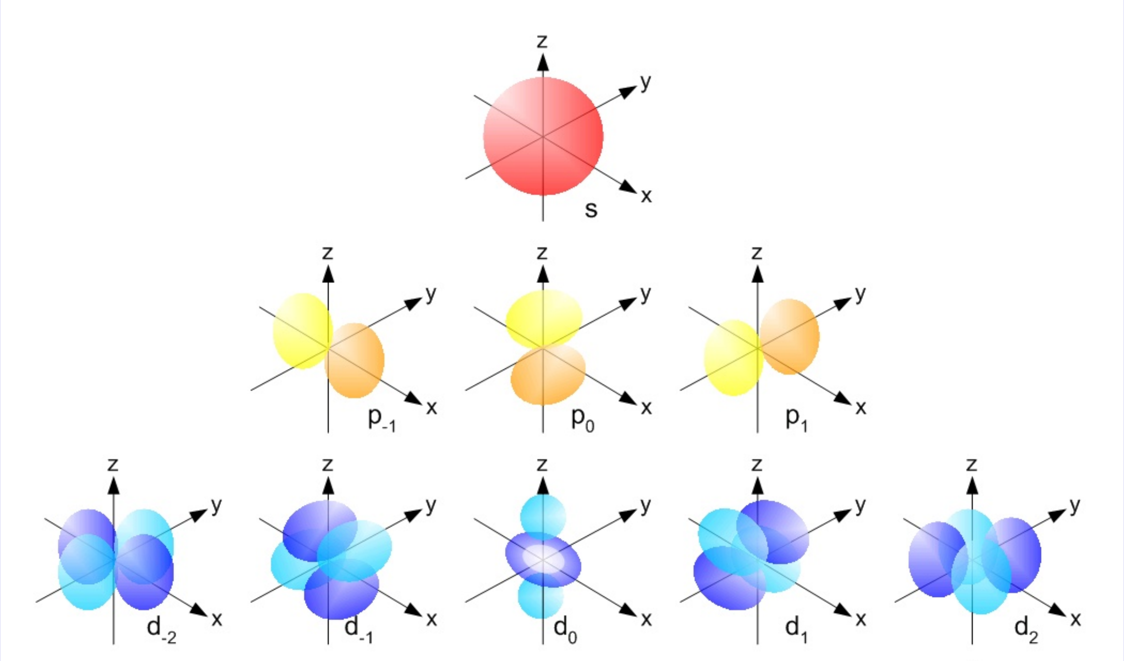
$$I(\vec{K}) = A_{\mathrm{el}}^2 \left[Z + \underbrace{Z(Z-1)\, f_e^2}_{} \right]$$

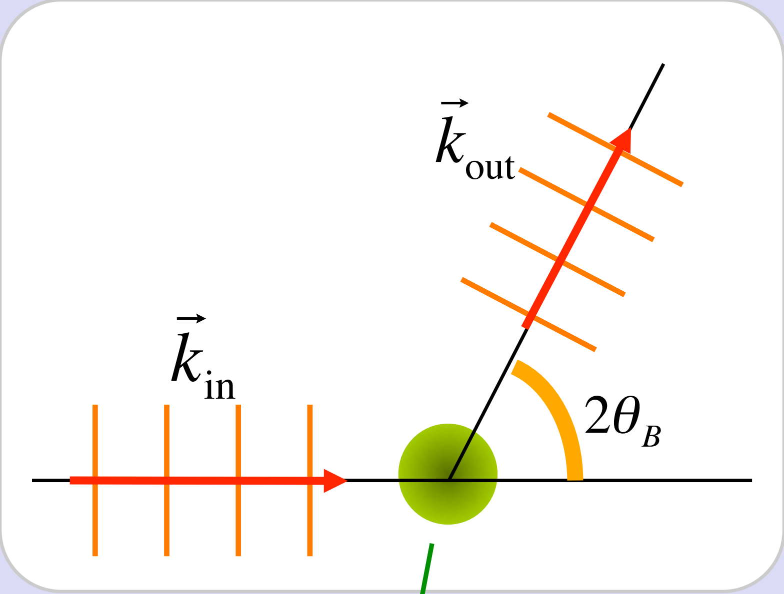
Independent scattering by single electrons

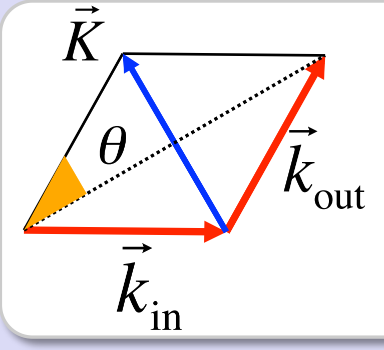
Interference: Z(Z-1) terms

> Deviations from classical treatment
Electrons distribution

Atomic orbitals





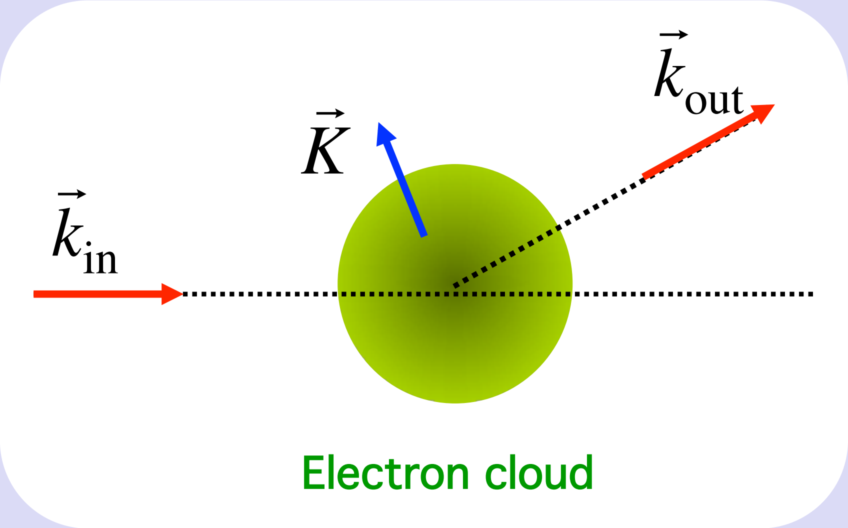


$$\left|\vec{K}\right| = 4\pi \frac{\sin\theta_B}{\lambda}$$

$$\boxed{A(\vec{K}) = A_{\text{el}} \int \rho_e(\vec{r})\, e^{i\vec{K}\cdot\vec{r}}\, dV}$$

Interference !

Electron scattering factor – electronic units



$$\boxed{A(\vec{K}) = A_{\text{el}} \int \rho_e(\vec{r})\, e^{i\vec{K}\cdot\vec{r}}\, dV}$$

$$\boxed{f_e(\vec{K})}$$

$$\boxed{I(\vec{K}) = |A(\vec{K})|^2 = |A_{\text{el}}|^2 \, |f_e(\vec{K})|^2}$$

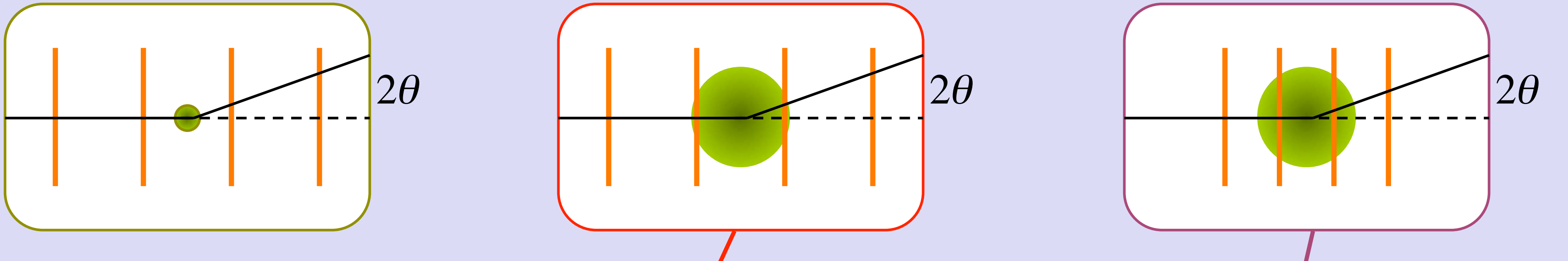
Electronic units

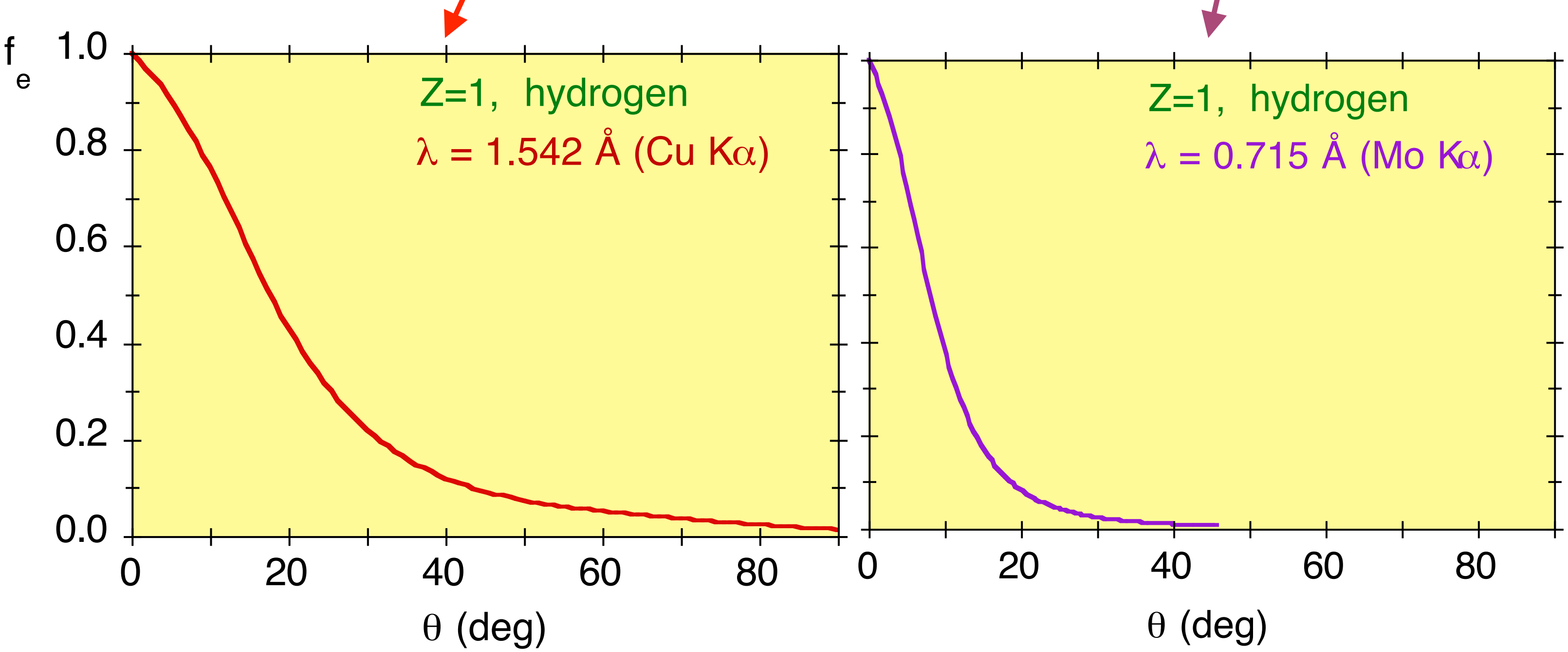
$$\boxed{A_{\text{e.u.}}(\vec{K}) = \frac{A(\vec{K})}{A_{\text{el}}} = f_e(\vec{K})}$$

$$\boxed{I_{\text{e.u.}}(\vec{K}) = \frac{|A(\vec{K})|^2}{|A_{\text{el}}|^2} = |f_e(\vec{K})|^2}$$

Interference depends on wavelength

Point-like scatterer





Hydrogen scattering factor

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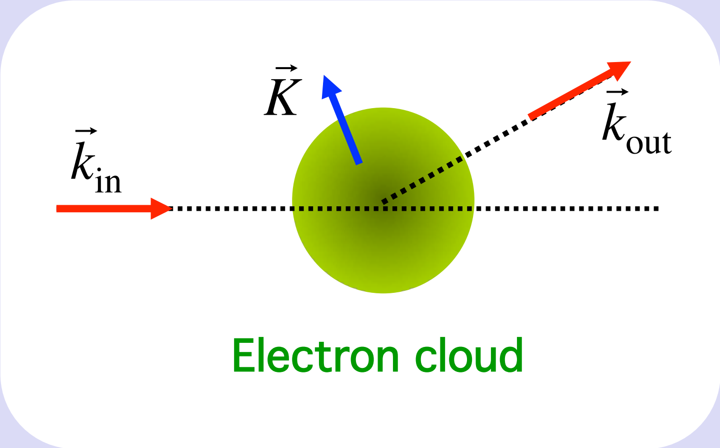
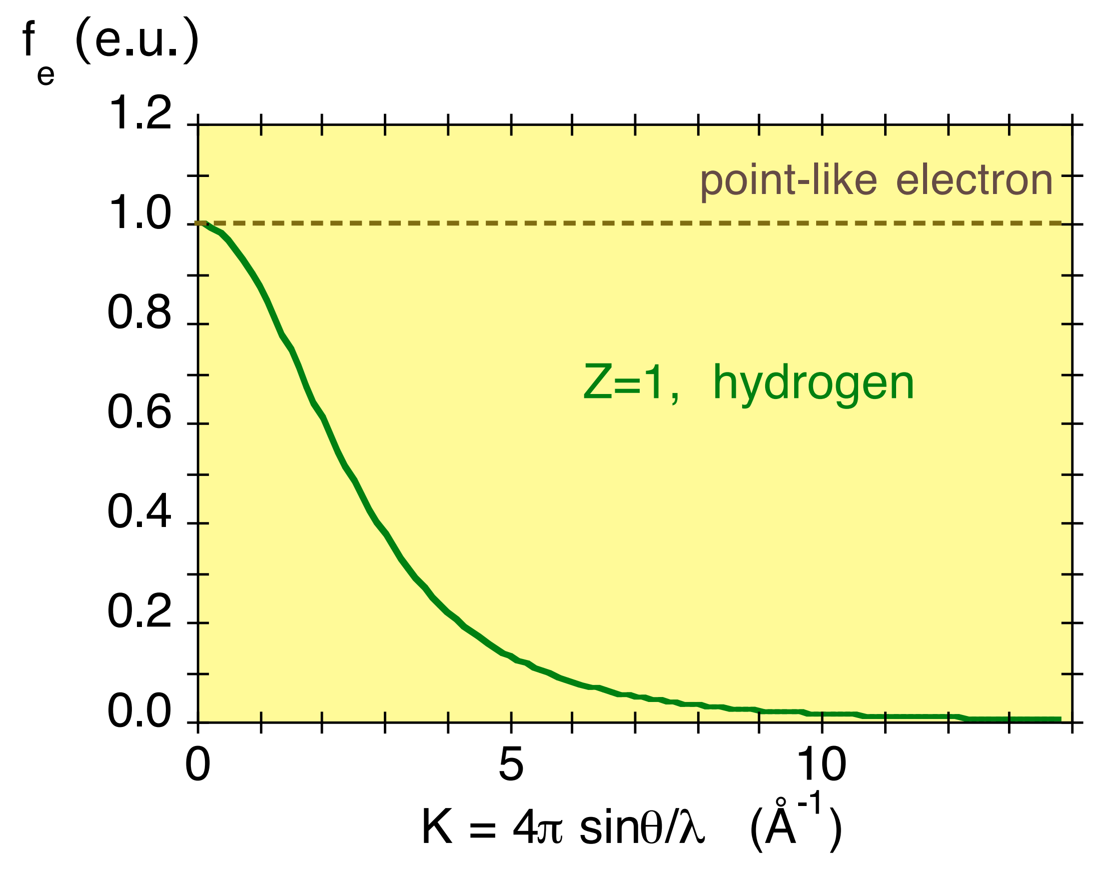


$$f_e\left(\vec{K}\right) = \int \rho_e(\vec{r})\, e^{i\vec{K}\cdot\vec{r}}\, dV$$

$$= 4\pi\int_0^\infty r^2 \rho_e(r)\,\frac{\sin Kr}{Kr}\,dr$$

for spherical symmetry



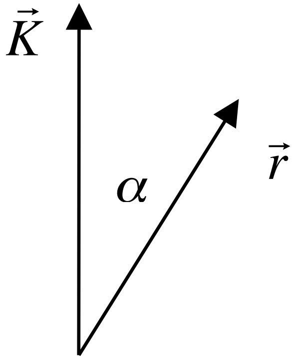
Plot independent of wavelength

Spherical symmetry

$$f_0(\vec{K}) \;=\; \int \rho(\vec{r})\, e^{i\vec{K}\cdot\vec{r}}\, dV$$

$$\begin{aligned} dV &= (dr)\;(2\pi r\sin\alpha)\;(r\,d\alpha) \\ &= 2\pi r^2\,\sin\alpha\,dr\,d\alpha \end{aligned}$$

$0 \le r < \infty$ and $0 \le \alpha < \pi$.



$$\begin{aligned} f_0(\vec{K}) &= 2\pi \int_0^\infty r^2\rho(r)\,dr \int_0^\pi e^{iKr\cos\alpha}\,\sin\alpha\,d\alpha \\ &= 2\pi \int_0^\infty r^2\,\rho(r)\,dr \left[\int_0^\pi \cos(Kr\cos\alpha)\;\sin\alpha\,d\alpha + i\int_0^\pi \sin(Kr\cos\alpha)\;\sin\alpha\,d\alpha\right] \\ &= 4\pi \int_0^\infty r^2\,\rho(r)\,\frac{\sin(Kr)}{Kr}\,dr \;=\; f_0(K)\,, \end{aligned}$$

K-dependence

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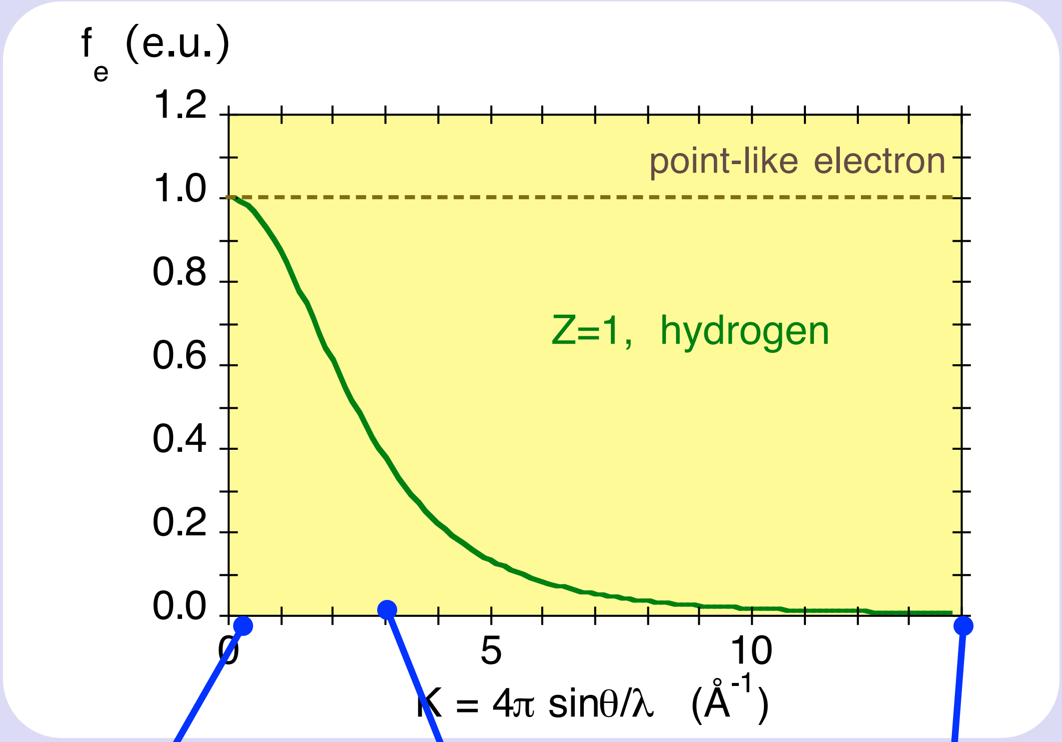
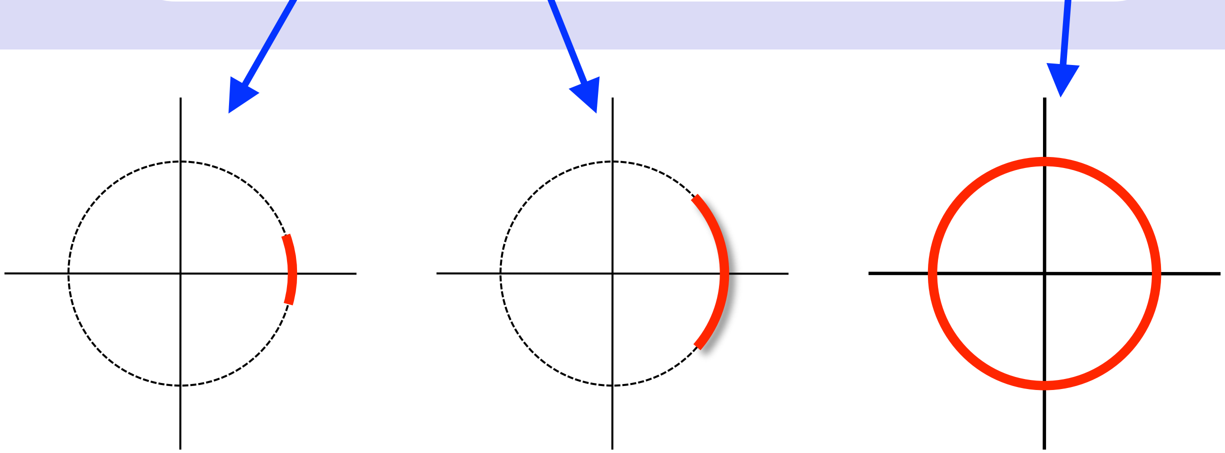
$$\boxed{f_e(\vec{K}) = \int \rho_e(\vec{r})\, e^{i\vec{K}\cdot\vec{r}}\, dV}$$

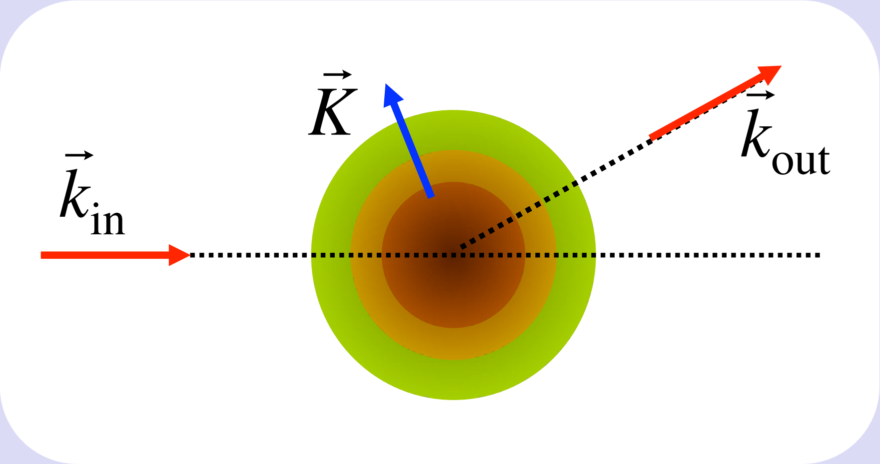


Imaginary plane

$$e^{i\vec{K}\cdot\vec{r}}$$



The atomic scattering factor



sum over electrons

$$f_0\left(\vec{K}\right) = \sum_n f_{e,n}\left(\vec{K}\right)$$

$$= \sum_n \int \rho_{e,n}(\vec{r}) e^{i\vec{K}\cdot\vec{r}} dV$$

$$= \int \boxed{\rho(\vec{r})} e^{i\vec{K}\cdot\vec{r}} dV$$

$$= 4\pi \int_0^\infty r^2 \rho_e(r) \frac{\sin Kr}{Kr} dr$$

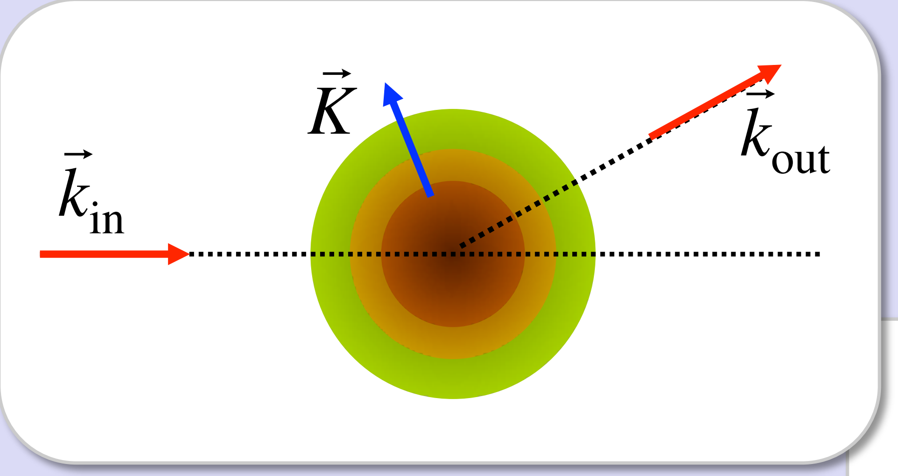
total electronic density

for spherical symmetry

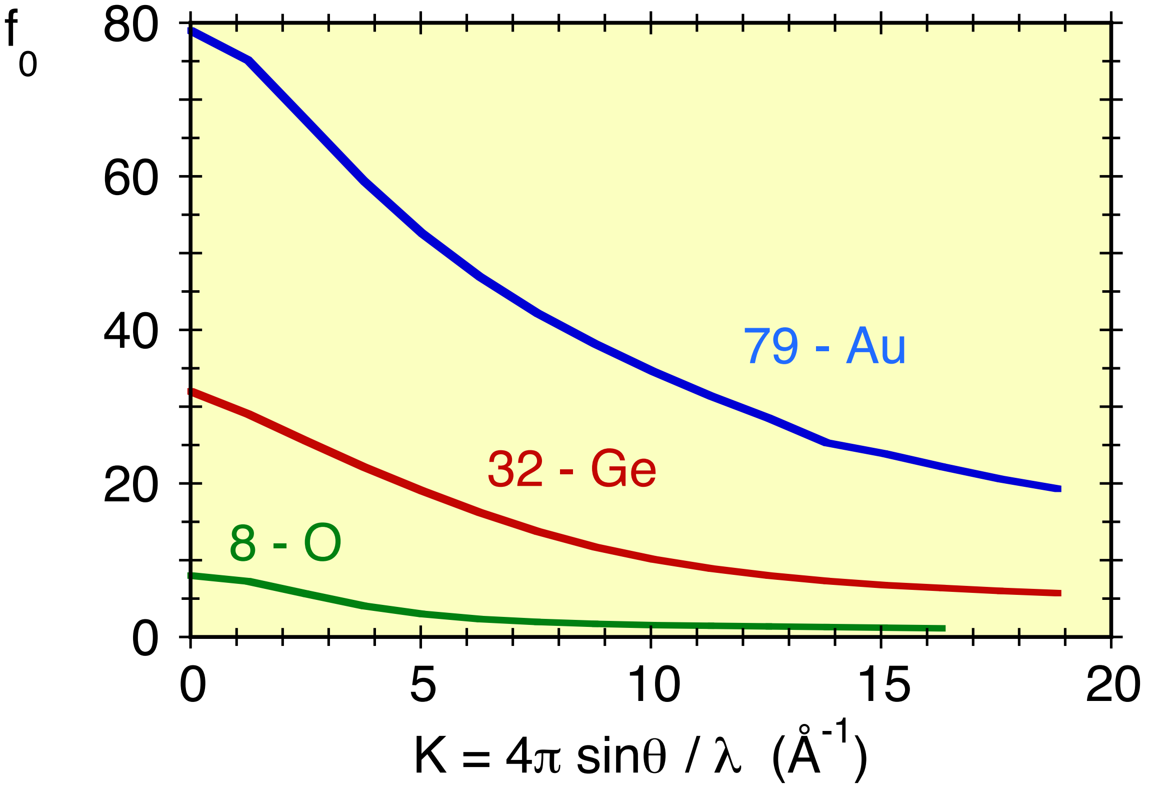
$$A_{\text{e.u.}}\left(\vec{K}\right) = f_0\left(\vec{K}\right)$$

$$I_{\text{e.u.}}\left(\vec{K}\right) = \left|f_0\left(\vec{K}\right)\right|^2$$

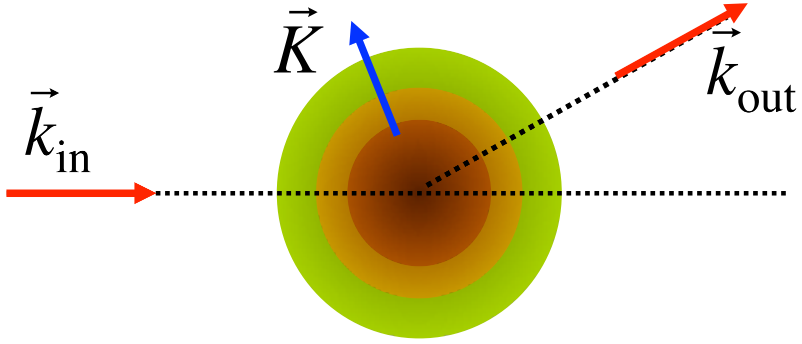
Scattering amplitudes



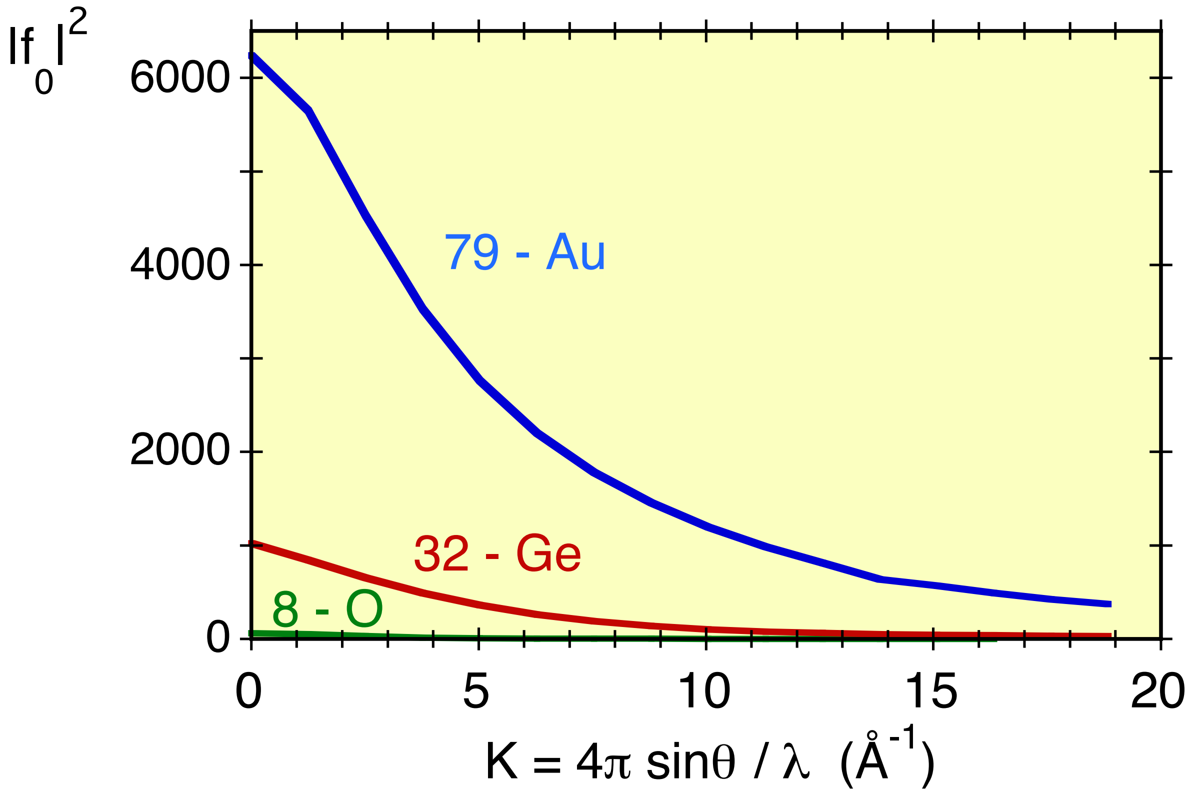
$$A_{\mathrm{e.u.}}\left(\vec{K}\right) = f_0\left(\vec{K}\right)$$



Scattering intensities



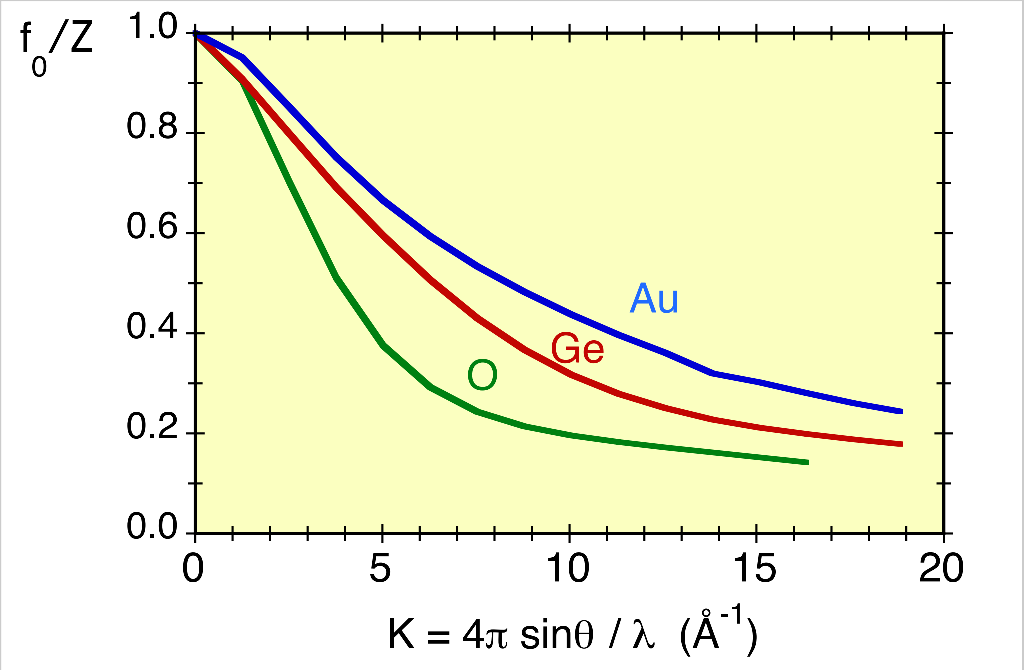
$$I_{\text{e.u.}}\left(\vec{K}\right) = \left|f_0\left(\vec{K}\right)\right|^2$$



Sensitivity to heavier atoms

K-dependence of intensity

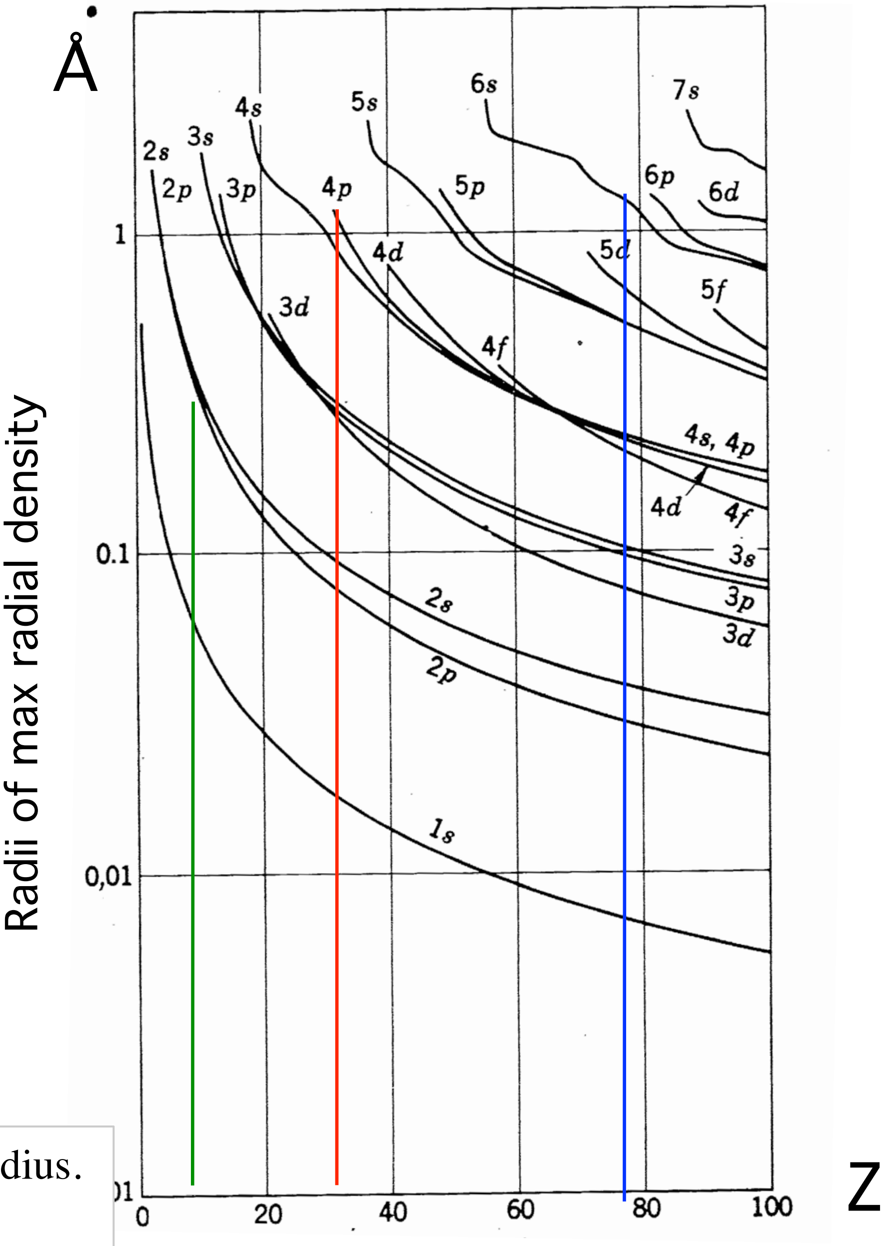
Scattering factors and electron densities



$$f_0(K) = 4\pi \int_0^\infty r^2 \rho_e(r) \frac{\sin Kr}{Kr} dr$$

Atomic radii

8 - O	0.48 Å	$1s^2\ 2s^2\ 2p^4$
32 Ge	1.25 Å	[Ar] $3d^{10}\ 4s^2\ 4p^2$
79 Au	1.74 Å	[Xe] $4f^{14}\ 5d^{10}\ 6s^1$



The scattering factor of Au is broader in spite of the larger atomic radius.
The electron density of Au is concentrated at short distances.

X-ray scattering intensity

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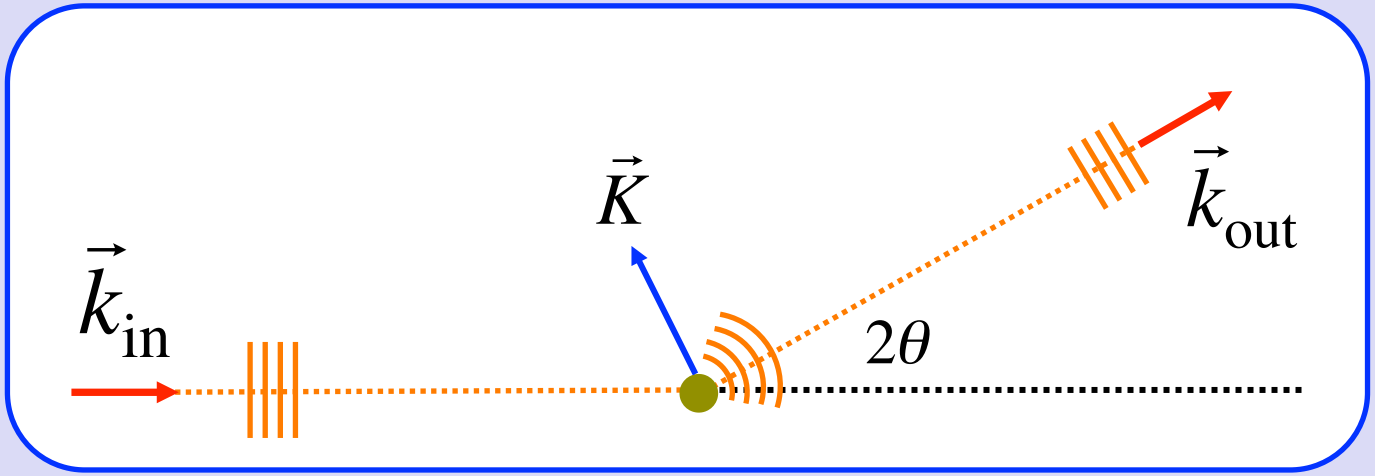


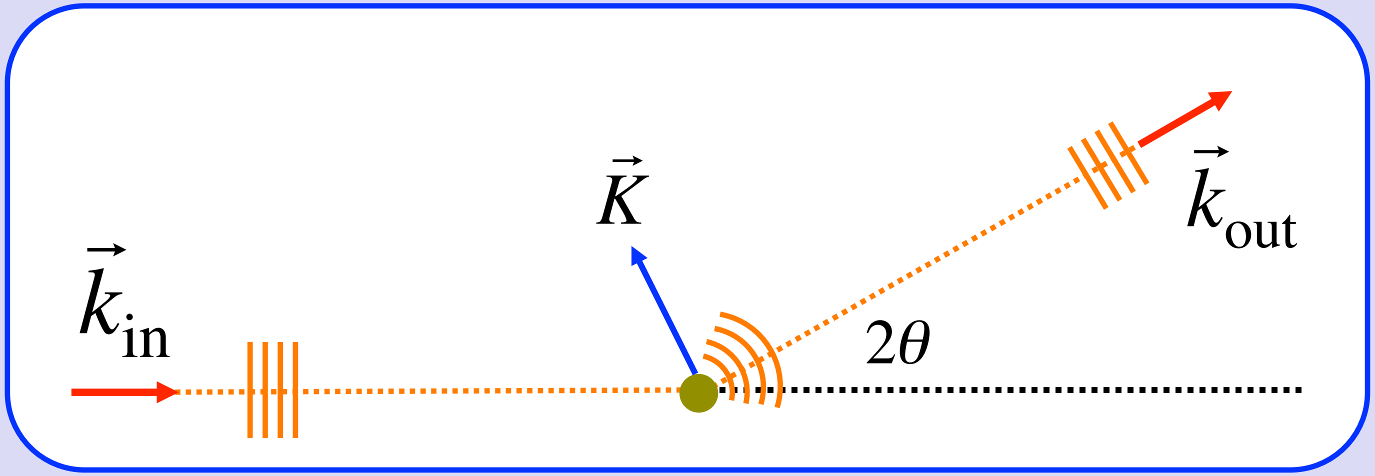
$$\left|\vec{K}\right| = 4\pi \frac{\sin\theta}{\lambda}$$

$$I(\vec{K}) \propto \begin{cases} r_e^2 \\ r_e^2 \left|f_0\left(\vec{K}\right)\right|^2 \end{cases}$$

r_e^2 → Point-like electron (independent of θ, λ)

$r_e^2 \left|f_0\left(\vec{K}\right)\right|^2$ → Atom (depending on θ, λ and Z)

X-ray scattering cross-section

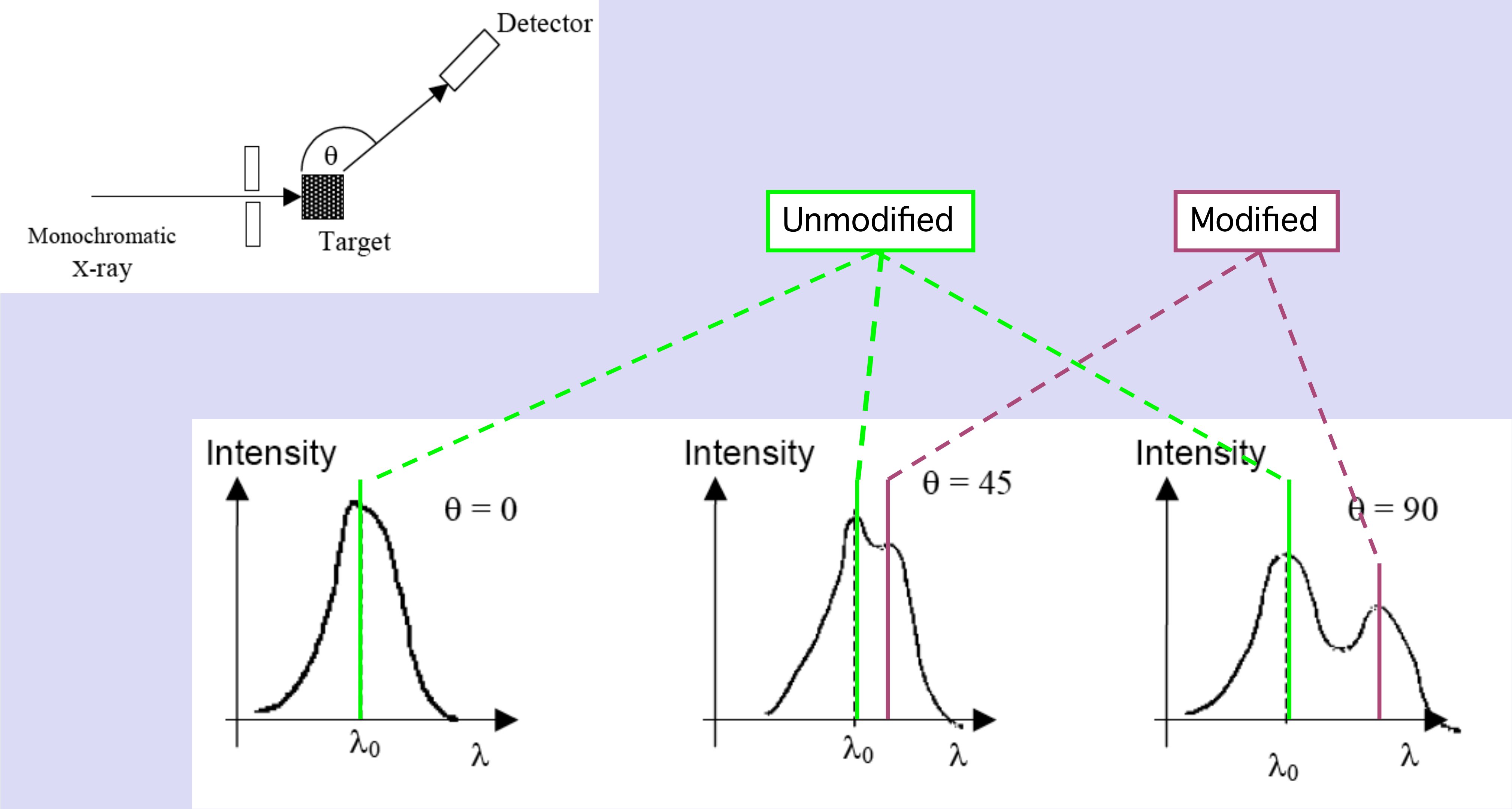


$$\left|\vec{K}\right| = 4\pi \frac{\sin\theta}{\lambda}$$

$$\frac{d\sigma}{d\Omega} = \begin{cases} r_e^2 & \longrightarrow \text{Point-like electron (independent of } \theta, \lambda) \\ r_e^2 \left|f_0\left(\vec{K}\right)\right|^2 & \longrightarrow \text{Atom (depending on } \theta, \lambda \text{ and Z)} \end{cases}$$

> Deviations from classical treatment
Compton scattering

Compton experiment (1922)



Compton scattering from free electrons (a)

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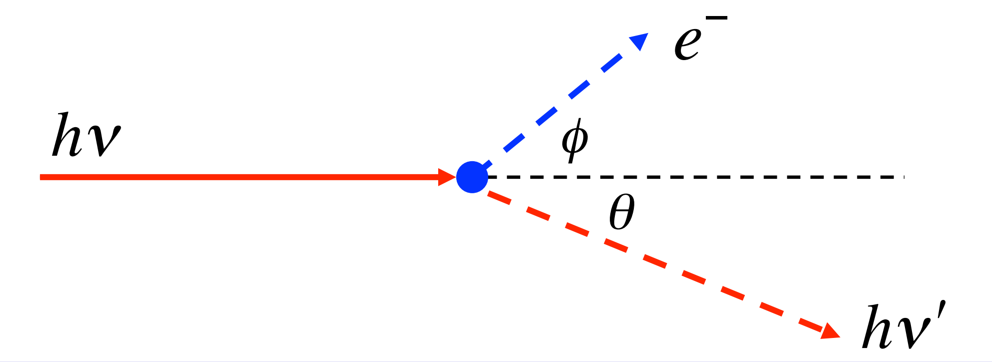


Recoil electron

Incoming photon

Scattered photon

$$\left.\begin{aligned} \frac{h\nu}{c} &= \frac{h\nu'}{c}\cos\theta + P_e\cos\phi \\ 0 &= \frac{h\nu'}{c}\sin\theta + P_e\sin\phi \end{aligned}\right\}$$

Conservation of linear momentum

$$h\nu = h\nu' + mc^2(\gamma - 1)$$

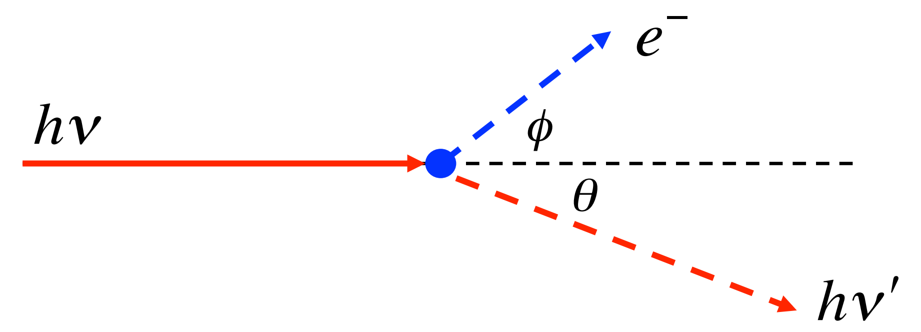
Conservation of energy

$mc^2(\gamma - 1) = E_k$ Electron kinetic energy

Assuming that the electron is initially at rest.

⇨ ν', E_k, ϕ as a function of ν, θ

Compton scattering from free electrons (b)



ν', E_k, ϕ as a function of ν, θ

$\lambda' = c/\nu'$

$\lambda = c/\nu$

Scattered photon

$$\Delta\lambda = \lambda' - \lambda = \frac{h}{mc}(1-\cos\theta) = \lambda_c(1-\cos\theta)$$

- Dependent on angle
- Independent of wavelength

0.02426 Å
(Compton wavelength)

$$mc^2 = h\nu_c = \frac{hc}{\lambda_c}$$

Recoil electron

$$E_k = h\nu \, \frac{\left(h\nu/mc^2\right)(1-\cos\theta)}{1+\left(h\nu/mc^2\right)(1-\cos\theta)}$$

$$\cot\phi = -\left[1+\left(h\nu/mc^2\right)\right]\tan(\theta/2)$$

Assuming that the electron is initially at rest.

Klein-Nishina scattering cross section

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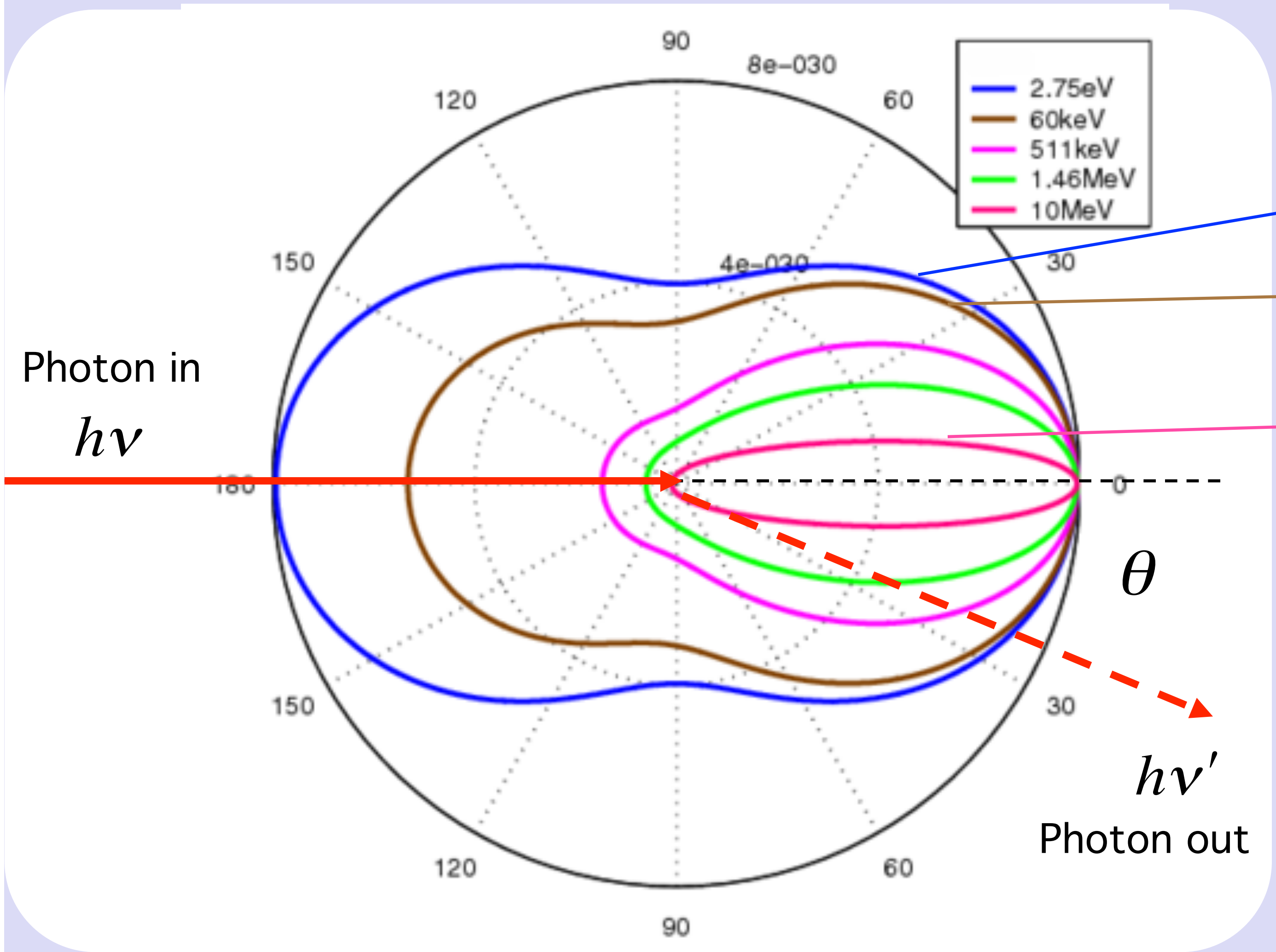
From Q.E.D.

$$\left(\frac{d\sigma}{d\Omega}\right)_{KN} = \frac{1}{2}\; r_0^2\; \frac{1}{\left[1+a(1-\cos\theta)\right]^2}\left[1+\cos^2\theta+\frac{a^2(1-\cos\theta)^2}{1+a(1-\cos\theta)}\right]$$

$$a = \frac{h\nu}{m_e c^2}$$



2.75 keV

60 keV

10 MeV

Scattering from free electrons

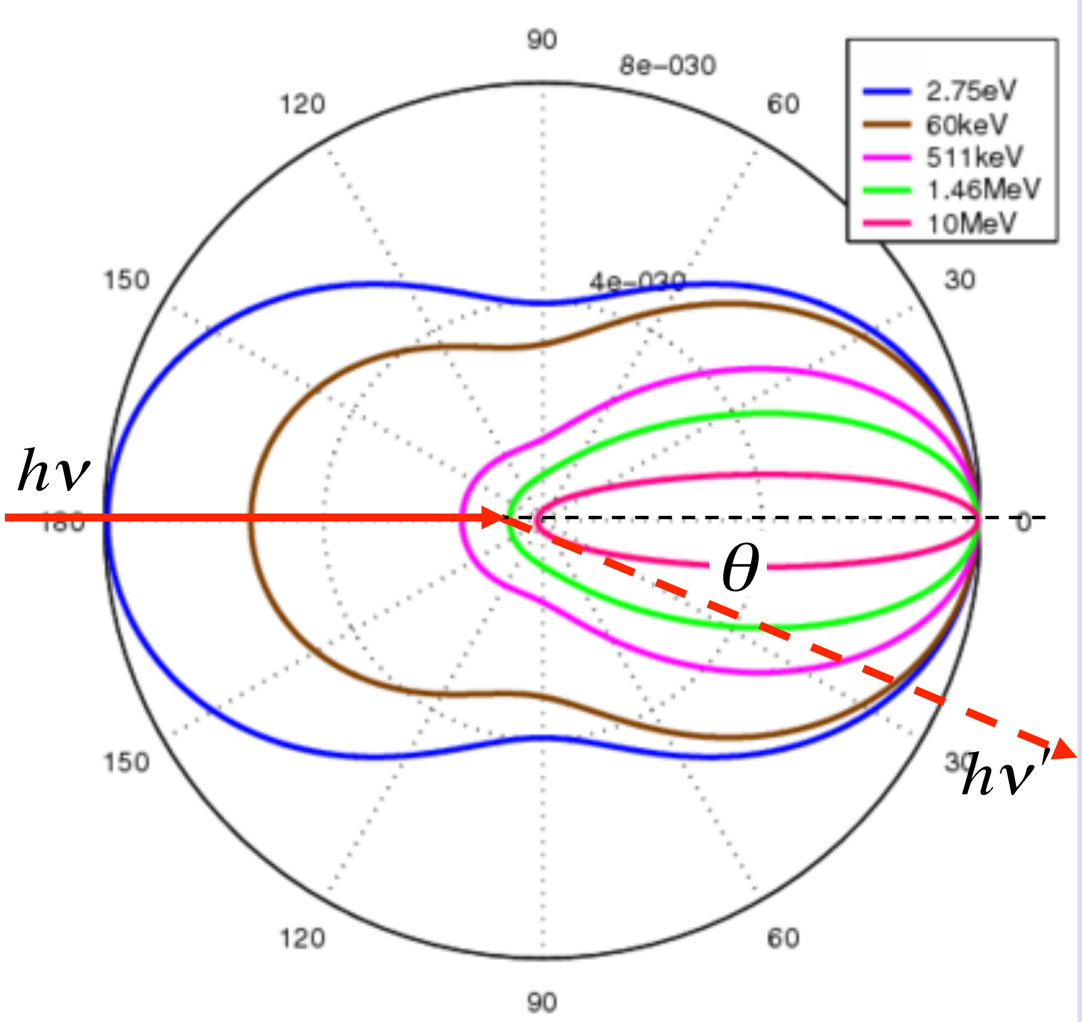
Forward peaked
at high energies

Klein-Nishina cross-section at low energies

$$\left(\frac{d\sigma}{d\Omega}\right)_{KN} = \frac{1}{2}\; r_0^2 \;\frac{1}{\left[1+a(1-\cos\theta)\right]^2}\left[1+\cos^2\theta+\frac{a^2(1-\cos\theta)^2}{1+a(1-\cos\theta)}\right]$$

$$a = \frac{h\nu}{m_e c^2}$$

Klein-Nishina formula



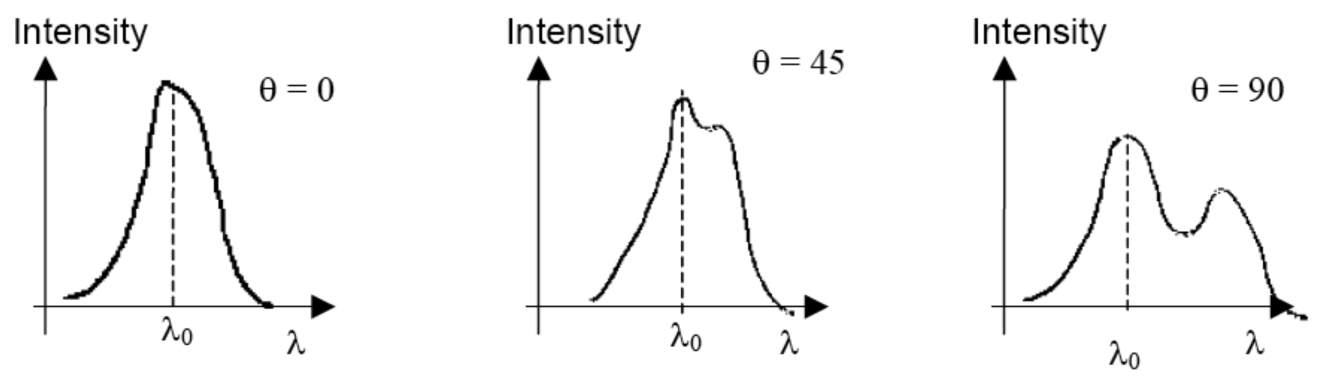
$$h\nu << m_e c^2$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{KN} \rightarrow \left(\frac{d\sigma}{d\Omega}\right)_{TH} = r_0^2\;\frac{1+\cos^2\theta}{2}$$

$$= 1 \quad \text{(in e.u.)}$$

Isotropic scattering

Scattering by atomic electrons



Scattering from electrons bound to atoms:

- both Compton and Thomson scattering can coexist
- balance: ratio (electron binding energy)/(Compton ΔE)

For rest electrons

$$\Delta E_{\mathrm{compton}} = \hbar\omega_0 - \hbar\omega' = hc\left[\frac{1}{\lambda_0} - \frac{1}{\lambda'}\right] \approx \hbar\omega_0 \frac{\Delta\lambda}{\lambda_0}$$

Modified scattering - 1 electron

From Q.E.D. (Klein-Nishina at low energies):

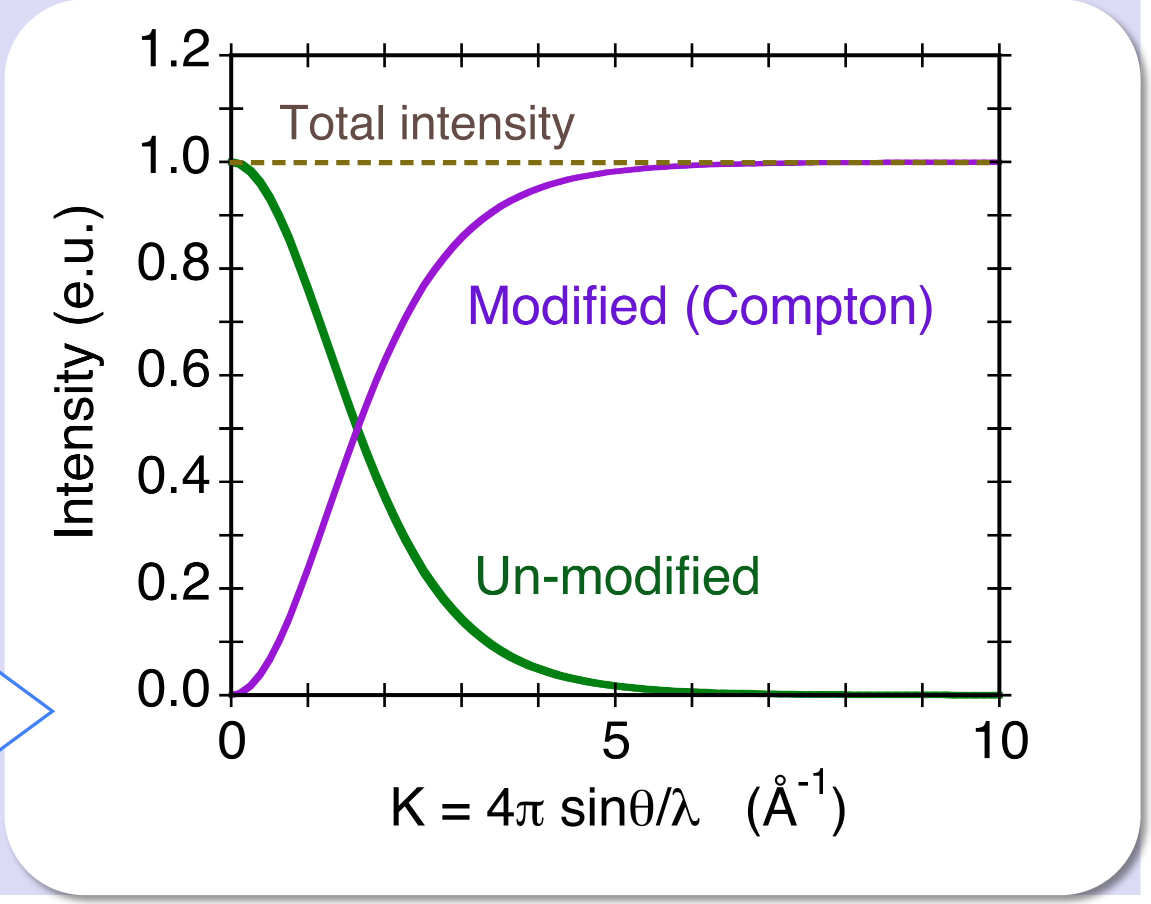
$$I_{e,\text{unmod}} + I_{e,\text{mod}} = 1$$

Intensity from a point-like classical electron (in e.u.)

$$f_e^2 + I_{e,\text{mod}} = 1$$

$$I_{e,\text{mod}} = 1 - f_e^2$$

Hydrogen



Modified scattering - atoms

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Unmodified

$$I_{\mathrm{un\,mod}} = \left| \sum_{n=1}^{Z} f_{e,n} \right|^2$$

$$\leq Z^2$$

coherent scattering
(sum of amplitudes)

Modified (Compton)

$$I_{\mathrm{mod}} = \sum \left(I_{e,\mathrm{mod}} \right)_n$$

$$= \sum (1 - f_{e,n}^2)$$

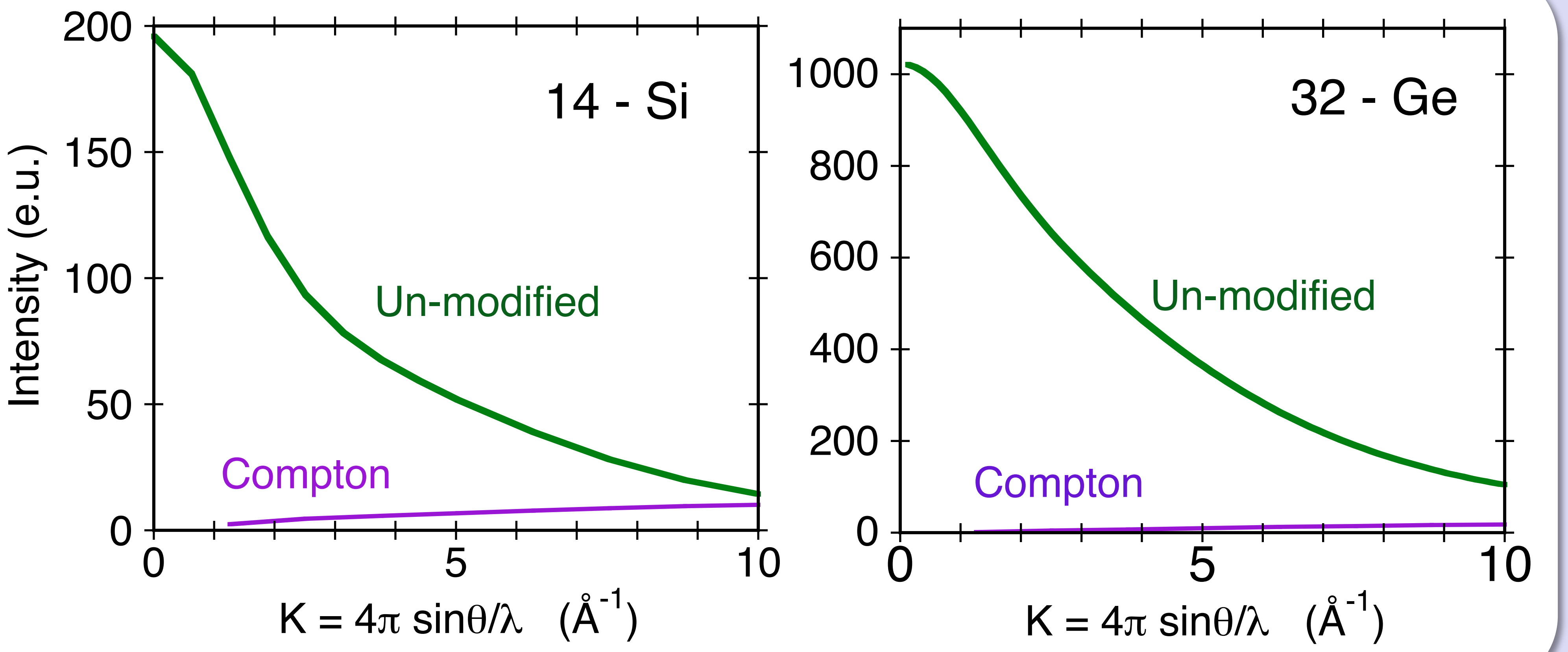
$$= Z - \sum_{n=1}^{Z} f_{e,n}^2$$

$$\leq Z$$

uncoherent scattering
(sum of intensities)

Intensities in electronic units !

Thomson .vs. Compton



Connection with Thomson theory

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Scattering from Z independent electrons (see above)

Total

equal electrons

$$I_{\text{tot}}(\vec{K}) = \left| \sum_{m=1}^{Z} e^{i\vec{K}\cdot\vec{r}_m} \right|^2 = Z + Z(Z-1)\, f_e^{\,2} = Z + Z^2 f_e^{\,2} - Z f_e^{\,2}$$

different orbitals

$$I_{\text{tot}}(\vec{K}) = \left| \sum_{m=1}^{Z} e^{i\vec{K}\cdot\vec{r}_m} \right|^2 = Z + \left| \sum_{n=1}^{Z} f_n \right|^2 - \sum_{n=1}^{Z} \left| f_n \right|^2$$

Unmodified

$$I_{\text{unmod}}(\vec{K}) = I_{\text{coherent}}(\vec{K}) = \left| \sum_{n=1}^{Z} f_n \right|^2$$

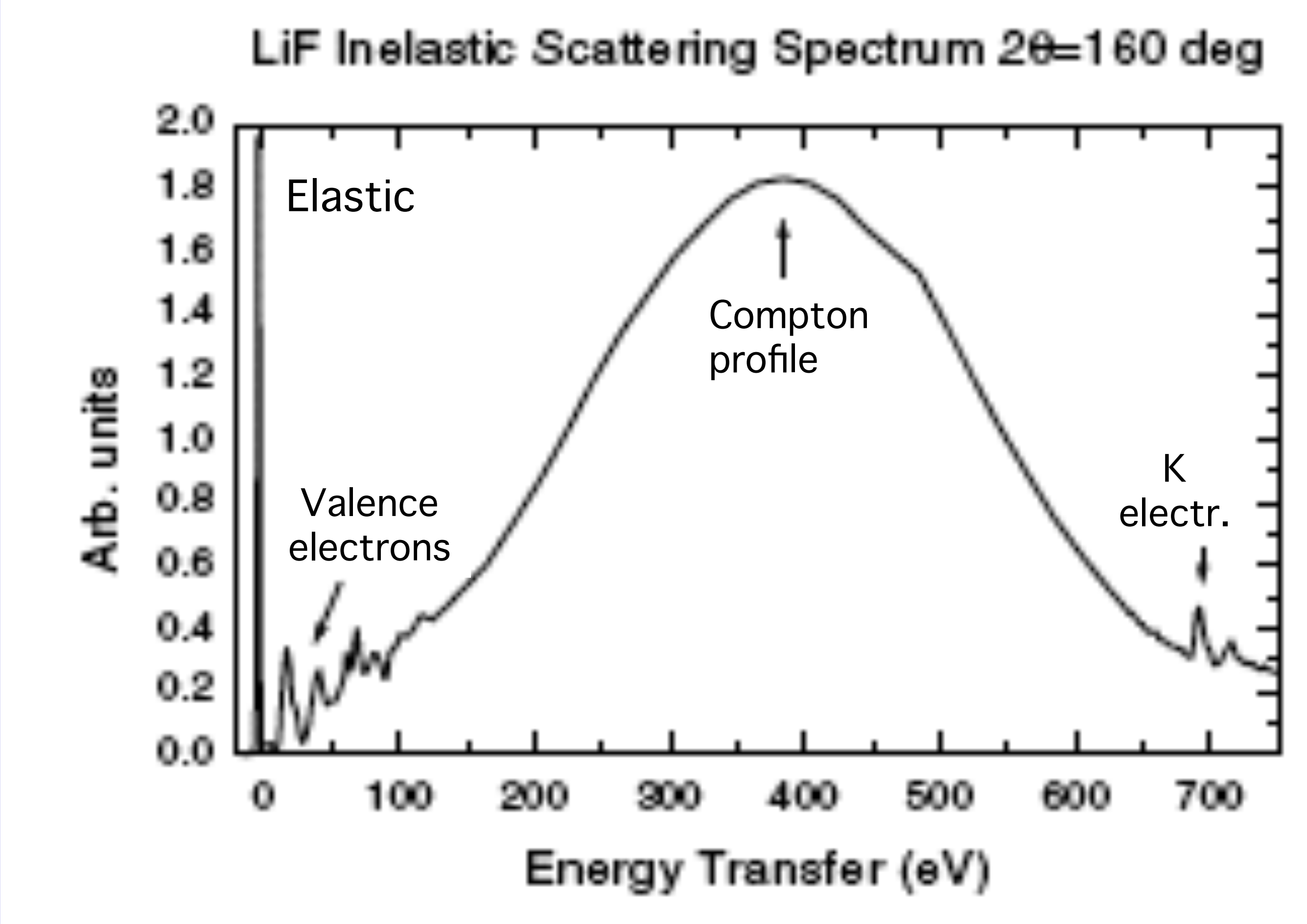
Modified (Compton)

$$\begin{aligned} I_{\text{mod}}(\vec{K}) &= I_{\text{incoherent}}(\vec{K}) \\ &= I_{\text{tot}}(\vec{K}) - I_{\text{coherent}}(\vec{K}) \\ &= Z - \sum_{n=1}^{Z} \left| f_n \right|^2 \end{aligned}$$

Intensities in electronic units !

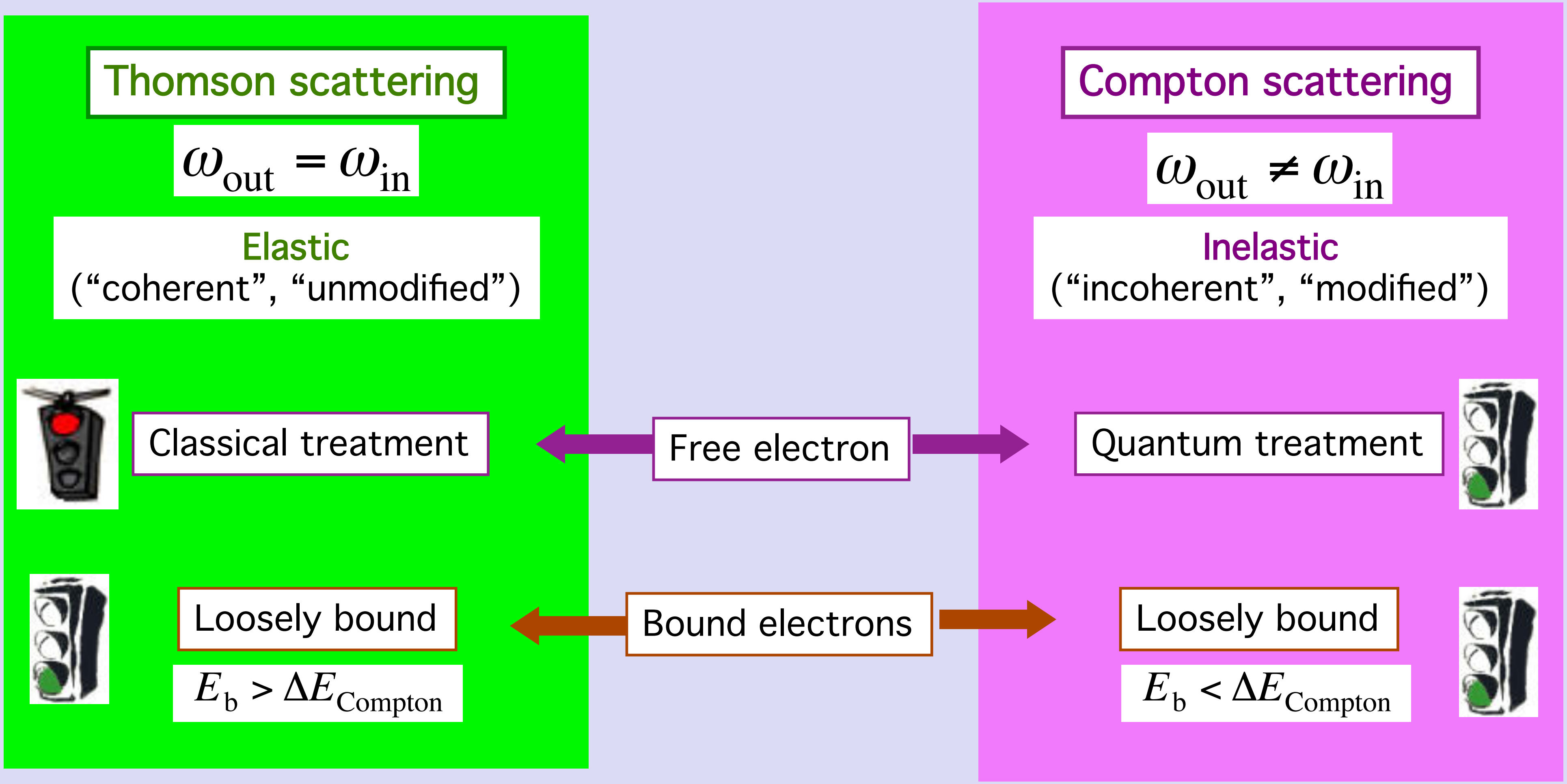
Compton profile

The electrons are not at rest initially. Compton radiation is scattered around the nominal wavelength.



Info on electron momentum distribution.
The profile is wider, the more strongly the electron is bound.

Scattering of X-rays from an electron



Thomson scattering

$\omega_{\text{out}} = \omega_{\text{in}}$

Elastic
(“coherent”, “unmodified”)

Classical treatment

Loosely bound

$E_{\text{b}} > \Delta E_{\text{Compton}}$

Free electron

Bound electrons

Compton scattering

$\omega_{\text{out}} \neq \omega_{\text{in}}$

Inelastic
(“incoherent”, “modified”)

Quantum treatment

Loosely bound

$E_{\text{b}} < \Delta E_{\text{Compton}}$

> Deviations from classical treatment Electron binding

Classical oscillator model (a)

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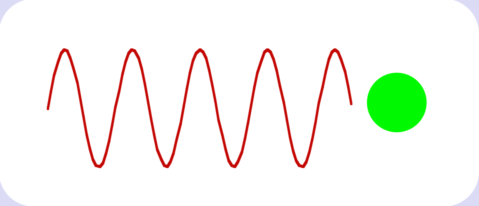
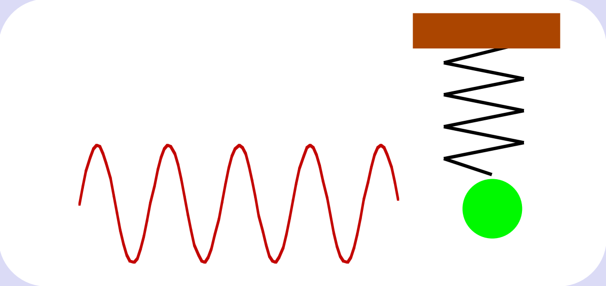




Free electron

$$\frac{d^2\vec{r}}{dt^2} = -\frac{e}{m}\vec{E}_0 e^{i\omega t}$$

E field

Bound electron

$$\frac{d^2\vec{r}}{dt^2} + 2\gamma\frac{d\vec{r}}{dt} + \omega_0^2\vec{r} = -\frac{e}{m}\vec{E}_0 e^{i\omega t}$$

Complex notation

Damping force

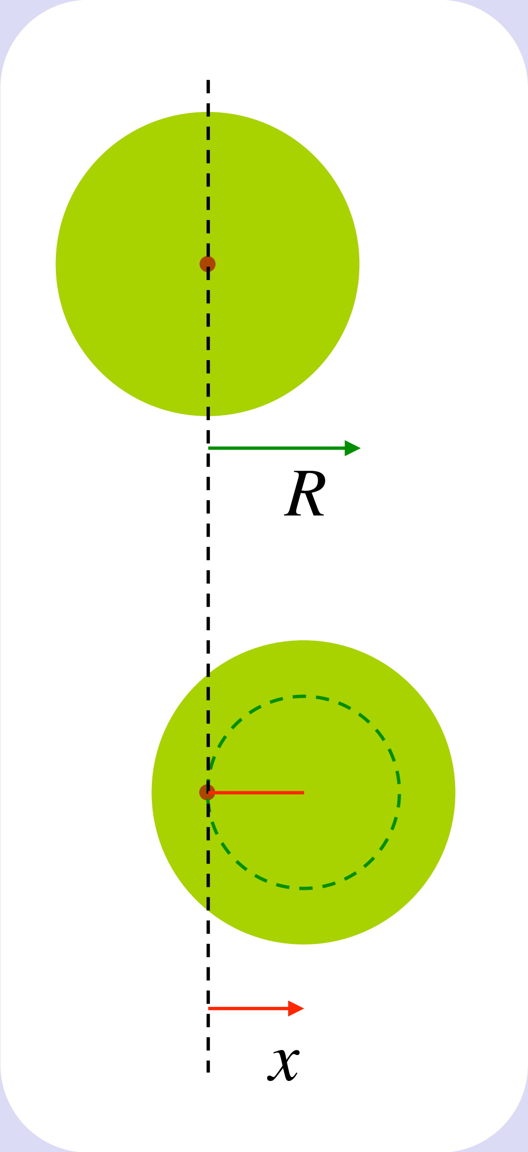
Elastic force

E field

Thomson model

Damped and forced oscillator model

Oscillator model of bound electron



Spherical distribution of negative charge centered on the positive nucleus

Displacement x

Restoring force

$$|F| = \frac{1}{4\pi\varepsilon_0}\frac{Qq_x}{x^2} \approx \frac{1}{4\pi\varepsilon_0}\frac{Q^2}{x^2}\frac{x^3}{R^3}$$

$$|F| \propto x$$

Classical oscillator model (b)

Free electron

$$\frac{d^2\vec{r}}{dt^2} = -\frac{e}{m}\vec{E}_0 e^{i\omega t}$$

Bound electron:

$$\frac{d^2\vec{r}}{dt^2} + 2\gamma\frac{d\vec{r}}{dt} + \omega_0^2\vec{r} = -\frac{e}{m}\vec{E}_0 e^{i\omega t}$$

Oscillating solution

$$\vec{r}(t) = \vec{r}_0 e^{i\omega t}$$

Complex notation

Amplitude of oscillation

$$\vec{r}_0 = \frac{e\vec{E}_0}{m}\frac{1}{\omega^2}$$

$$\vec{r}_0 = -\frac{e\vec{E}_0}{m}\frac{1}{\omega_0^2 - \omega^2 + 2i\gamma\omega}$$

$$= \frac{e\vec{E}_0}{m}\frac{1}{\omega^2 - \omega_0^2 - 2i\gamma\omega}$$

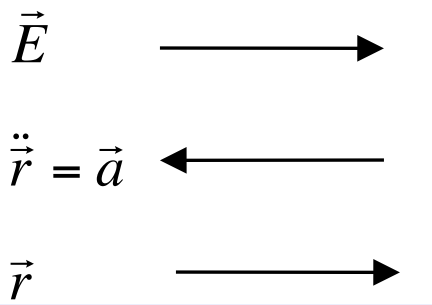
Complex amplitude

Complex displacement amplitude

Free electron

$$\vec{r}_0 = \frac{e\vec{E}_0}{m}\frac{1}{\omega^2} = \vec{R}_0\, e^{i\phi}$$

$$\phi = 0$$



Bound electron

$$\vec{r}_0 = \frac{e\vec{E}_0}{m}\frac{1}{\omega^2 - \omega_0^2 - 2i\gamma\omega} = \frac{e\vec{E}_0}{m}\frac{\omega^2 - \omega_0^2 + 2i\gamma\omega}{\left(\omega^2 - \omega_0^2\right)^2 + 4\gamma^2\omega^2} = \vec{R}_0\; e^{i\phi}$$

$$R_0 = \frac{eE_0}{m}\frac{1}{\sqrt{\left(\omega^2 - \omega_0^2\right)^2 + 4\gamma^2\omega^2}}$$

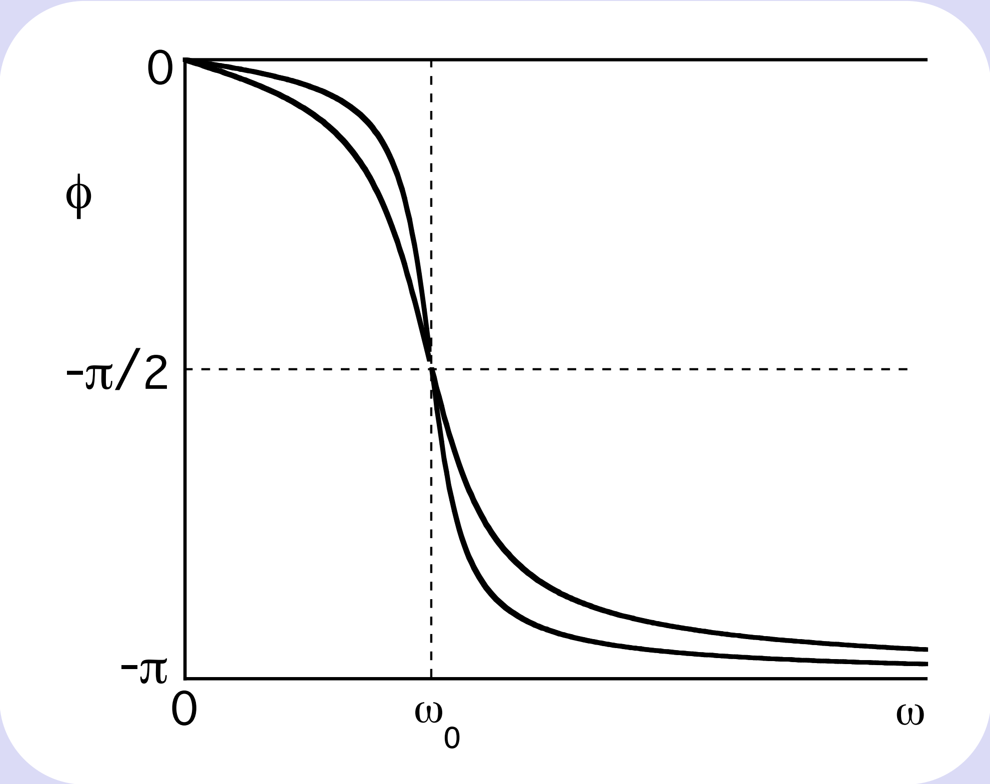
$$\tan\phi = \frac{2\gamma\omega}{\omega^2 - \omega_0^2}$$

Resonance

Phaseshift

Displacement .vs. electric field phaseshift

$$\tan\phi = \frac{2\gamma\omega}{\omega^2 - \omega_0^2}$$



Thomson model

$$\gamma = \omega_0^2 = 0$$

$$\phi = 0$$

Polarizability – 1 electron

Macroscopic electric field $P = \varepsilon_0 \chi\, E$ Electric susceptibility

Microscopic local electric field $p = \varepsilon_0 \alpha\, E$ Electric polarisability of an atom

Polarisation $\vec{p}(t) = -e\vec{r}(t) = \vec{p}_0 e^{i\omega t}$

Free electron

$$\vec{p}_0 = -\left(\frac{e^2}{\varepsilon_0 m}\,\frac{1}{\omega^2}\right)\vec{E}_0 = \boxed{\alpha(\omega)}\,\vec{E}_0$$

$$\alpha(\omega) = -\frac{e^2}{\varepsilon_0 m}\,\frac{1}{\omega^2}$$

Bound electron:

$$\vec{p}_0 = -\left(\frac{e^2}{\varepsilon_0 m}\,\frac{1}{\omega^2 - \omega_0^2 - 2i\gamma\omega}\right)\vec{E}_0 = \boxed{\alpha(\omega)}\,\vec{E}_0$$

$$\alpha(\omega) = \frac{e^2}{\varepsilon_0 m}\left(\frac{1}{\omega_0^2 - \omega^2 + 2i\gamma\omega}\right)$$

Polarizability – many electrons

Total atomic polarizability

oscillator strengths

$$\boxed{\alpha(\omega) = \frac{e^2}{\varepsilon_0 m} \sum_i \frac{f_i}{\omega_i^2 - \omega^2 + 2i\gamma\omega}}$$

sum over the frequencies
of the electromagnetic spectrum

Susceptibility

atoms per unit volume

$$\boxed{\chi(\omega) = n\alpha(\omega) = \frac{ne^2}{\varepsilon_0 m} \sum_i \frac{f_i}{\omega_i^2 - \omega^2 + 2i\gamma\omega}}$$

Dielectric constant and refractive index

Complex dielectric constant

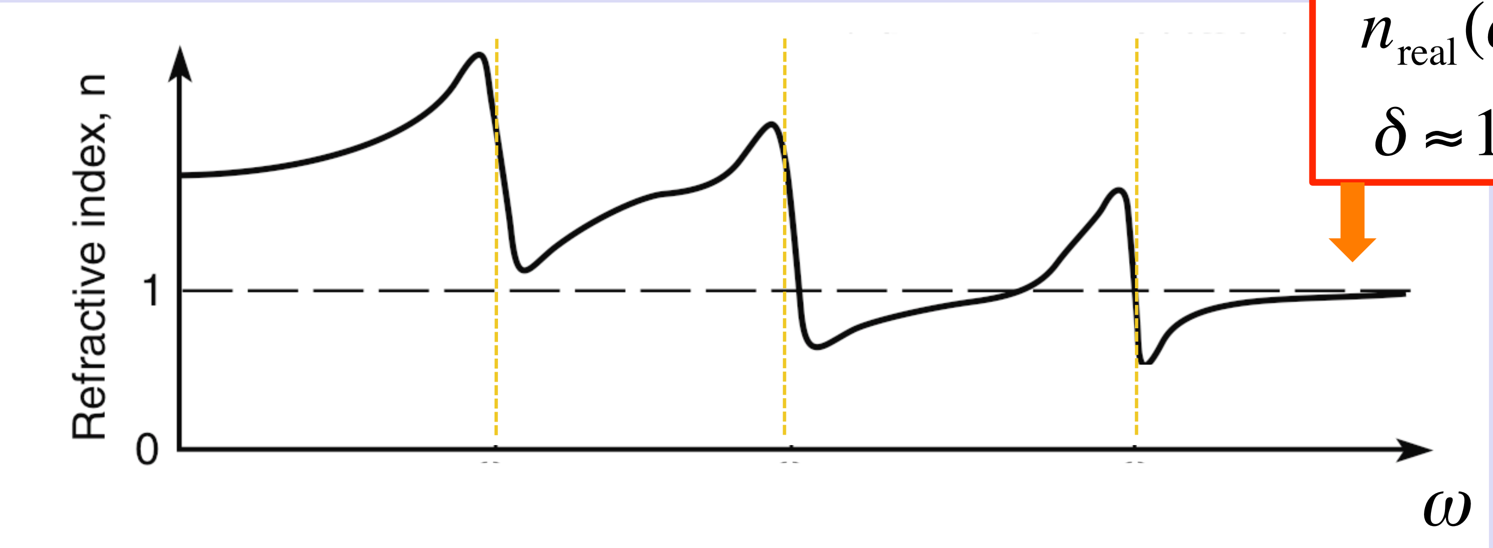
$$\varepsilon_r(\omega) = 1 + \chi(\omega) = 1 + \frac{ne^2}{\varepsilon_0 m} \sum_i \frac{f_i}{\omega_i^2 - \omega^2 + 2i\gamma\omega}$$

Real part

$$\varepsilon_{\mathrm{real}}(\omega) = 1 + \frac{ne^2}{\varepsilon_0 m} \sum_i \frac{\left(\omega_i^2 - \omega^2\right) f_i}{\left(\omega_i^2 - \omega^2\right)^2 + 4\gamma^2\omega^2}$$

Refractive index real part

$$n_{\mathrm{real}}(\omega) \approx \sqrt{\varepsilon_{\mathrm{real}}(\omega)}$$



X-rays

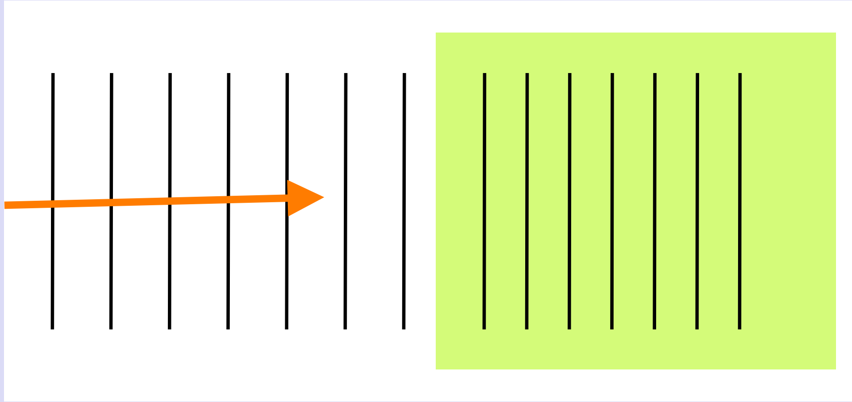
$$n_{\mathrm{real}}(\omega) \approx 1 - \delta$$

$$\delta \approx 10^{-5} - 10^{-6}$$

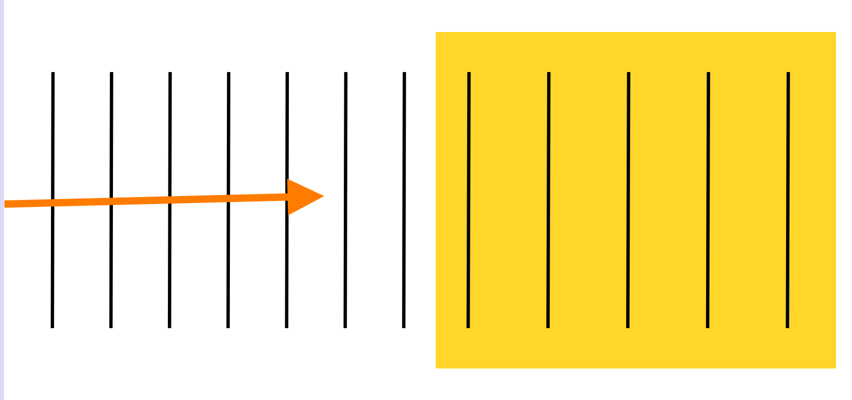
Refractive index and phase velocity

$$n_{\text{real}}(\omega) = \frac{c}{v(\omega)}$$

Interference between incoming wave and waves scattered by all atoms → Phase velocity



$$\omega << \omega_0 \begin{cases} \phi \approx 0 \\ n > 0 \end{cases}$$



$$\omega >> \omega_0 \begin{cases} \phi \approx -\pi \\ n < 0 \end{cases}$$

Very difficult
rigorous treatment.

See:
> Feymnan 1, ch. 31
>Als-Nielsen, McMorrow
ch. 3

Dielectric constant and absorption

Complex dielectric constant

$$\boxed{\varepsilon_r(\omega) = 1 + \chi(\omega) = 1 + \frac{ne^2}{\varepsilon_0 m} \sum_i \frac{f_i}{\omega_i^2 - \omega^2 + 2i\gamma\omega}}$$

Imaginary part

$$\varepsilon_{\text{imag}}(\omega) = \sum_i \frac{e^2}{\varepsilon_0 m} \frac{\gamma\omega f_i}{\left(\omega_i^2 - \omega^2\right)^2 + 4\gamma^2\omega^2}$$

Refractive index

$$n = n_{\text{real}} + i\beta$$

$$\beta(\omega) \approx \frac{\varepsilon_{\text{imag}}(\omega)}{2n_{\text{real}}}$$

Attenuation coefficient

$$\mu(\omega) = \frac{2\beta(\omega)\omega}{c} = \frac{4\pi\beta(\omega)}{\lambda}$$

Acceleration and emitted field

Free electron

$$\vec{r}(t) = \frac{e\vec{E}_0}{m}\frac{1}{\omega^2}e^{i\omega t}$$

$$\vec{a}(t) = -\frac{e\vec{E}_0}{m}e^{i\omega t}$$

$$\vec{E}_{\text{out}} = -\frac{\vec{E}_0}{r}r_e$$

Bound electron:

$$\vec{r}(t) = \frac{e\vec{E}_0}{m}\frac{1}{\omega^2-\omega_0^2-2i\gamma\omega}e^{i\omega t}$$

$$\vec{a}(t) = -\frac{e\vec{E}_0}{m}\frac{\omega^2}{\omega^2-\omega_0^2-2i\gamma\omega}e^{i\omega t}$$

$$\vec{E}_{\text{out}} = -\frac{\vec{E}_0}{r}r_e\frac{\omega^2}{\omega^2-\omega_0^2-2i\gamma\omega}$$

Acceleration

Out field
π polarisation

$$\boxed{r_e = \frac{e^2}{4\pi\varepsilon_0 c^2 m}}$$

Scattering amplitude (one point-like electron)

Free electron

$$A(\vec{K}) = \underbrace{\underbrace{-E_0\,\frac{e^{-ik_{\mathrm{out}}R}}{R}\,e^{i\omega t}\,r_e}_{\boxed{A_{\mathrm{el}}}} \left\{\begin{matrix}\boxed{1}\\[2ex] \boxed{\dfrac{\omega^2}{\omega^2-\omega_0^2-2i\gamma\omega}}\end{matrix}\right\}}_{\boxed{A}}\; e^{i\vec{K}\cdot\vec{r}}$$

Bound electron

Point-like electron

Resonant terms (one point-like electron)

$$A = A_{\mathrm{el}} \left[\frac{\omega^2}{\omega^2 - \omega_0^2 - 2i\gamma\omega} \right]$$

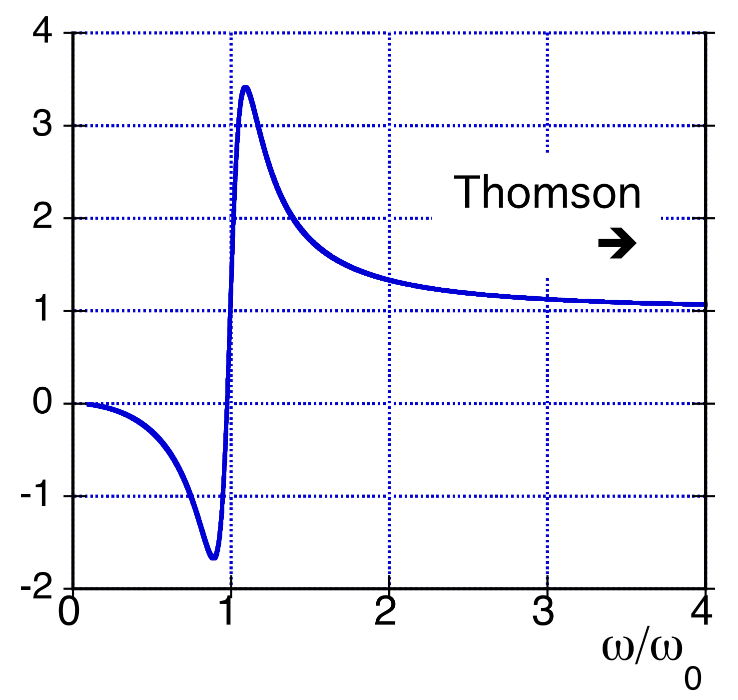
$$= A_{\mathrm{el}} \left[1 + \frac{\omega_0^2 + 2i\gamma\omega}{\omega^2 - \omega_0^2 - 2i\gamma\omega} \right] \approx A_{\mathrm{el}} \left[1 + \frac{\omega_0^2}{\omega^2 - \omega_0^2 - 2i\gamma\omega} \right]$$

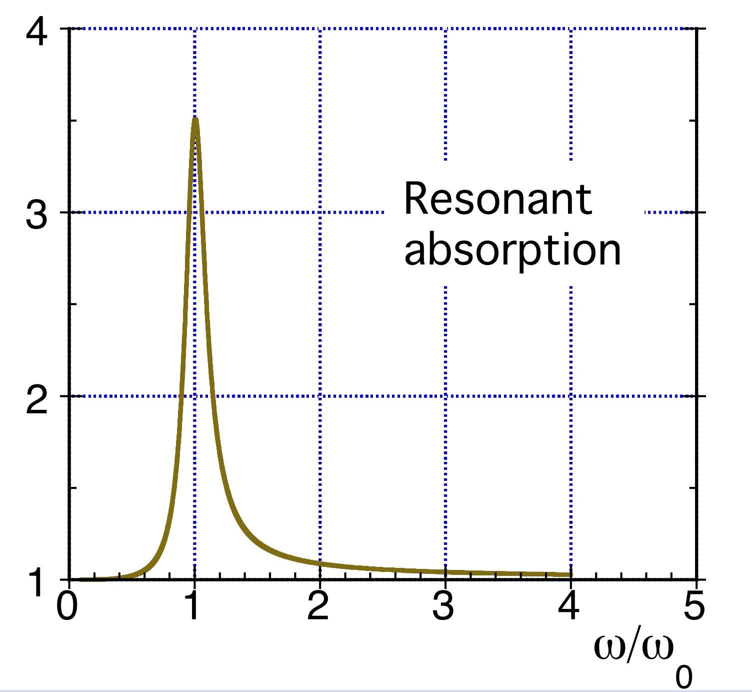
$$= A_{\mathrm{el}} \left[1 + \frac{\omega_0^2\left(\omega^2 - \omega_0^2\right) + 2i\gamma\omega\omega_0^2}{\left(\omega^2 - \omega_0^2\right)^2 + 4\gamma^2\omega^2} \right]$$

$$= A_{\mathrm{el}} \left[\underbrace{1}_{\text{Thomson term}} + \underbrace{\frac{\omega_0^2\left(\omega^2 - \omega_0^2\right)}{\left(\omega^2 - \omega_0^2\right)^2 + 4\gamma^2\omega^2}}_{\text{Real resonant term}} + i \underbrace{\frac{2\gamma\omega\omega_0^2}{\left(\omega^2 - \omega_0^2\right)^2 + 4\gamma^2\omega^2}}_{\text{Imaginary resonant term}} \right]$$

Resonant terms (one point-like electron)

$$A \;=\; A_{\mathrm{el}}\left[\underbrace{1\;+\frac{\omega_0^2\left(\omega^2-\omega_0^2\right)}{\left(\omega^2-\omega_0^2\right)^2+4\gamma^2\omega^2}}_{}\;+\;\underbrace{i\;\frac{2\gamma\omega\omega_0^2}{\left(\omega^2-\omega_0^2\right)^2+4\gamma^2\omega^2}}_{}\right]$$





connection with
refractive index

$$\propto 2-\varepsilon_{\mathrm{real}} = 2-n_{\mathrm{real}}^2$$

Resonant absorption (one point-like electron)

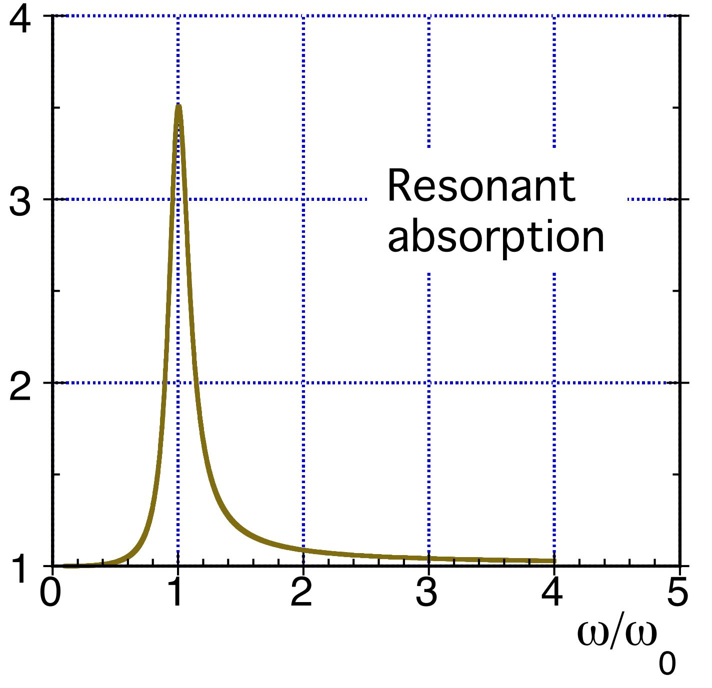
Absorption coefficient
(imaginary part of the refractive index)

$$\mu(\omega) = \frac{2\omega}{c}\beta(\omega) \approx \frac{2\omega}{c}\frac{\varepsilon_{\text{imag}}(\omega)}{2} \propto \frac{\gamma\omega^2}{\left(\omega^2 - \omega_0^2\right)^2 + 4\gamma^2\omega^2}$$

$$\Updownarrow$$

Imaginary part
of scattering amplitude

$$A_{\text{imag}} \propto \frac{2\gamma\omega\omega_0^2}{\left(\omega^2 - \omega_0^2\right)^2 + 4\gamma^2\omega^2}$$



Total cross-section (one point-like electron)

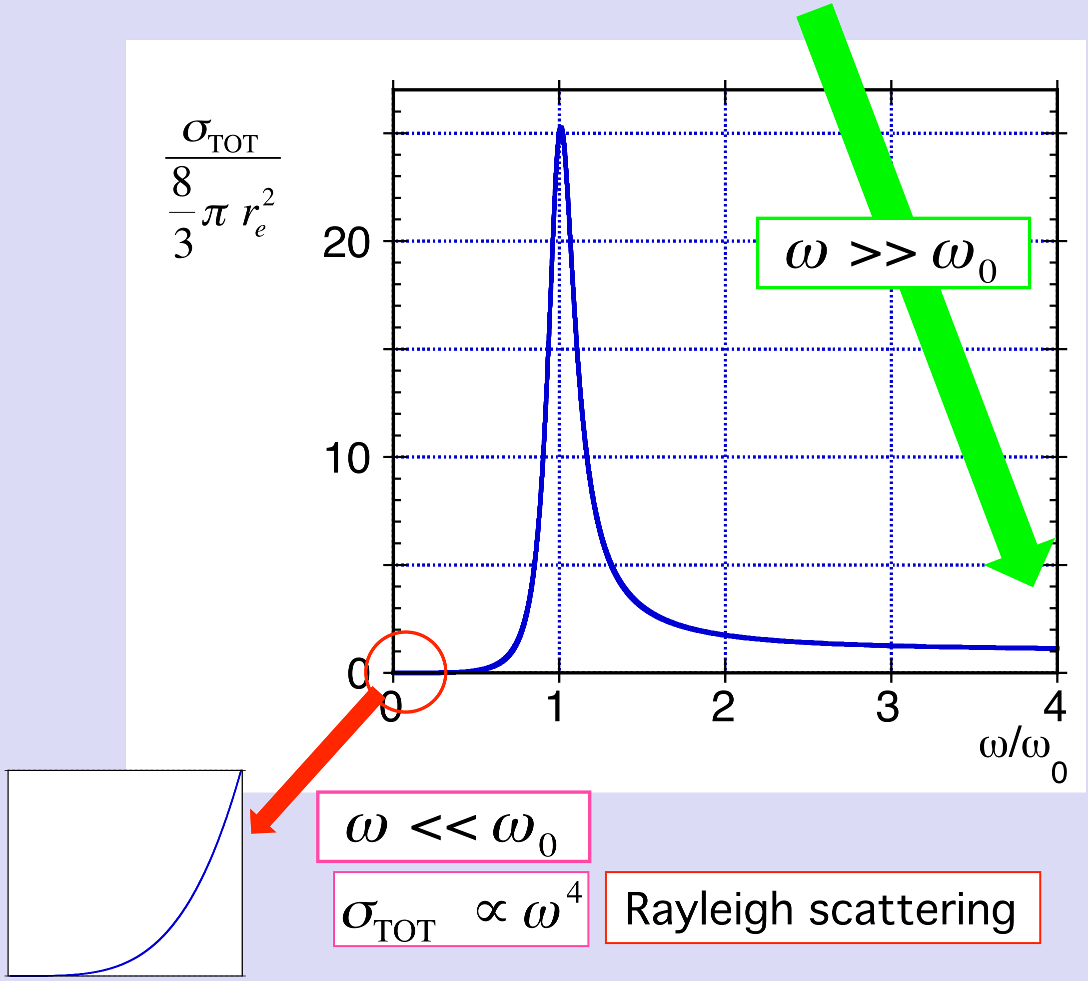
Total Thomson cross-section

$$\sigma_{\mathrm{Th}} = \frac{8}{3}\pi\, r_e^2$$

Including the resonant factor

$$\sigma_{\mathrm{TOT}} = \frac{8}{3}\pi\, r_e^2 \left| \frac{\omega^2}{\omega^2 - \omega_0^2 - 2i\gamma\omega} \right|^2$$

$$= \frac{8}{3}\pi\, r_e^2 \frac{\omega^4}{\left(\omega^2 - \omega_0^2\right)^2 + 4\gamma^2\omega^2}$$



$\omega >> \omega_0$

$\omega << \omega_0$

$\sigma_{\mathrm{TOT}} \propto \omega^4$

Rayleigh scattering

One-electron atomic scattering factor

$$A(\vec{K}) = \underbrace{-E_0 \frac{e^{-ik_{\text{out}}R}}{R} e^{i\omega t} r_e}_{A_{\text{el}}} \frac{\omega^2}{\omega^2 - \omega_0^2 - 2i\gamma\omega} e^{i\vec{K}\cdot\vec{r}}$$

Electronic charge distribution

$$\boxed{f_e(\vec{K}) = \int \rho_e(\vec{r})\, e^{i\vec{K}\cdot\vec{r}} dV}$$

$$A(\vec{K}) = A_{\text{el}}\, f_e(\vec{K}) \left[\frac{\omega^2}{\omega^2 - \omega_0^2 - 2i\gamma\omega}\right]$$

$$= A_{\text{el}} \left[\underbrace{f_e(\vec{K})} + \underbrace{f_e(\vec{K}) \frac{\omega_0^2(\omega^2 - \omega_0^2)}{(\omega^2 - \omega_0^2)^2 + 4\gamma^2\omega^2}} + \underbrace{i\, f_e(\vec{K}) \frac{\gamma\omega\omega_0^2}{(\omega^2 - \omega_0^2)^2 + 4\gamma^2\omega^2}} \right]$$

$$A(\vec{K}) = A_{\text{el}} \left[f_e(\vec{K}) + \underbrace{f'_e(K,\omega) + if_e''(K,\omega)}_{\text{Resonant terms}} \right]$$

Many-electrons atoms, quantum picture

Classical oscillator frequencies

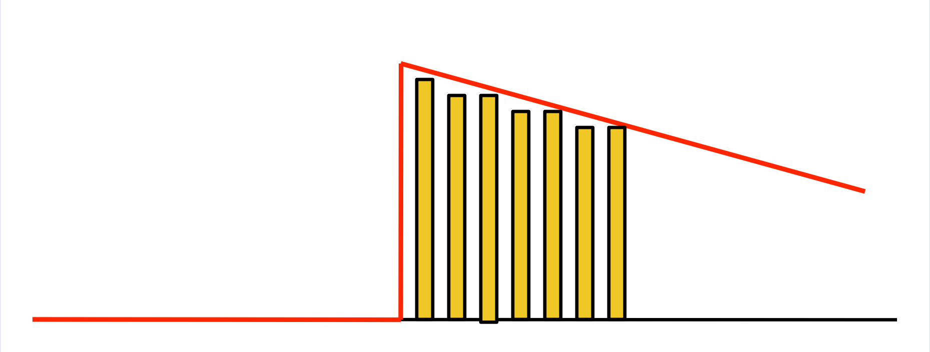
Oscillations damping

→

Bohr frequencies, transitions between stationary states
> large number of bound and
> infinite free states

Photo-electric absorption

$$\mu(\omega) \propto \sum_s g(\omega_s)\delta(\omega - \omega_s)$$



X-rays:
resonance for localised inner shells,
peaked density ρ(r)

$$f_e''(\omega,Z)$$

$$f'_e(\omega,Z)$$

largely independent of K

Resonant scattering factor (a)

Atom = assembly of oscillators at different frequencies

$$f\left(\vec{K},Z\right)=\overbrace{f_0\left(\vec{K},Z\right)}^{\text{Normal term (dep. on angle)}}+\overbrace{\underbrace{f'(\hbar\omega,Z)}_{\text{Real}}+i\,\underbrace{f''(\hbar\omega,Z)}_{\text{Imaginary}}}^{\text{Resonant ('anomalous') terms (~ indep. of angle)}}$$

$f\left(\vec{K},Z\right)$ ↕ Sum of contributions from all electrons

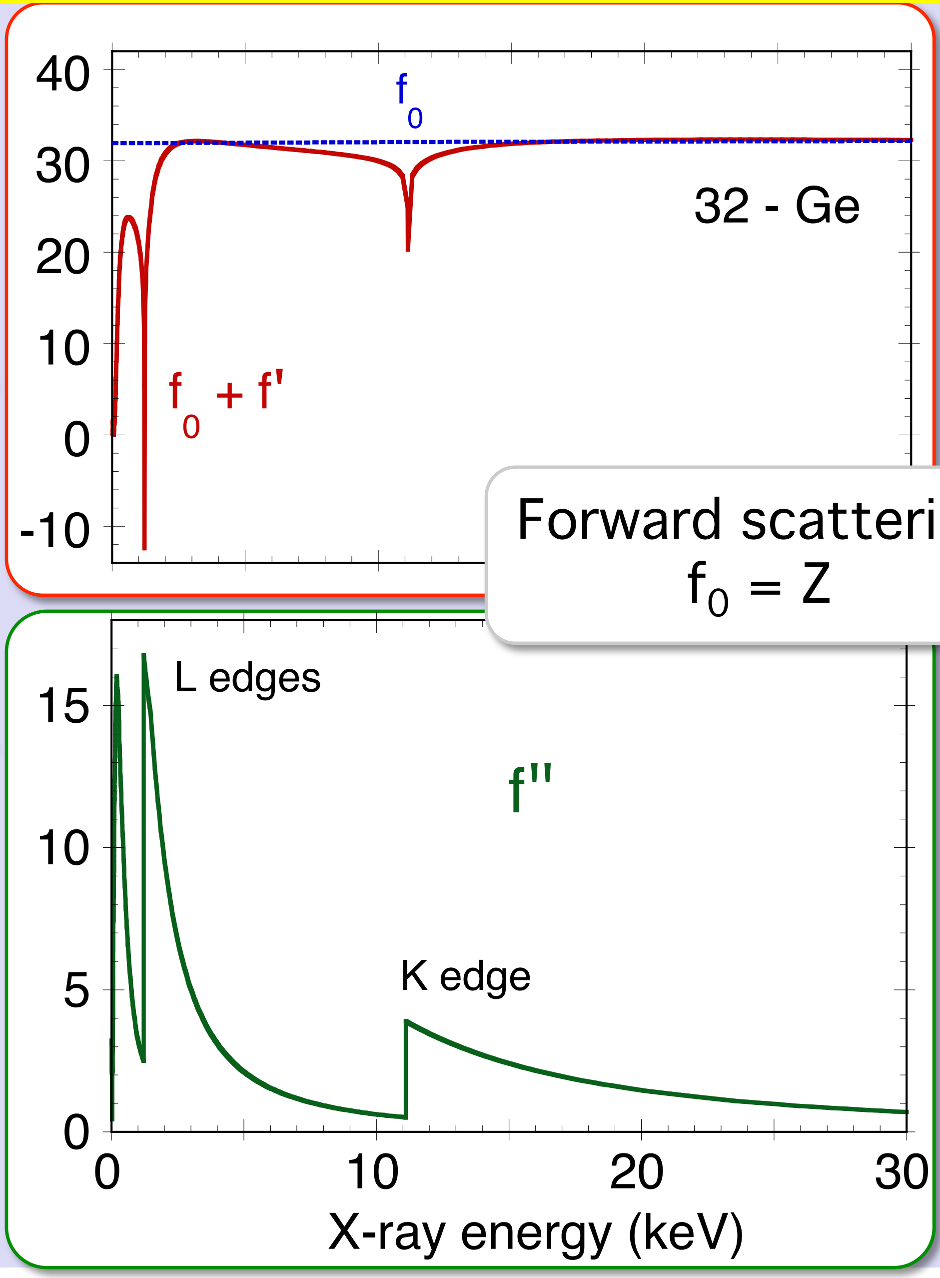
Imaginary ↕ Absorption

Resonant scattering factor (b)

$$f\left(\vec{K},Z\right) = f_0\left(\vec{K},Z\right) + f'(\hbar\omega,Z) + i\, f''(\hbar\omega,Z)$$

Real

Imaginary



Forward scattering
$f_0 = Z$

For K≠0, f_0 diminishes
and the resonant terms become
more relevant

> Thermal neutrons and electron scattering

X-rays and electrons

X-rays
(neglecting polarisation factor)

$$\left(\frac{d\sigma}{d\Omega}\right)_0 = r_e^2 \left|f_0\left(\vec{K},Z\right)\right|^2$$

$$= \left|f_X\left(\vec{K},Z\right)\right|^2$$

Radiation – matter interaction

$$f_0\left(\vec{K}\right) = \int \rho_e\left(\vec{r}\right) e^{i\vec{K}\cdot\vec{r}} dV$$

Electrons

$$\left(\frac{d\sigma}{d\Omega}\right)_0 = \left|f_{\text{el}}\left(\vec{K},Z\right)\right|^2$$

Central potential scattering
– Born approx.

$$f_{\text{el}}\left(\vec{K}\right) \approx \int \Phi\left(\vec{r}\right) e^{i\vec{K}\cdot\vec{r}} dV$$

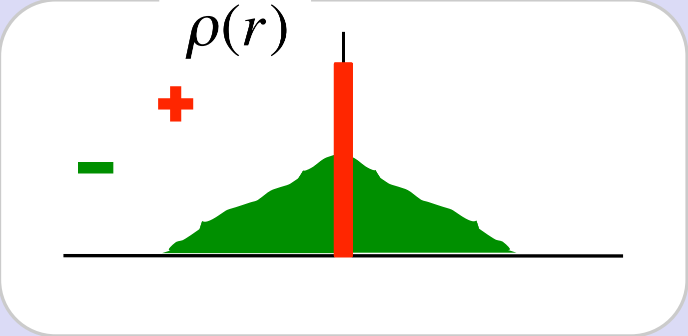
Scattering lengths
(form factors)

Fourier transforms

Electron scattering: Poisson equation

Poisson equation:

$$\nabla^2\Phi(\vec{r}) = -\left[\frac{\rho_+(\vec{r})}{\varepsilon_0} - \frac{\rho_-(\vec{r})}{\varepsilon_0}\right]$$



... for spherical symmetry:

$$\frac{\partial^2\Phi(r)}{\partial r^2} + \frac{2}{r}\frac{\partial\Phi(r)}{\partial r} = -\frac{1}{\epsilon_0}\left[\rho_+(r) - \rho_-(r)\right]$$

Potential:

$$\Phi(r) = \Phi_+(r) + \Phi_-(r)$$

Boundary condition:

$$\Phi(r) \to 0 \quad \text{for} \quad r \to \infty\,.$$

Potential energy

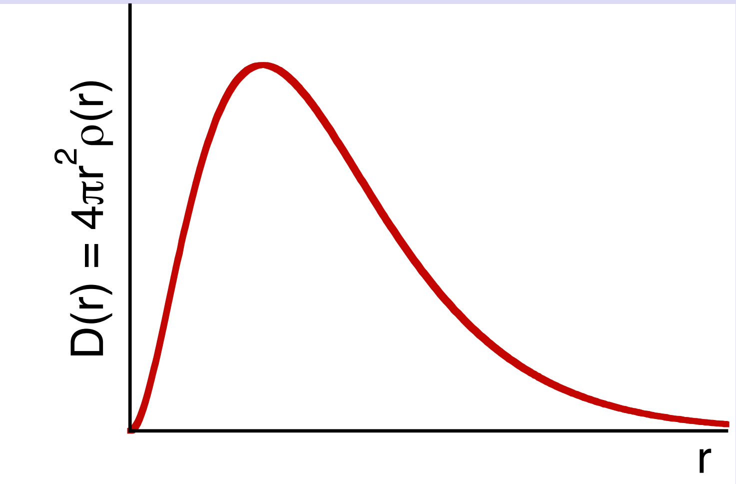
$$E_p(r) = -e\Phi(r).$$

Electron scattering: potential energy

Electrons negative charge

Radial distribution

$$D(r) \;=\; 4\pi r^2\, \rho_-(r)$$

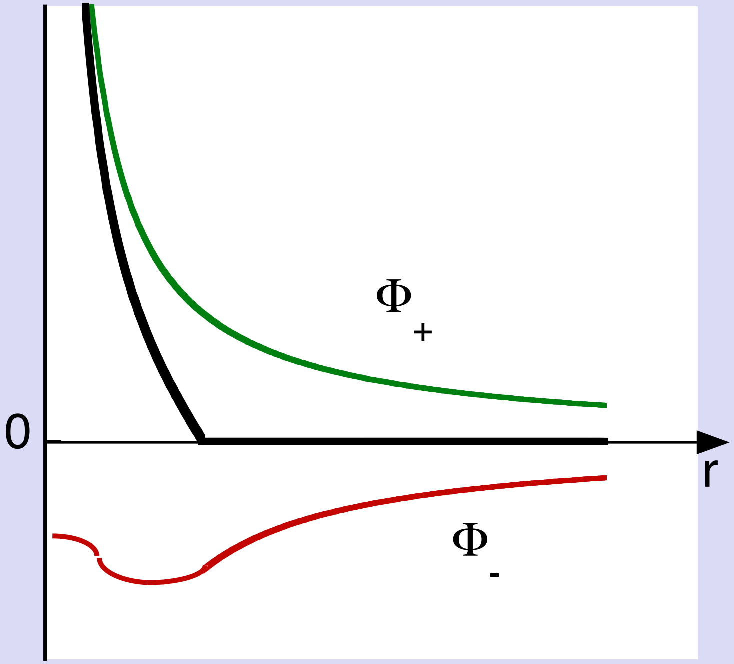


$$\Phi_-(r) \;=\; \frac{1}{4\pi\epsilon_0}\left[\frac{\int_0^r D(r')\,dr'}{r'} + \int_0^{\infty} \frac{D(r')}{r'}\,dr'\right]$$

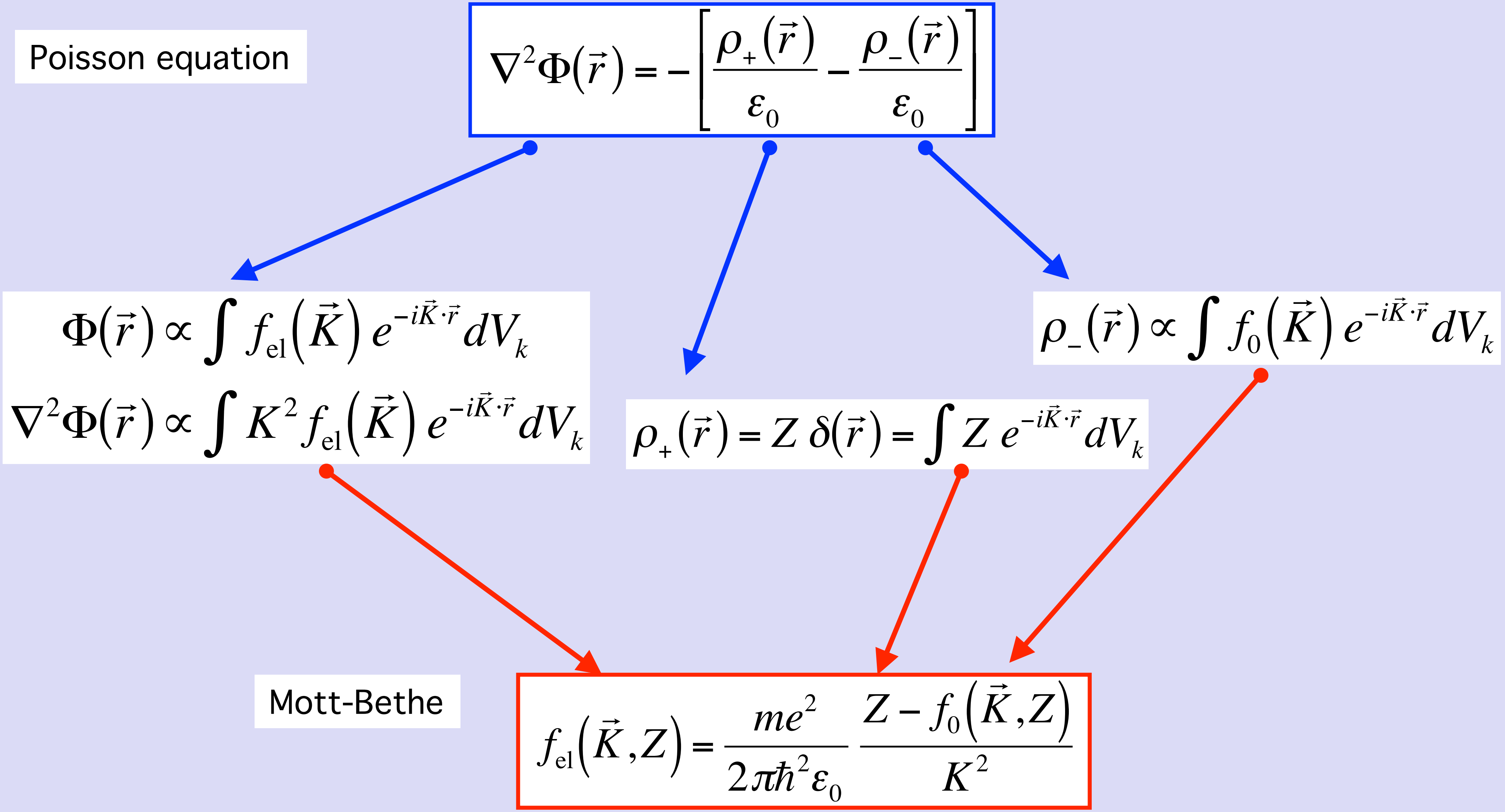
Nuclear positive charge

$$\rho_+(r) \;=\; +Ze\,\delta(r)$$

$$\Phi_+(r) \;=\; \frac{1}{4\pi\epsilon_0}\,\frac{Ze}{r}\,.$$



Electron scattering: Mott-Bethe formula



Poisson equation

$$\nabla^2\Phi(\vec{r}) = -\left[\frac{\rho_+(\vec{r})}{\varepsilon_0} - \frac{\rho_-(\vec{r})}{\varepsilon_0}\right]$$

$$\Phi(\vec{r}) \propto \int f_{\text{el}}\left(\vec{K}\right) e^{-i\vec{K}\cdot\vec{r}} dV_k$$

$$\nabla^2\Phi(\vec{r}) \propto \int K^2 f_{\text{el}}\left(\vec{K}\right) e^{-i\vec{K}\cdot\vec{r}} dV_k$$

$$\rho_+(\vec{r}) = Z\,\delta(\vec{r}) = \int Z\, e^{-i\vec{K}\cdot\vec{r}} dV_k$$

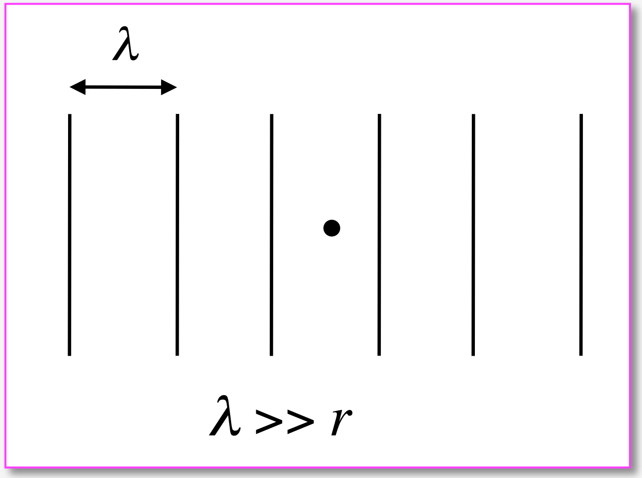
$$\rho_-(\vec{r}) \propto \int f_0\left(\vec{K}\right) e^{-i\vec{K}\cdot\vec{r}} dV_k$$

Mott-Bethe

$$f_{\text{el}}\left(\vec{K}, Z\right) = \frac{me^2}{2\pi\hbar^2\varepsilon_0}\,\frac{Z - f_0\left(\vec{K}, Z\right)}{K^2}$$

Thermal neutrons: interaction with matter

Paolo
Fornasini
Univ. Trento

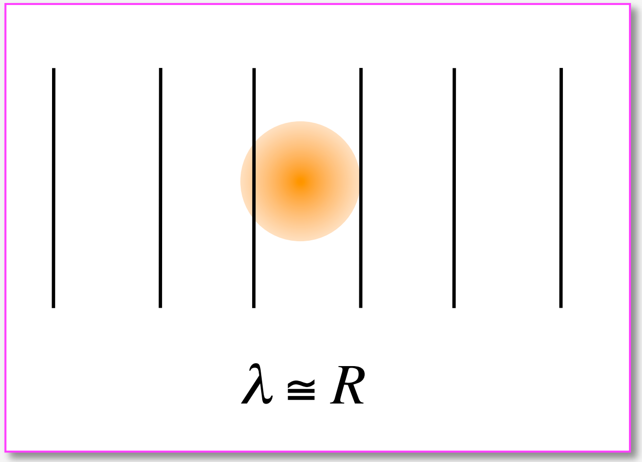


Nuclear interaction with nuclei

Strong interaction
> no classical approximation
> no perturbative treatment

Very short range (~10^{-15} m)
> isotropic scattering

Structural info



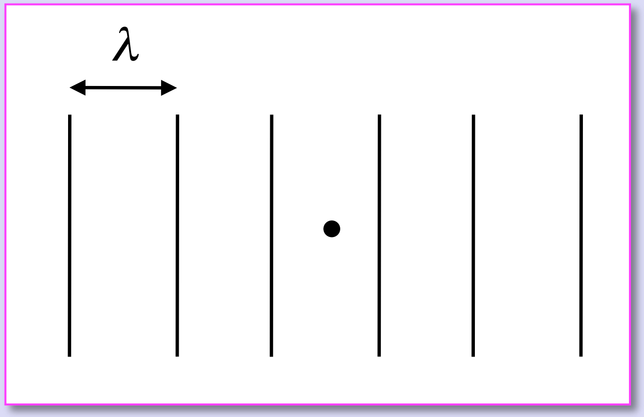
Magnetic interaction
of neutron spin
with unpaired electrons

Only for magnetic atoms

Extended electron clouds
> anisotropic scattering

Magnetic info

Thermal neutrons as structural probe



Interaction with nuclei:

$\lambda >> r$ → Isotropic scattering

[cfr. X-ray Thomson scattering
from point-like electrons]

Thomson scattering length r_e

↓

Neutrons scattering length b

- independent of scattering angle
- independent of neutron wavelength

- different for different isotopes
- depending on nuclear spin
- no correlation with Z

- experimentally determined

- Fermi pseudopotential $V(r) \propto b\,\delta(r)$

Nuclear scattering intensity

For one isotope:

$$I(\vec{K}) \propto |b|^2 = b^* b$$

Differential cross section $\frac{d\sigma}{d\Omega} = |b|^2 = b^* b$

Total cross section $\sigma_{\text{tot}} = 4\pi |b|^2$

For different isotopes
of the same atomic species
randomly distributed within the material.

$$I(\vec{K}) \propto \langle b_i b_j \rangle$$

i,j label atomic sites (including i=j)

$$K = Q = \frac{4\pi \sin\theta_B}{\lambda}$$

Neutron scattering lengths

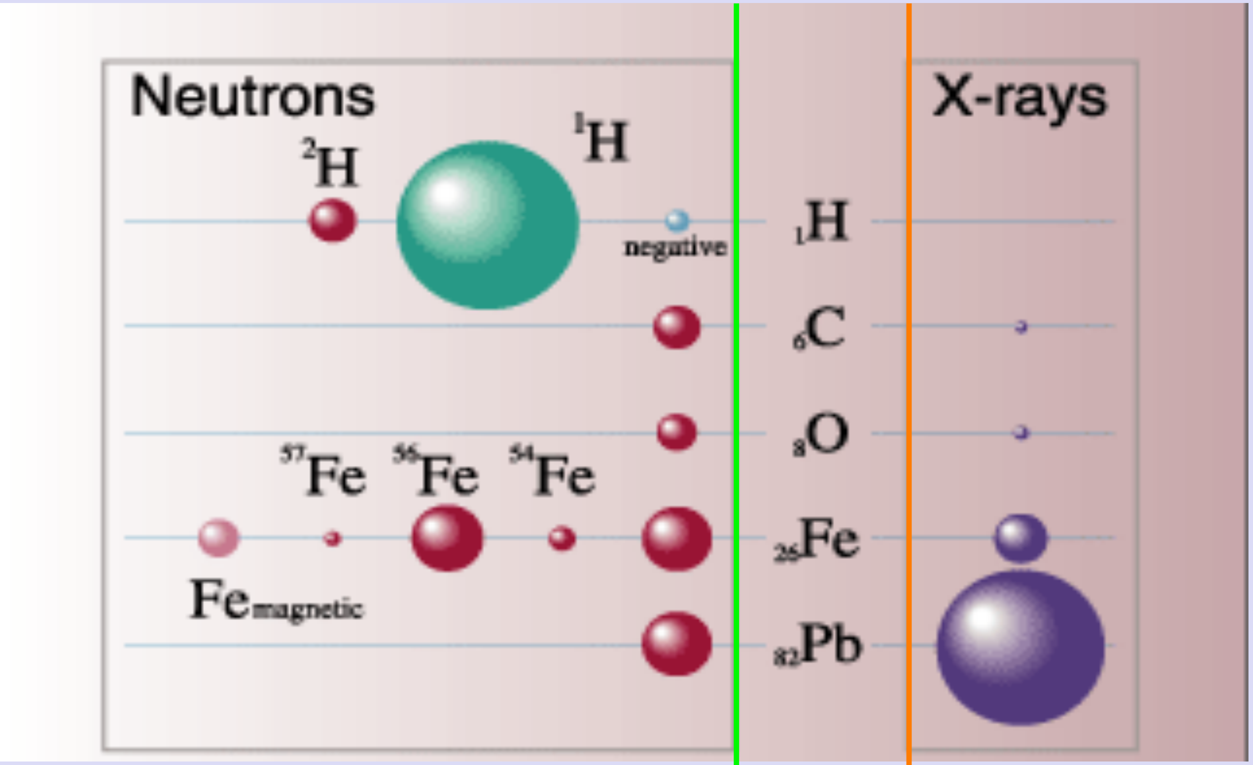
Isotope	**Z**	**A**	**b (10^{-15} m)**
Hydrogen Deuterium Tritium	1 1 1	1 2 3	-3.74 +6.67 +4.94
Silicon	14	28	+4.11
Germanium	32	70	+8.4
Lantanum	57	139	+8.2
Gold	79	197	+7.63

$b<0 \Rightarrow$ no π phase change on scattering

Scattering lengths (n .vs. X)

Scattering cross sections

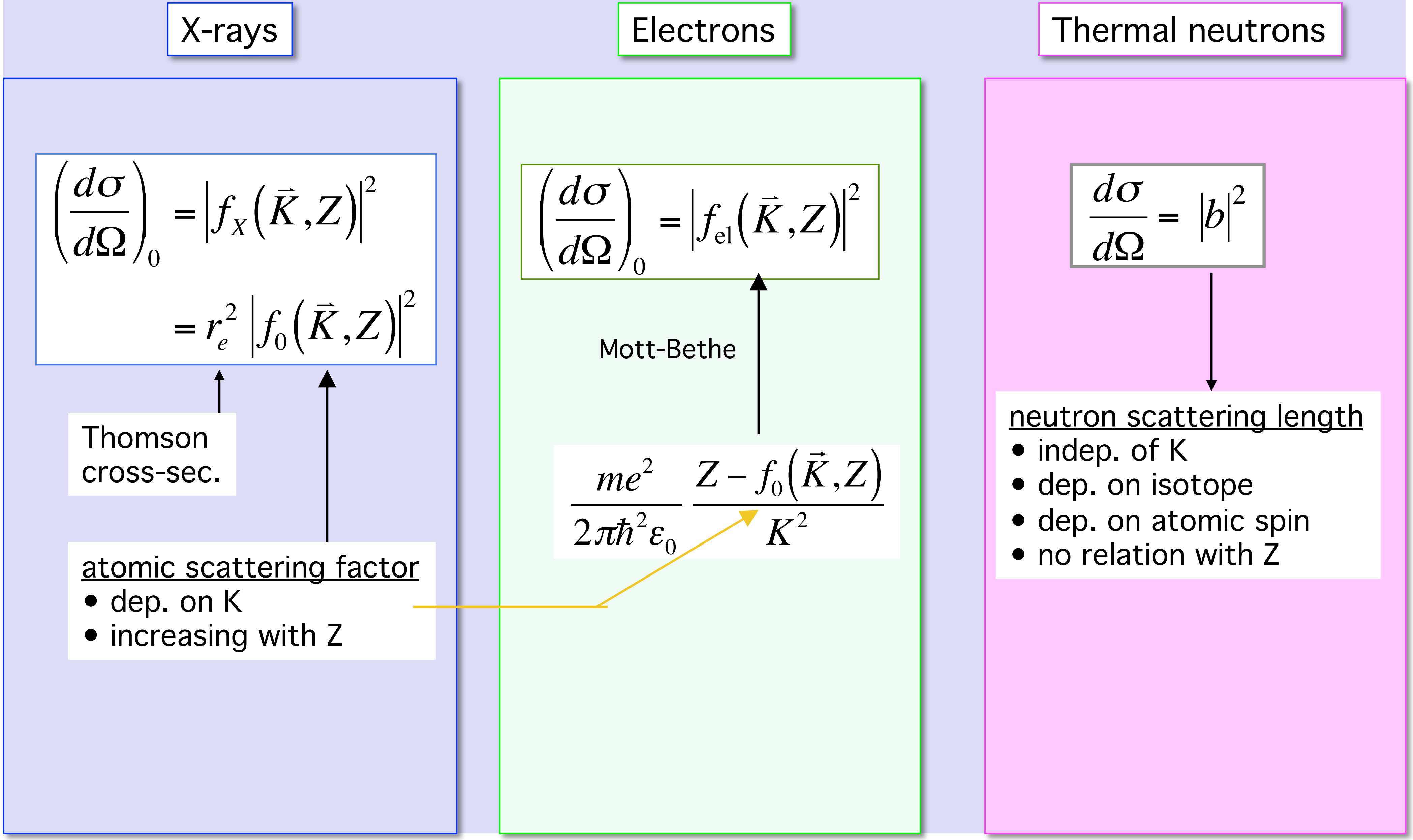
(proportional to sphere volume)



Scattering lengths
(indep. of scattering angle)

Atomic scattering factors
(dep on scattering angle)

Atomic cross sections



X-rays

$$\left(\frac{d\sigma}{d\Omega}\right)_0 = \left|f_X\left(\vec{K},Z\right)\right|^2$$

$$= r_e^2 \left|f_0\left(\vec{K},Z\right)\right|^2$$

Thomson
cross-sec.

atomic scattering factor
- dep. on K
- increasing with Z

Electrons

$$\left(\frac{d\sigma}{d\Omega}\right)_0 = \left|f_{\mathrm{el}}\left(\vec{K},Z\right)\right|^2$$

Mott-Bethe

$$\frac{me^2}{2\pi\hbar^2\varepsilon_0}\,\frac{Z - f_0\left(\vec{K},Z\right)}{K^2}$$

Thermal neutrons

$$\frac{d\sigma}{d\Omega} = |b|^2$$

neutron scattering length
- indep. of K
- dep. on isotope
- dep. on atomic spin
- no relation with Z

X-rays, electrons, neutrons

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Electrons

$$f_{\mathrm{el}}\left(\vec{K},Z\right)=\frac{me^2}{2\pi\hbar^2\varepsilon_0}\,\frac{Z-f_0\left(\vec{K},Z\right)}{K^2}$$

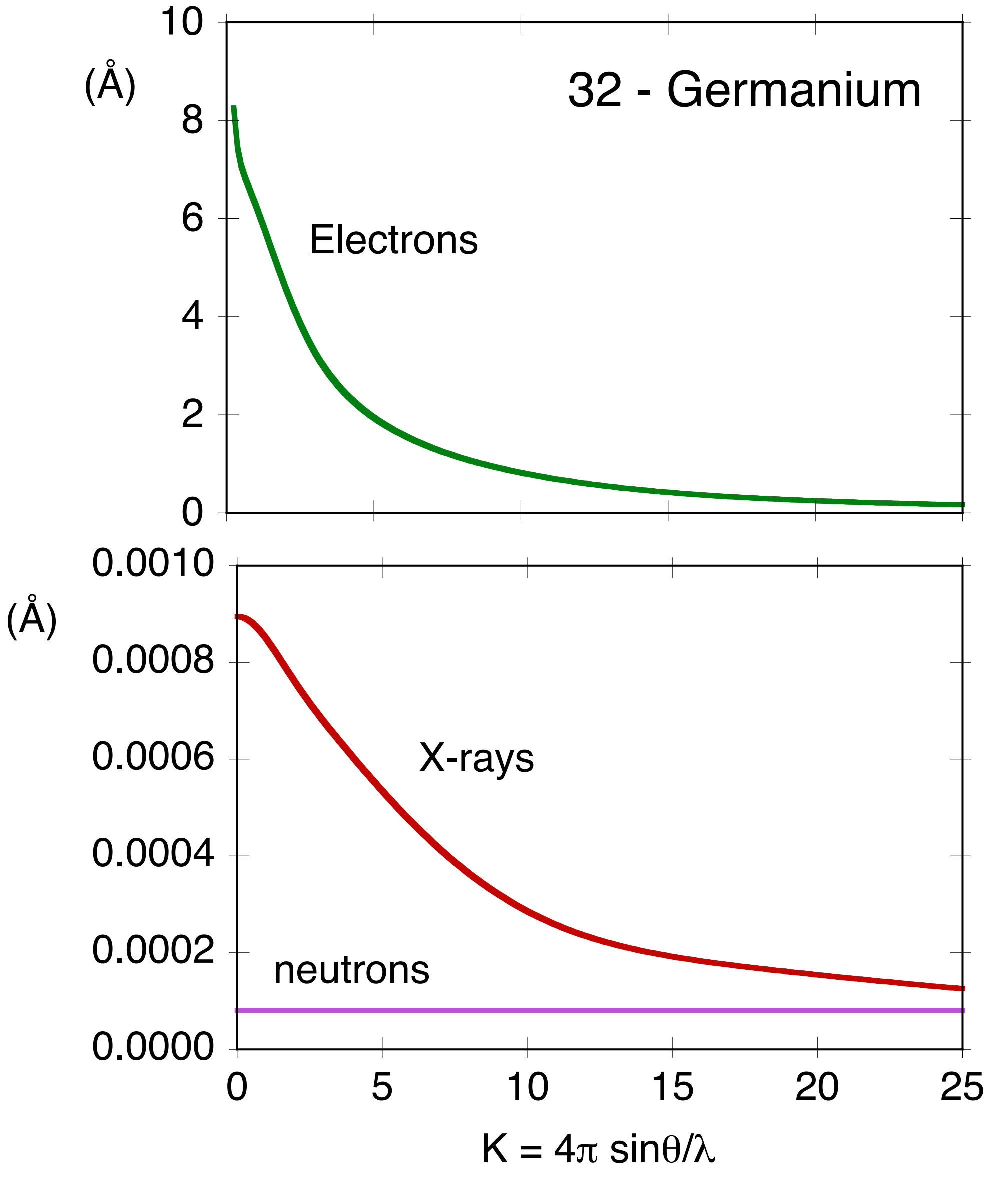
$$=3.77\,[\mathring{A}^{-1}]\,\frac{Z-f_0\left(\vec{K},Z\right)}{K^2[\mathring{A}^{-2}]}$$

X-rays

$$f_{\mathrm{X}}\left(\vec{K},Z\right)=r_e\;f_0\left(\vec{K},Z\right)$$

Neutrons

$$b_{\mathrm{coh}}(Z)$$



Comparisons

X-rays	Electrons	Thermal neutrons
Scattered by electron cloud	Scattered by Coulomb potential (long ranged)	Scattered by nuclear potential (short ranged)
Sensitivity to electron distribution	Sensitivity to electron distribution	Sensitivity only to nuclear position
Increases with Z	Increases with Z	No correlation with Z Isotope-dependent
Weak interaction	Strong interaction	Weak interaction
Strong penetration	Weak penetration	Strong penetration
Kinematical theory generally OK	Dynamical theory often necessary	Kinematical theory generally OK

Basic references

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