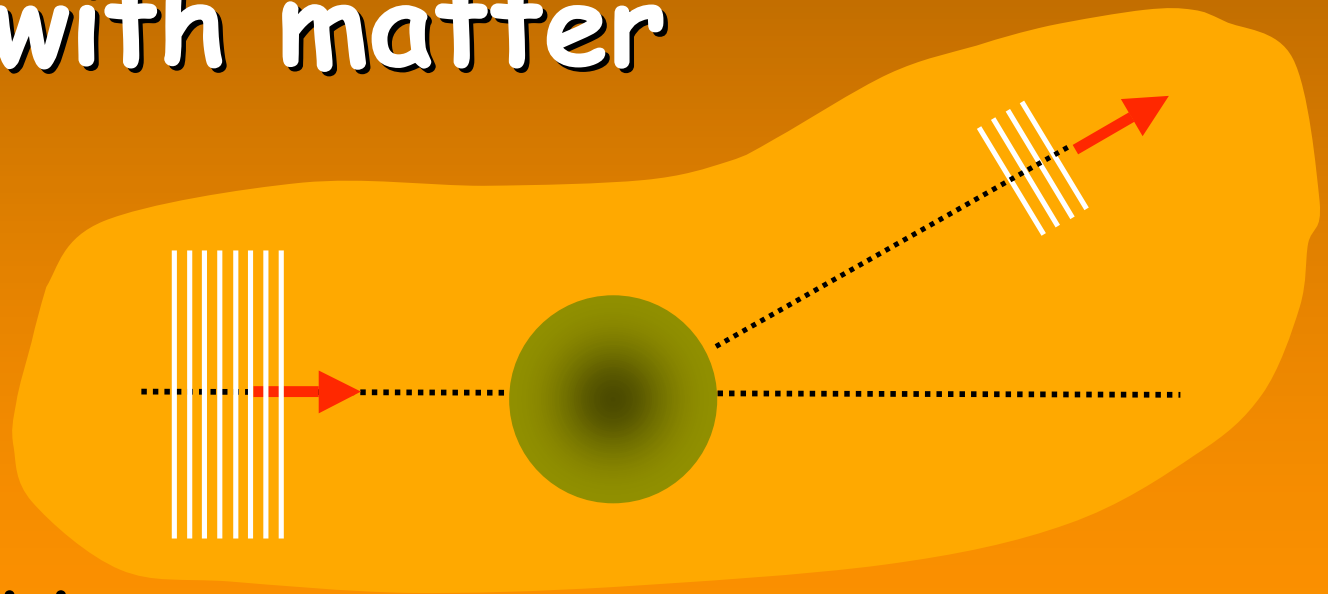




# Interaction of X-rays with matter



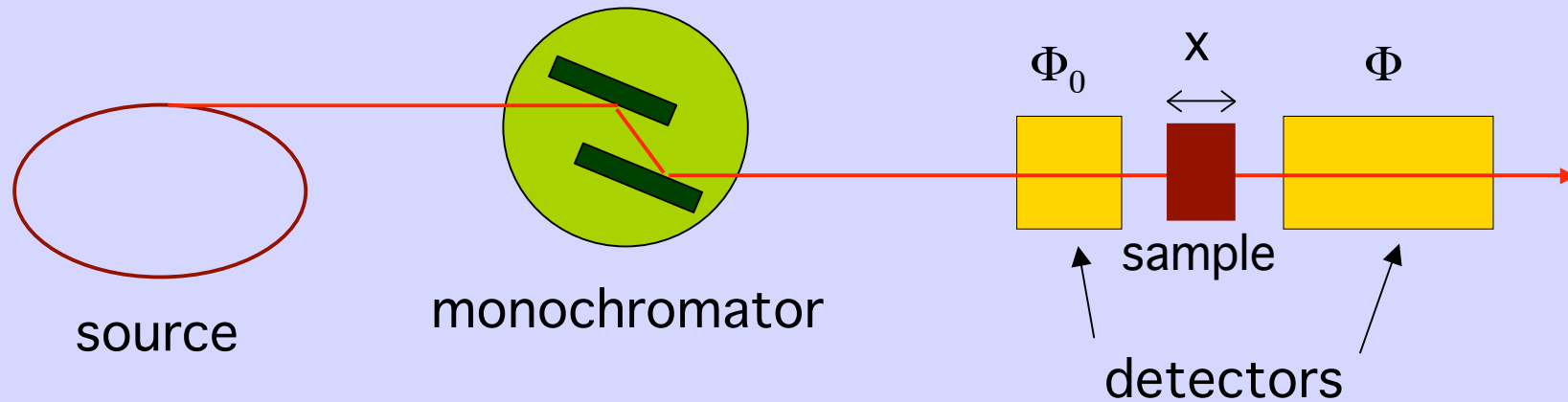
Paolo Fornasini  
Department of Physics  
University of Trento, Italy



## Overview

- Attenuation of x-rays
  - Classical Thomson scattering
  - Basic interference phenomenon
  - Scattering: deviations from classical behaviour
- ❖ Photoelectric absorption

# Attenuation of X-rays



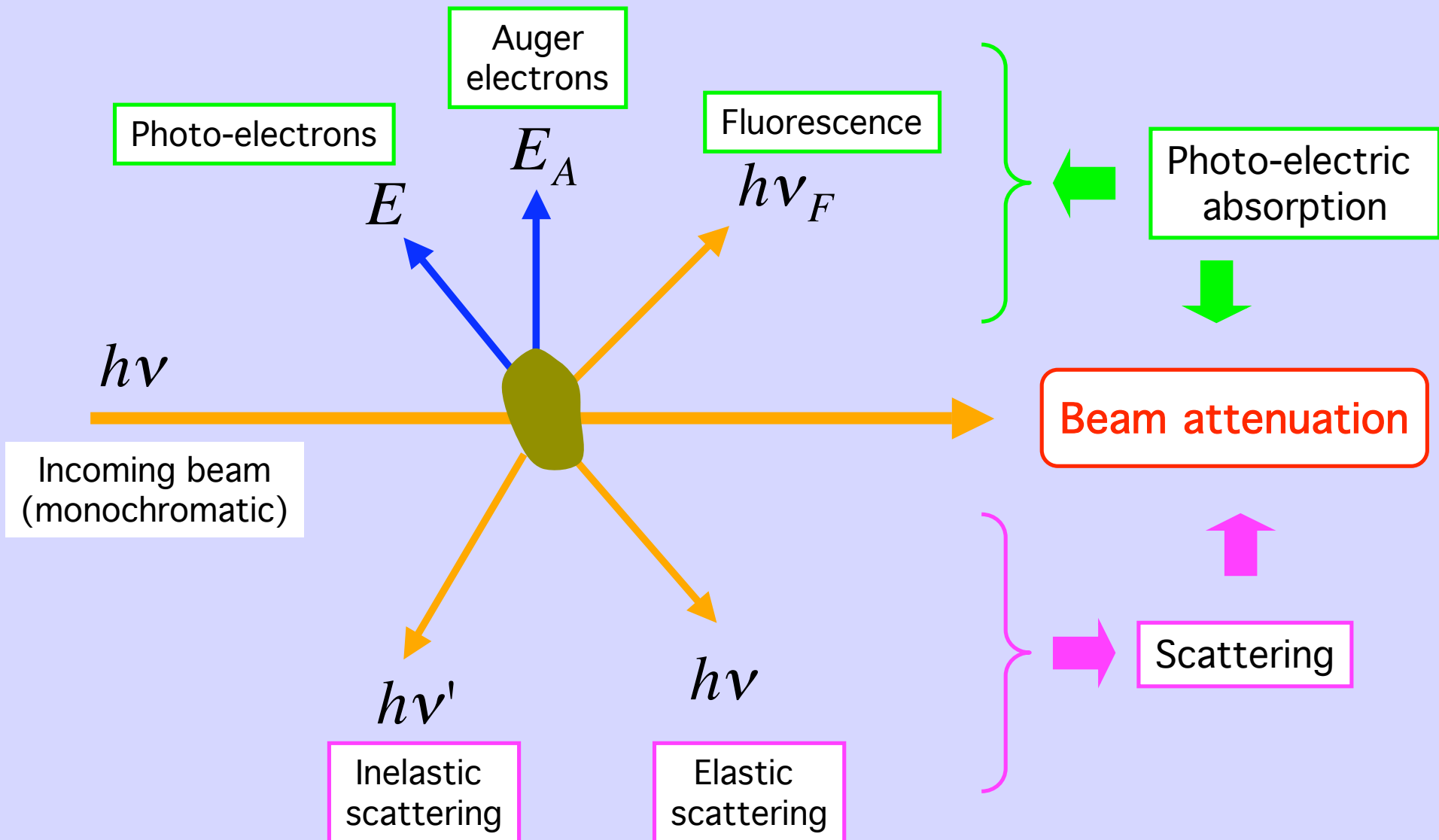
Exponential attenuation

$$\Phi = \Phi_0 \exp[-\mu(\omega) x]$$

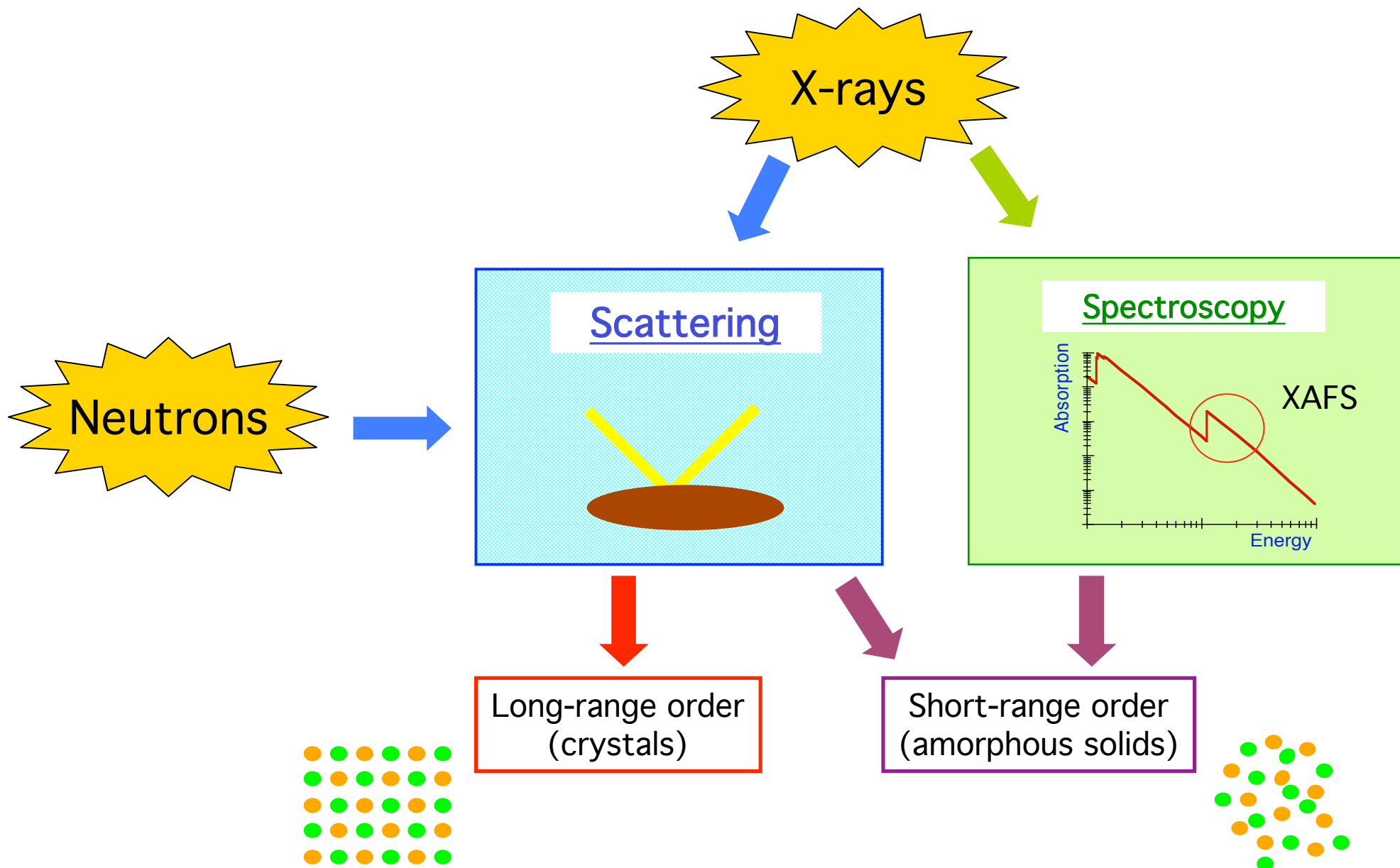
Attenuation coefficient

$$\mu(\omega) = \frac{1}{x} \ln \frac{\Phi_0}{\Phi}$$

# Interaction of x-rays with matter



# Structural techniques



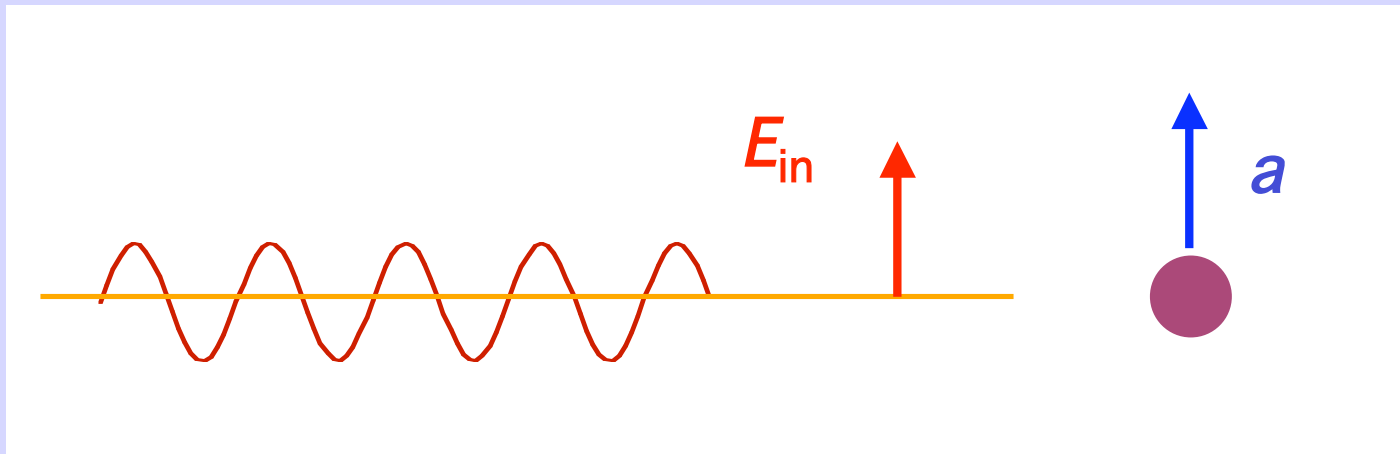
- Scattering from a free charge  
classical treatment (Thomson scattering)

Incoming electric field

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

Charge acceleration

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



Magnetic field effects are negligible

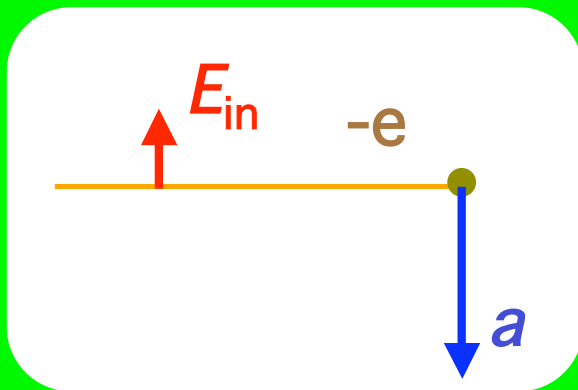
# Electrons .vs. protons

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

Electron

$$q = -e$$

$$\frac{e}{m} \approx 1.7 \times 10^{11} \text{ C/kg}$$



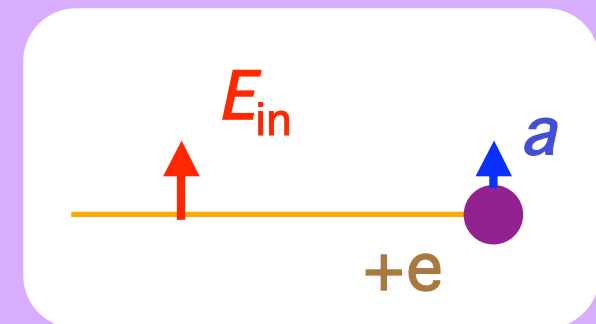
$\pi$  phase-shift

$$\frac{M}{m} \approx 1836$$

$$q = +e$$

Proton

$$\frac{e}{M} \approx 0.96 \times 10^8 \text{ C/kg}$$





# Dipole emission of radiation

## Accelerating charge $\Rightarrow$ electromagnetic field

Dipole approximation:

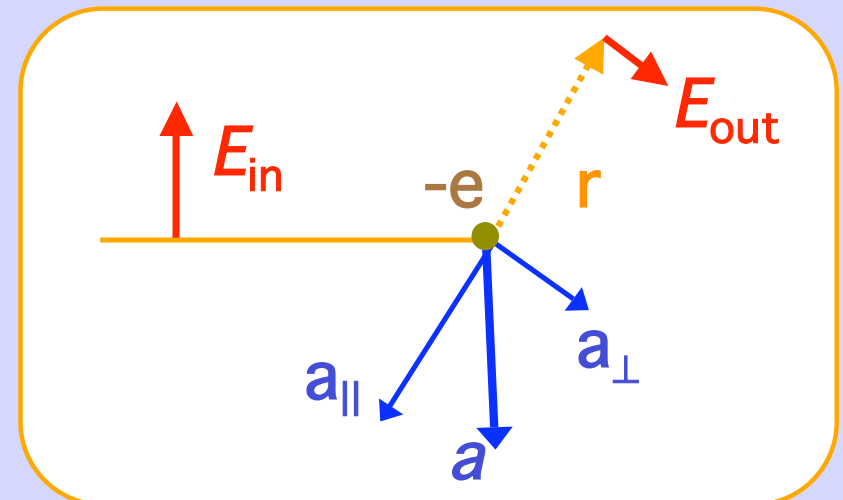
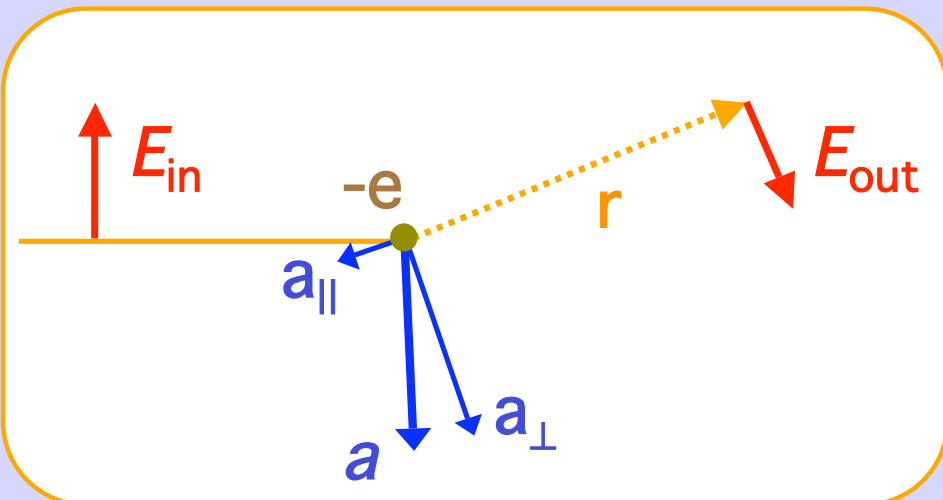
- charge velocity:  $v \ll c$
- charge distribution:  $d \ll \lambda$
- observer distance:  $r \gg \lambda$

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

Electron:

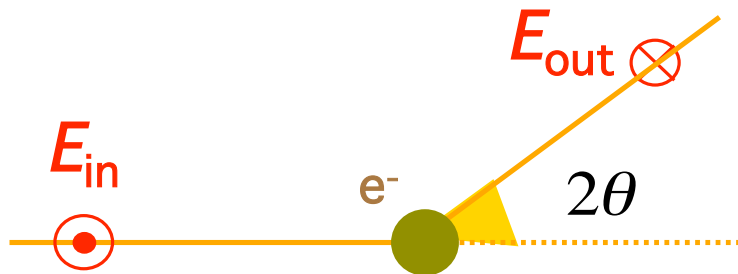
$$q = -e$$

$$\vec{E}_{\text{out}}(\vec{r}, t) = \frac{e \vec{a}_{\perp}(t')}{4\pi\epsilon_0 r c^2}$$



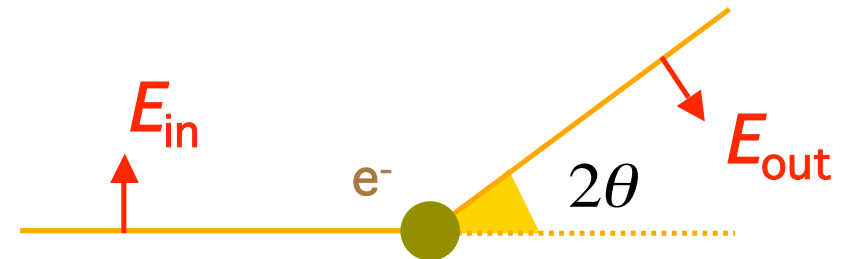
# Outgoing electric field

$\pi$  polarisation



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

$\sigma$  polarisation



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

$$r_e = \frac{e^2}{4\pi\epsilon_0 c^2 m}$$

Thomson scattering length

or

Classical electron radius

# Thomson scattering length

= Classical electron radius

Energy of a uniformly charged:

➤ spherical shell

$$U = \frac{1}{2} \left( \frac{1}{4\pi\epsilon_0} \frac{q^2}{r_e} \right)$$

➤ spherical volume

$$U = \frac{3}{5} \left( \frac{1}{4\pi\epsilon_0} \frac{q^2}{r_e} \right)$$

Electron

$$U \approx \frac{1}{4\pi\epsilon_0} \frac{e^2}{r_e} = mc^2$$

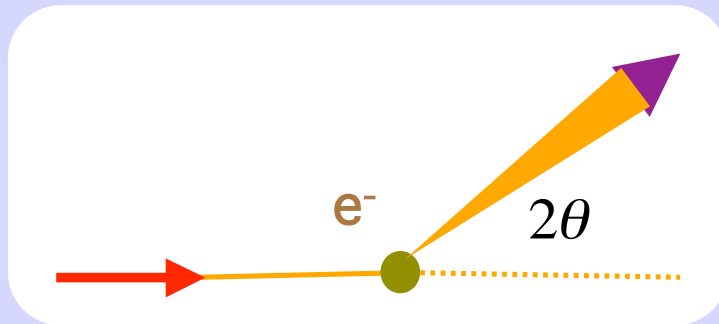
Relativistic  
rest energy



$$r_e = \frac{e^2}{4\pi\epsilon_0 c^2 m} = 2.8 \times 10^{-15} \text{ m} = 2.8 \times 10^{-5} \text{ \AA}$$

Incoming power flux

$$I_0 = \frac{1}{2} \epsilon_0 E_0^2 c \quad [\text{W/m}^2]$$



Un-polarized beam

Emitted power

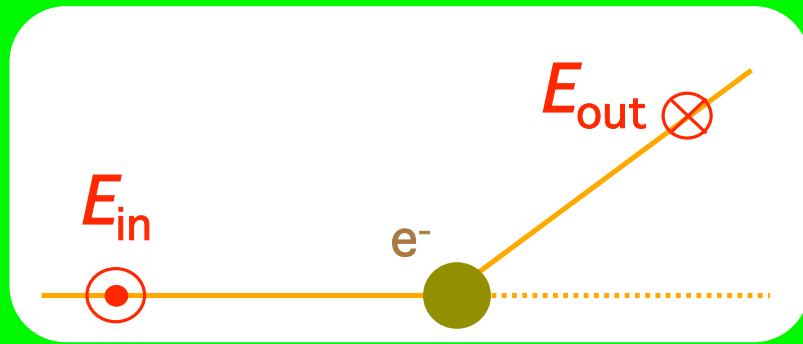
$$P(\theta) d\theta = r_e^2 \left[ \frac{1 + \cos^2(2\theta)}{2} \right] I_0 d\theta$$

Polarisation factor

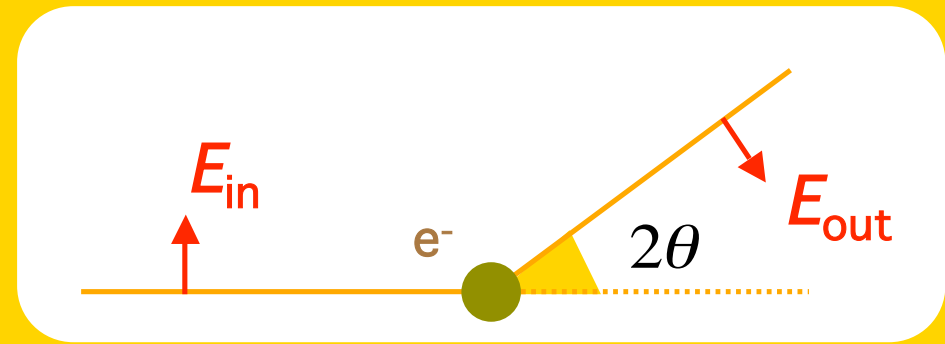
Independent from radiation wavelength

# Polarisation factor

$\pi$  polarisation



$\sigma$  polarisation



Un-polarised beam

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

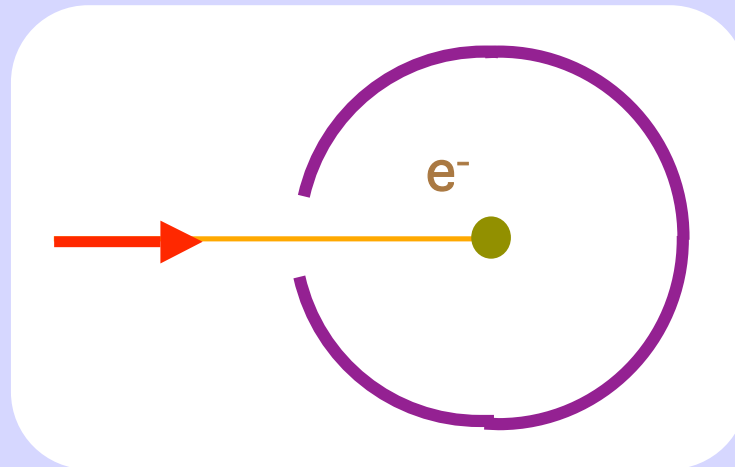
Laboratory x-ray sources

# Total electron cross-section

Incoming power flux

$$I_0 = \frac{1}{2} \epsilon_0 E_0^2 c \quad [\text{W/m}^2]$$

Un-polarized beam



Total radiated power

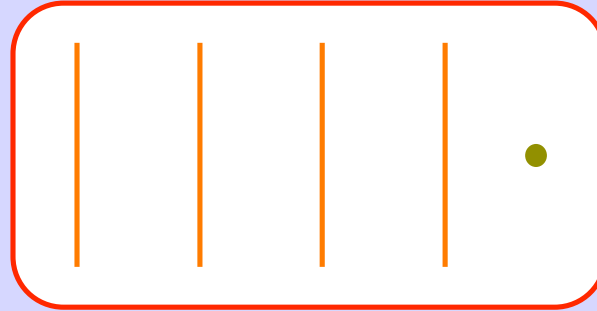
$$P = \frac{8}{3} \pi r_e^2 I_0$$

Electron cross-section  
 $\sigma_e = 6.66 \times 10^{-29} \text{ m}^2$

Independent from radiation wavelength

# Beyond classical treatment

Thomson scattering:



Free electron

Elastic scattering

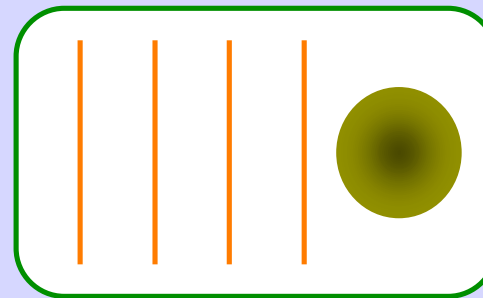
$$r_e \ll \lambda$$



Free electron  $\Rightarrow$  Inelastic scattering (Compton)

Electrons are bound in atoms

Probabilistic distribution of  $e^-$  charge



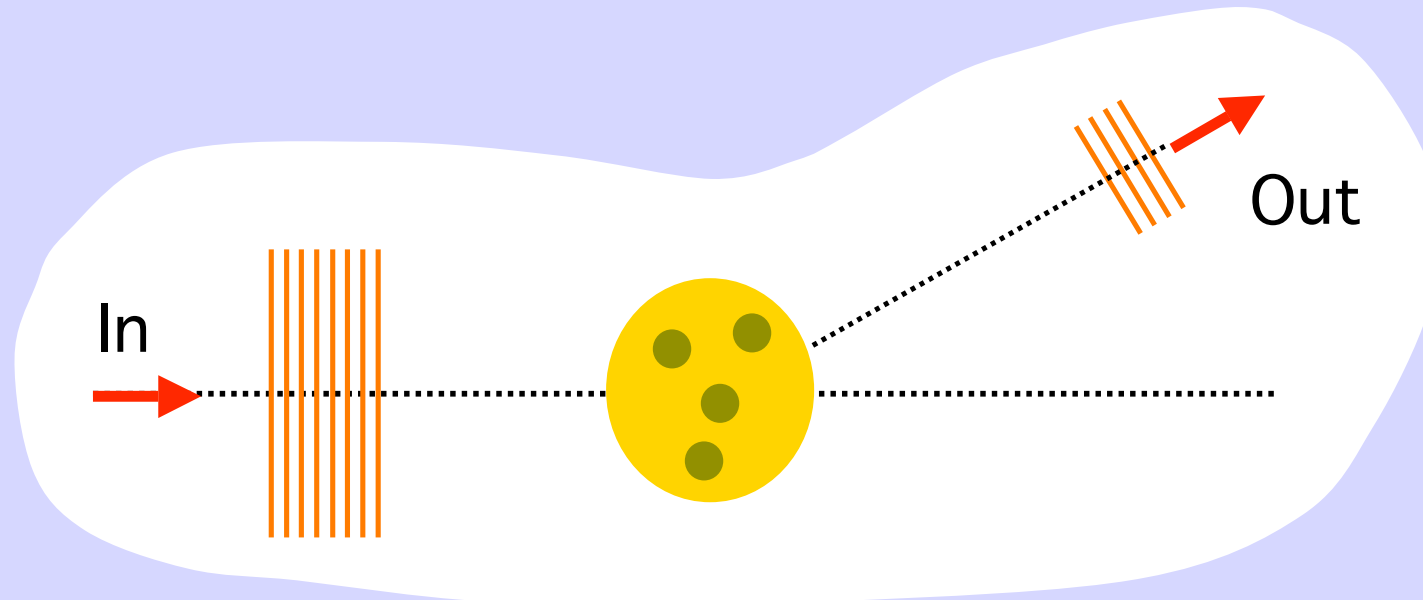
Interference



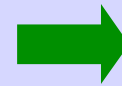
# Interference



# Scattering from many electrons



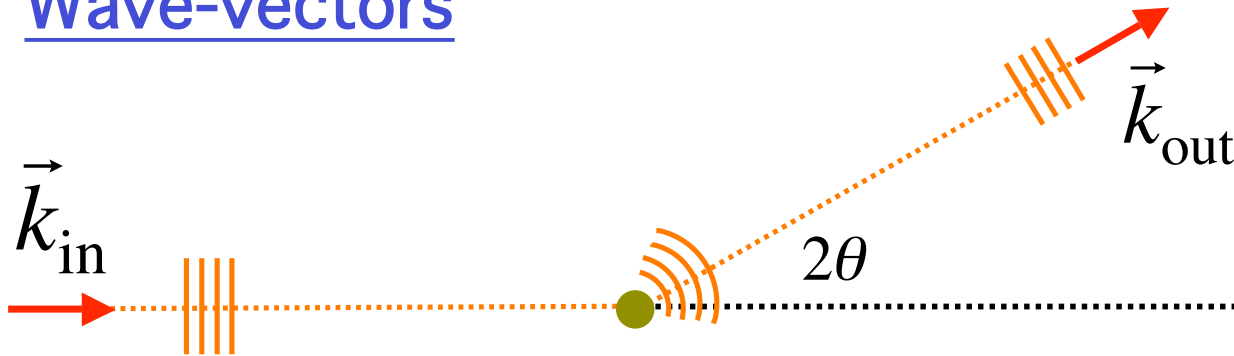
Waves from  
different electrons



**Interference**

Depending on radiation wavelength

## Wave-vectors



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

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

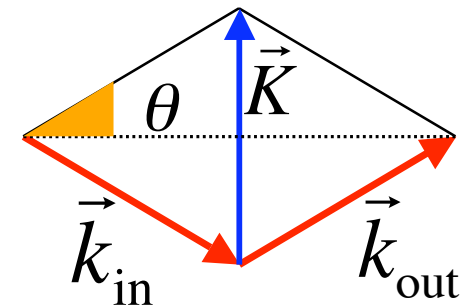
Elastic scattering

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

## Scattering vector

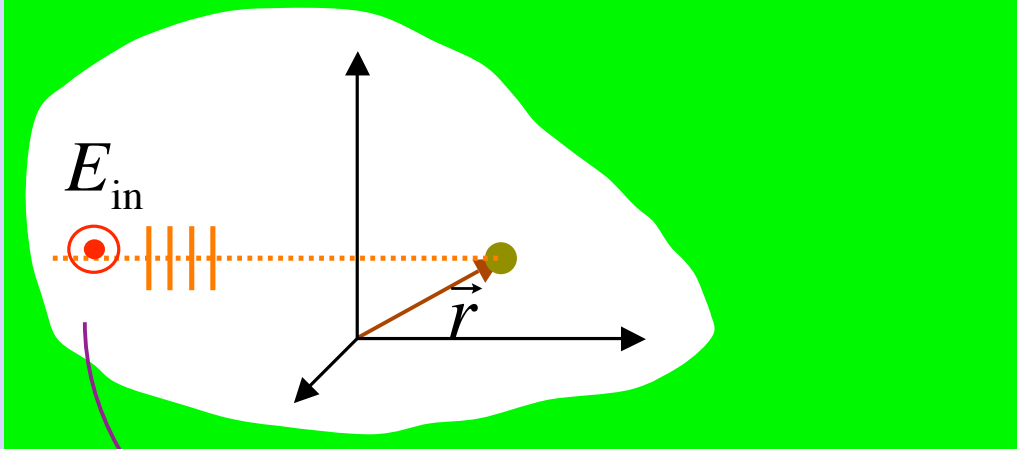
$$\vec{K} = \vec{k}_{\text{out}} - \vec{k}_{\text{in}}$$

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



# Incoming wave

$\pi$  polarisation



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

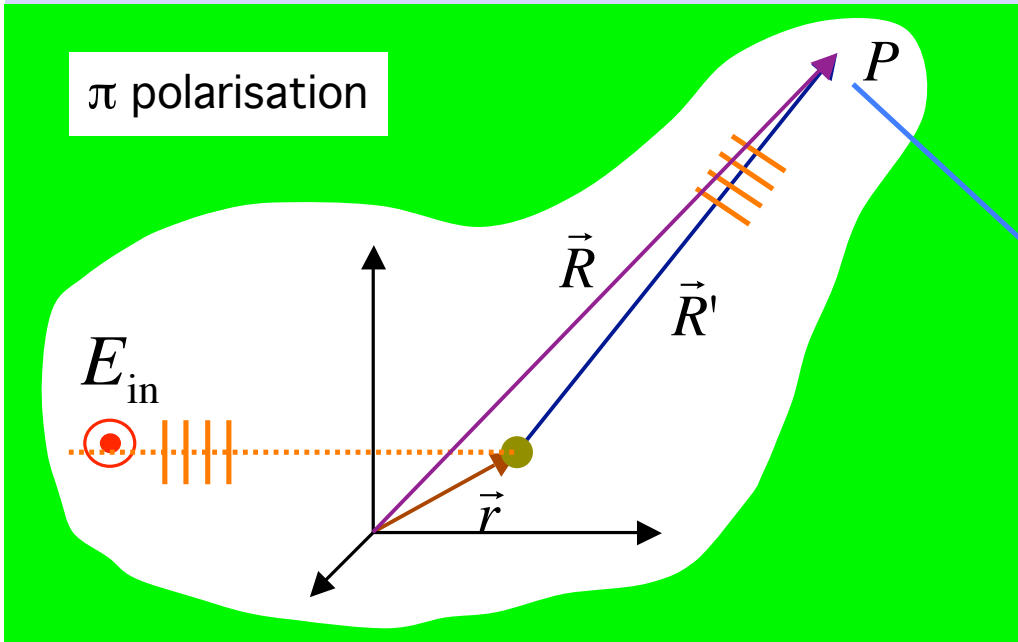
$$= \text{Re} \left\{ E_0 e^{i(\omega t - \vec{k}_{in} \cdot \vec{r})} \right\}$$

Complex notation

$A_0$

Input amplitude

# Outgoing wave



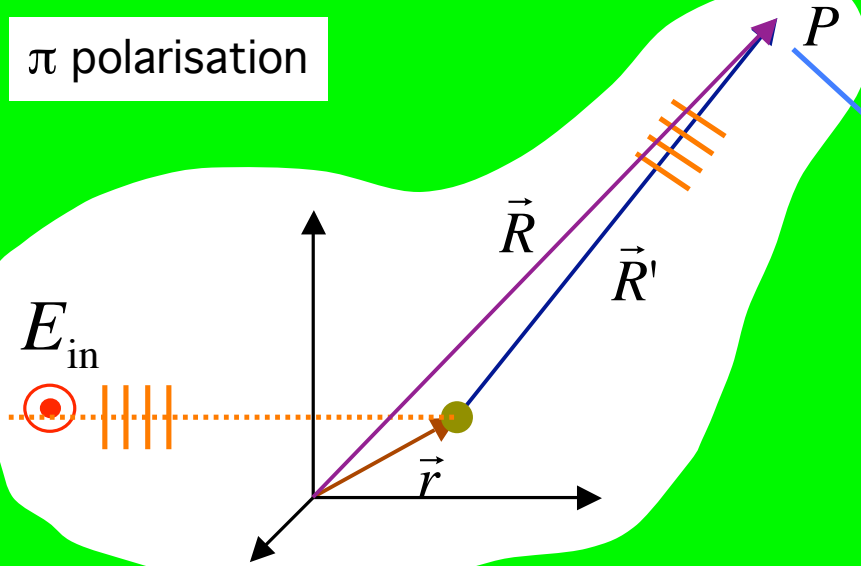
$$E_{out} = \text{Re} \left\{ \overbrace{E_0}^{A_0} e^{i(\omega t - \vec{k}_{in} \cdot \vec{r})} (-r_e) \frac{e^{-ik_{out} R'}}{R'} \right\}$$

$A$

Scattered amplitude

# Geometrical tricks

$\pi$  polarisation

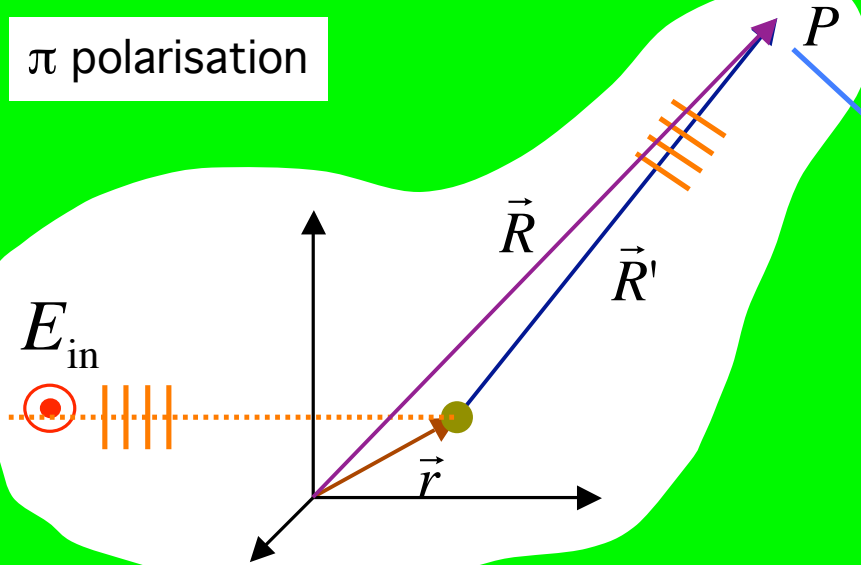


$$E_{out} = \text{Re} \left\{ E_0 e^{i(\omega t - \vec{k}_{in} \cdot \vec{r})} (-r_e) \frac{e^{-ik_{out} R'}}{R'} \right\}$$

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

# Scattered amplitude

$\pi$  polarisation



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

Scattered  
amplitude

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

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

Phase factor

# Amplitude and intensity

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

( $\pi$  polarisation)

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

Cannot be measured !

We measure:

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

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

( $\pi$  polarisation)

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

un-polarized beam

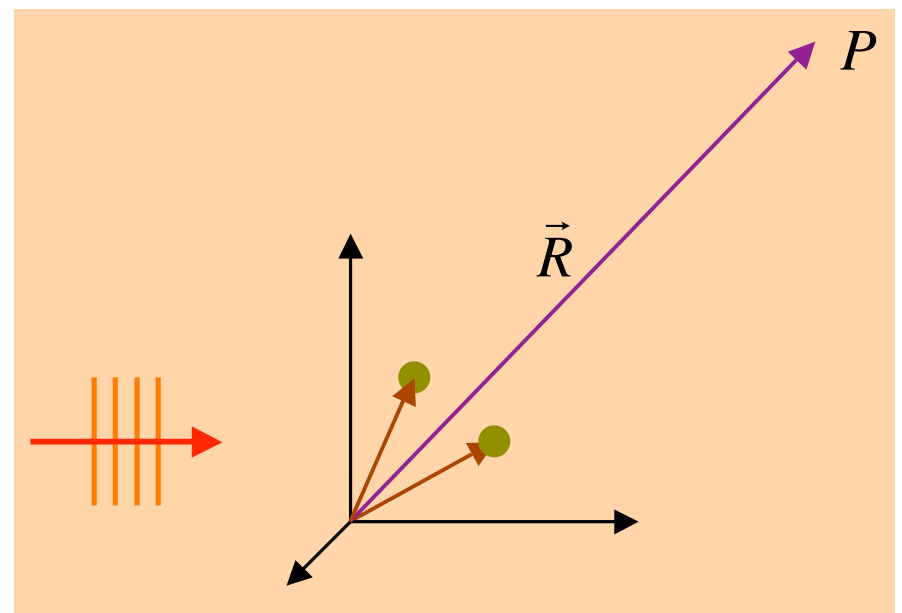
# Basic interference effect (a)

## 1 electron ( $\pi$ polarisation)

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

## 2 electrons ( $\pi$ polarisation)

$$A(\vec{K}) = A_1(\vec{K}) + A_2(\vec{K})$$
$$= A_{\text{el}} \left[ e^{i\vec{K}\cdot\vec{r}_1} + e^{i\vec{K}\cdot\vec{r}_2} \right]$$

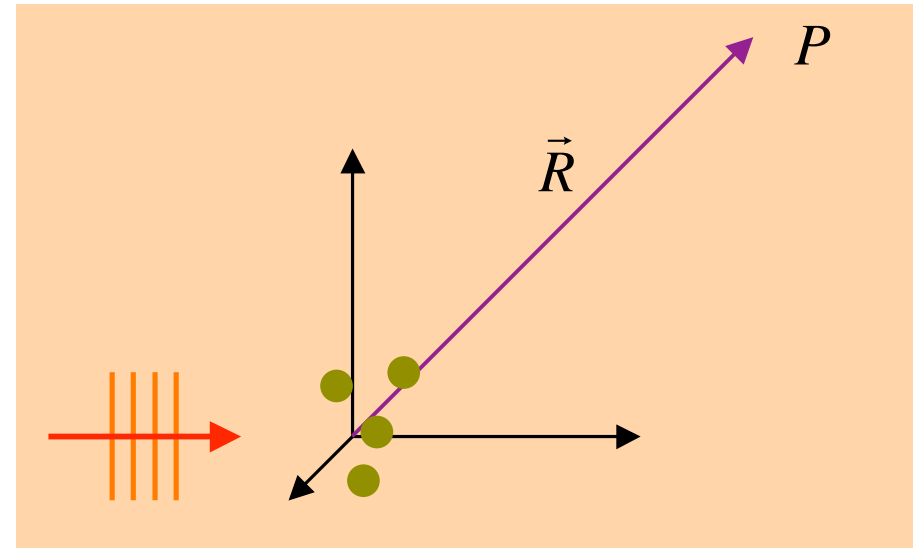




# Basic interference effect (b)

n electrons ( $\pi$  polarisation)

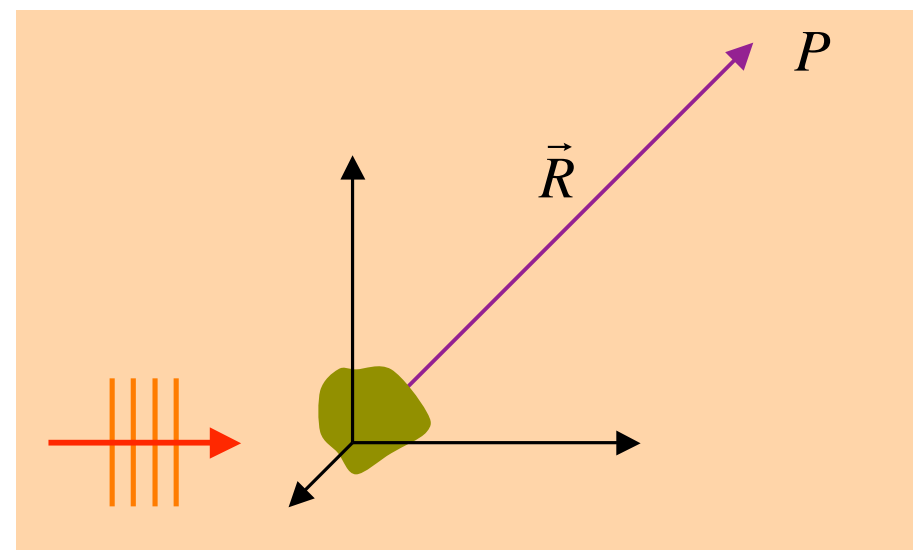
$$A(\vec{K}) = A_{\text{el}} \sum_i e^{i\vec{K} \cdot \vec{r}_i}$$



Continuous charge distribution

( $\rho$  = number density)

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



The **scattered amplitude** is the Fourier transform of the **electron density**

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

(number density)

# Amplitude and intensity (b)

## Amplitude

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

Cannot be measured !

## Intensity

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

Is measured,  
but  
phase information  
is lost !

Structural info

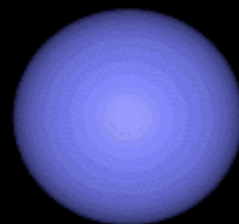
$$|A_{\text{el}}|^2 = r_e^2 E_0^2 \frac{1}{R^2} \left[ \frac{1 + \cos^2(2\theta)}{2} \right]$$

Polarisation factor  
for unpolarised beam

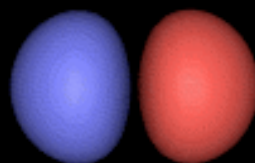
- 🛡 Deviations from classical treatment
  - a) Electronic distribution

# Electronic orbitals

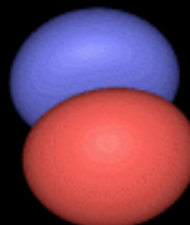
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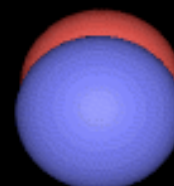
s



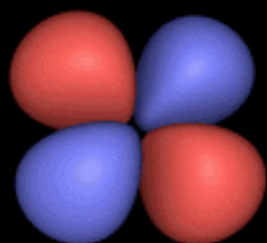
p<sub>x</sub>



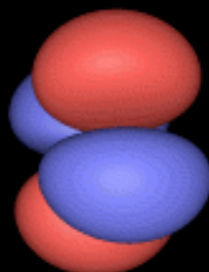
p<sub>y</sub>



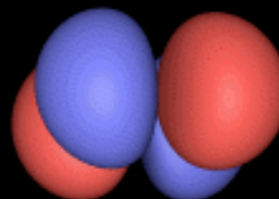
p<sub>z</sub>



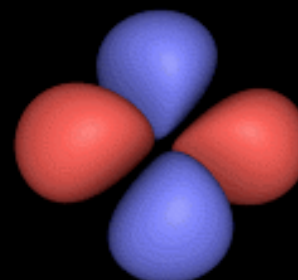
d<sub>xy</sub>



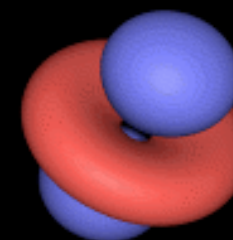
d<sub>xz</sub>



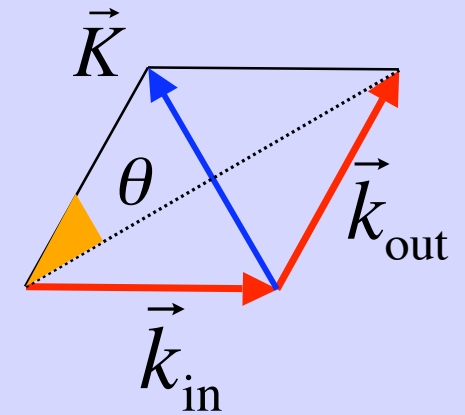
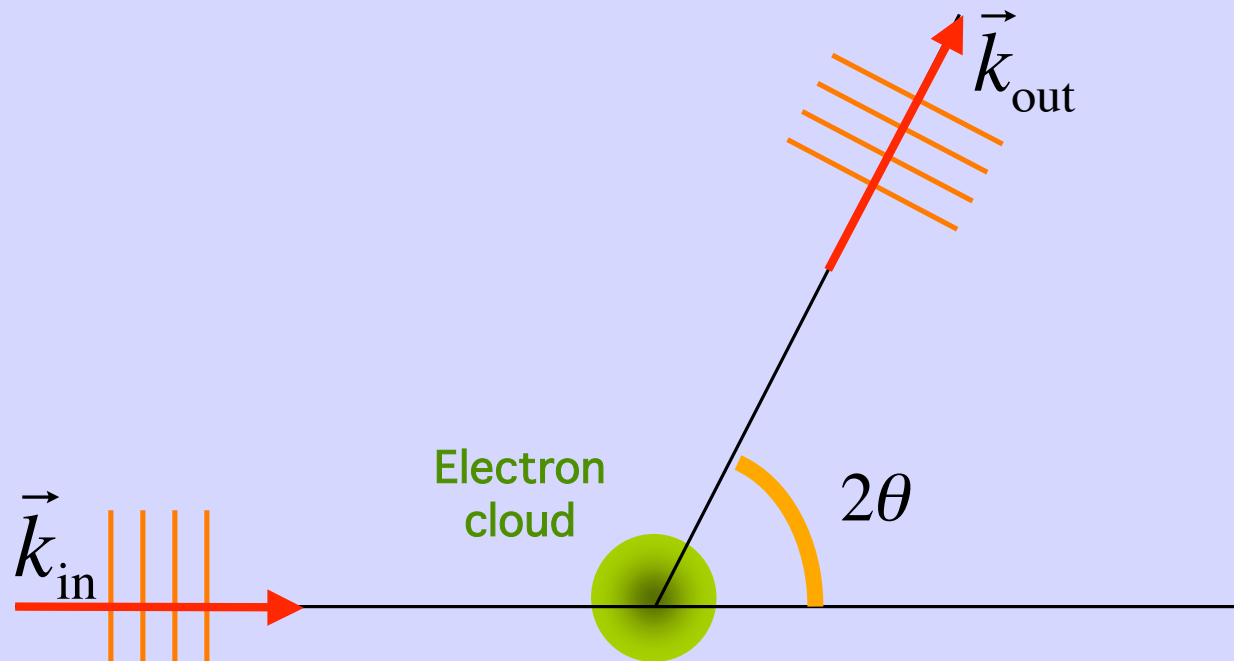
d<sub>yz</sub>



d<sub>x<sup>2</sup> - y<sup>2</sup></sub>



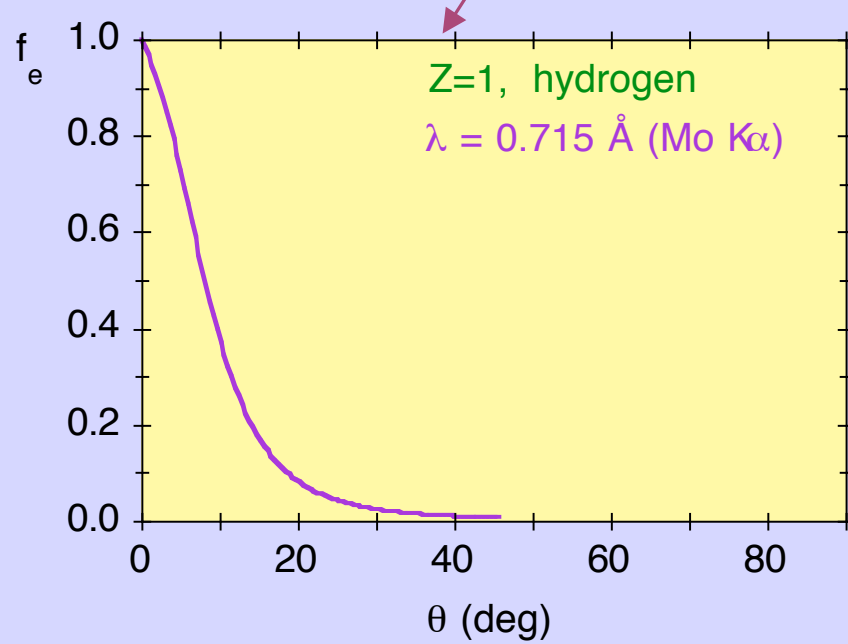
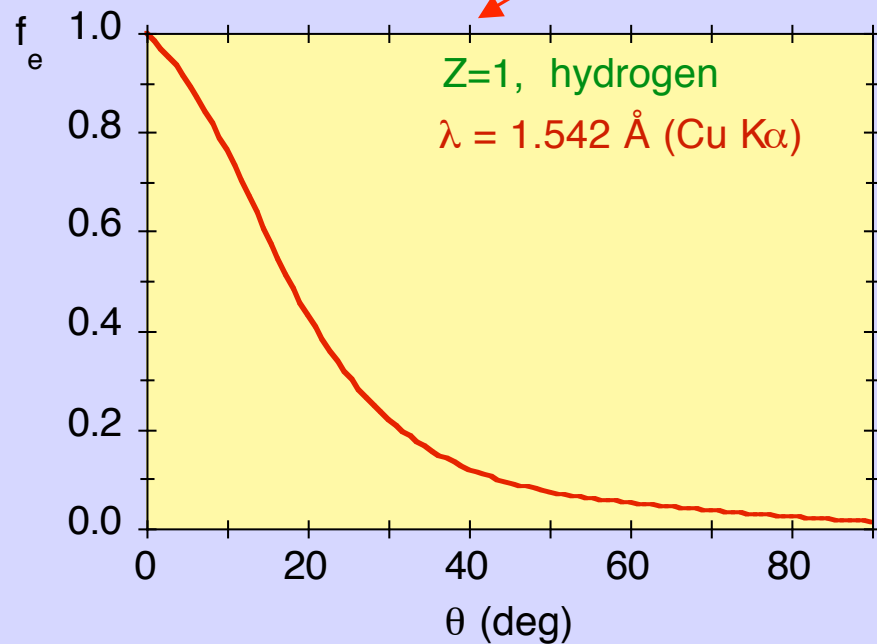
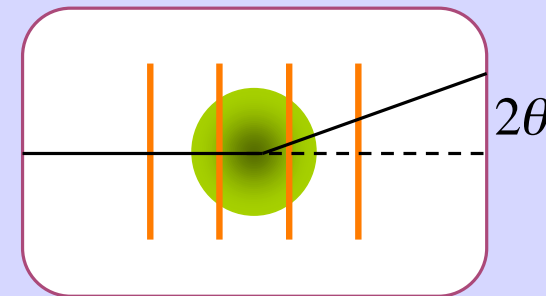
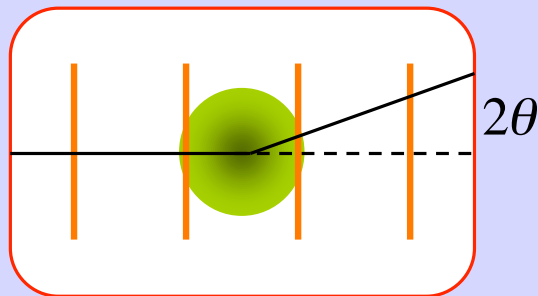
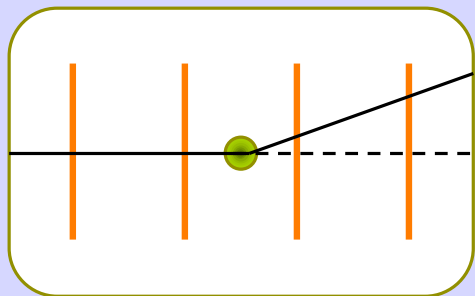
d<sub>z<sup>2</sup></sub>



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

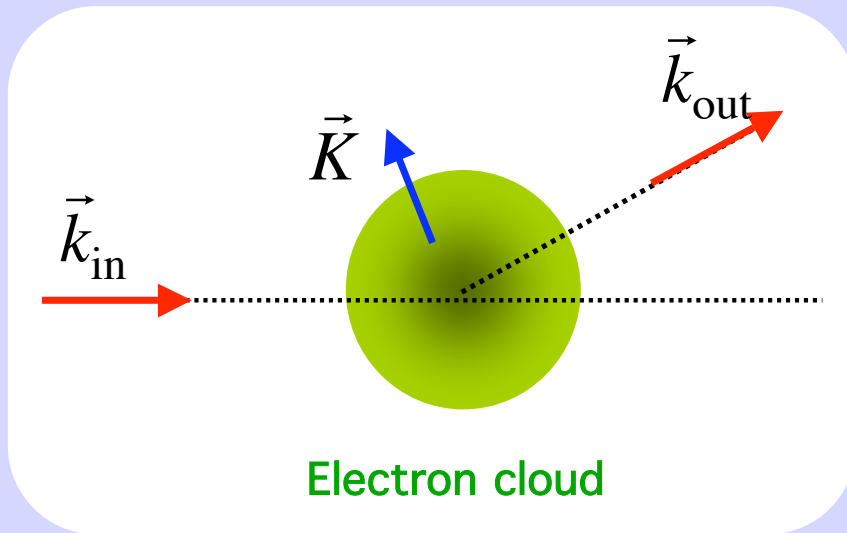
$$A(\vec{K}) = A_{el} \int \rho_e(\vec{r}) e^{i\vec{K} \cdot \vec{r}} dV$$

# Interference depends on wavelength



# Electron scattering factor

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

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

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

## Electronic units

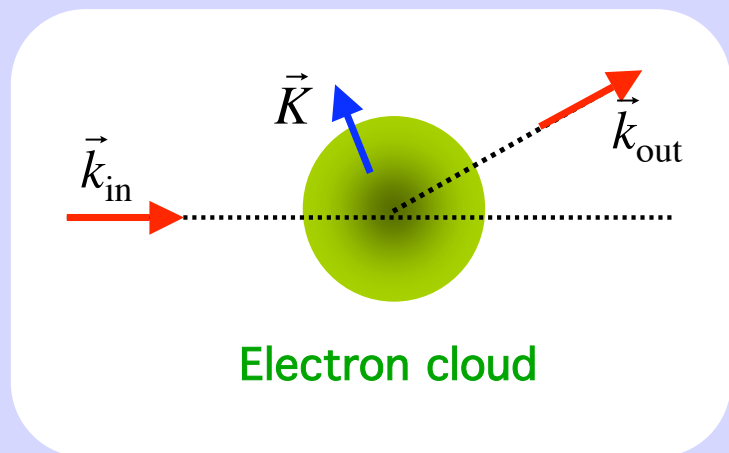
$$A_{e.u.}(\vec{K}) = \frac{A(\vec{K})}{A_{el}} = f_e(\vec{K})$$

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



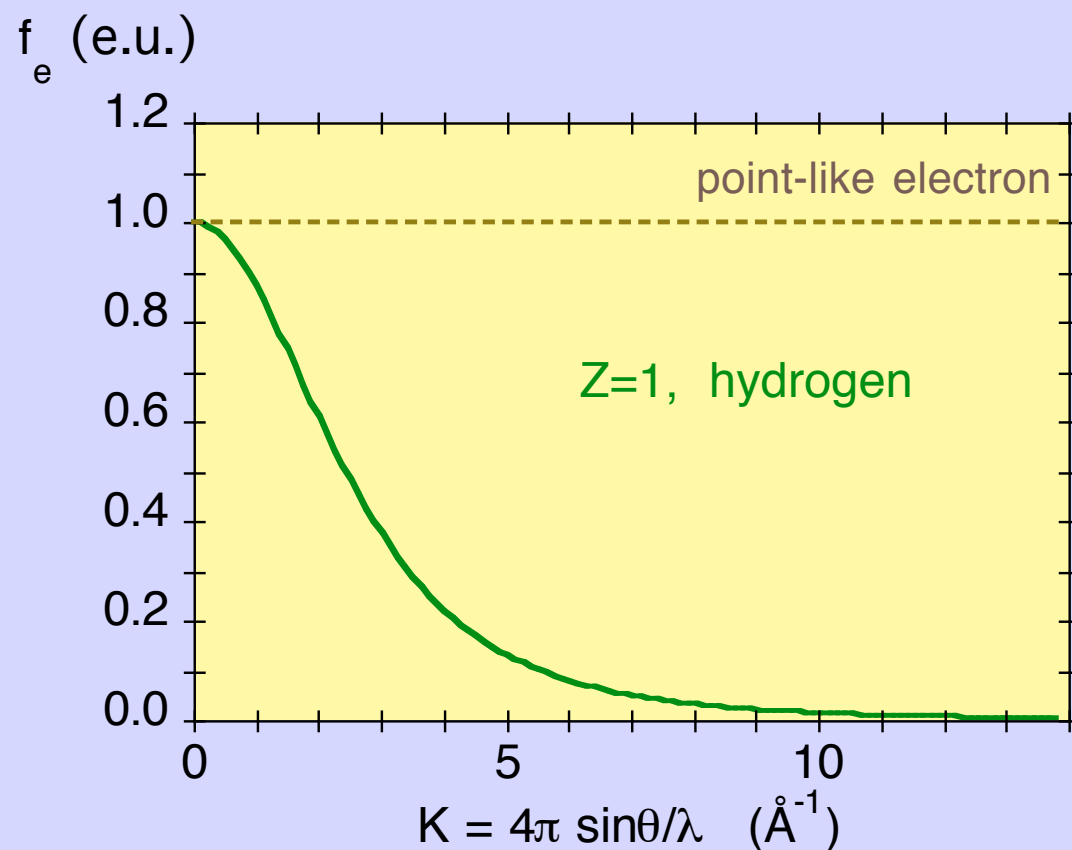
# Hydrogen scattering factor

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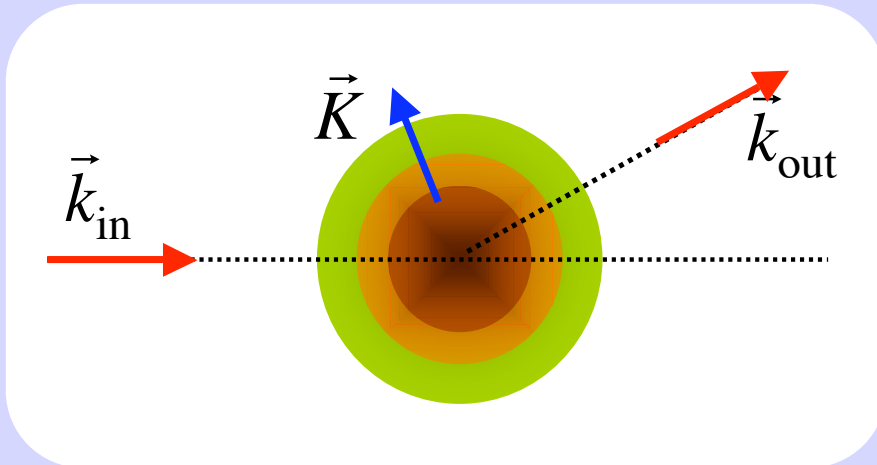


$$f_e(\vec{K}) = \int \rho_e(\vec{r}) e^{i\vec{K}\cdot\vec{r}} dV$$
$$= 4\pi \int_0^\infty r^2 \rho_e(r) \frac{\sin Kr}{Kr} dr$$

for spherical symmetry



# Atomic scattering factor (a)



sum over electrons

$$\begin{aligned} f_0(\vec{K}) &= \sum_n f_{e,n}(\vec{K}) \\ &= \sum_n \int \rho_{e,n}(\vec{r}) e^{i\vec{K}\cdot\vec{r}} dV \\ &= \int \rho(\vec{r}) e^{i\vec{K}\cdot\vec{r}} dV \\ &= 4\pi \int_0^\infty r^2 \rho_e(r) \frac{\sin Kr}{Kr} dr \end{aligned}$$

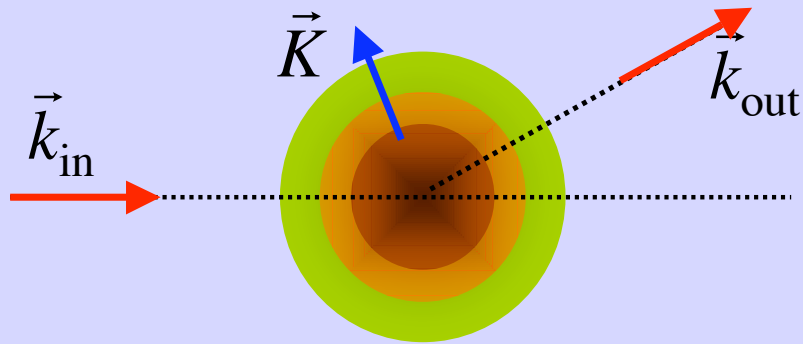
$$A_{e.u.}(\vec{K}) = f_0(\vec{K})$$

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

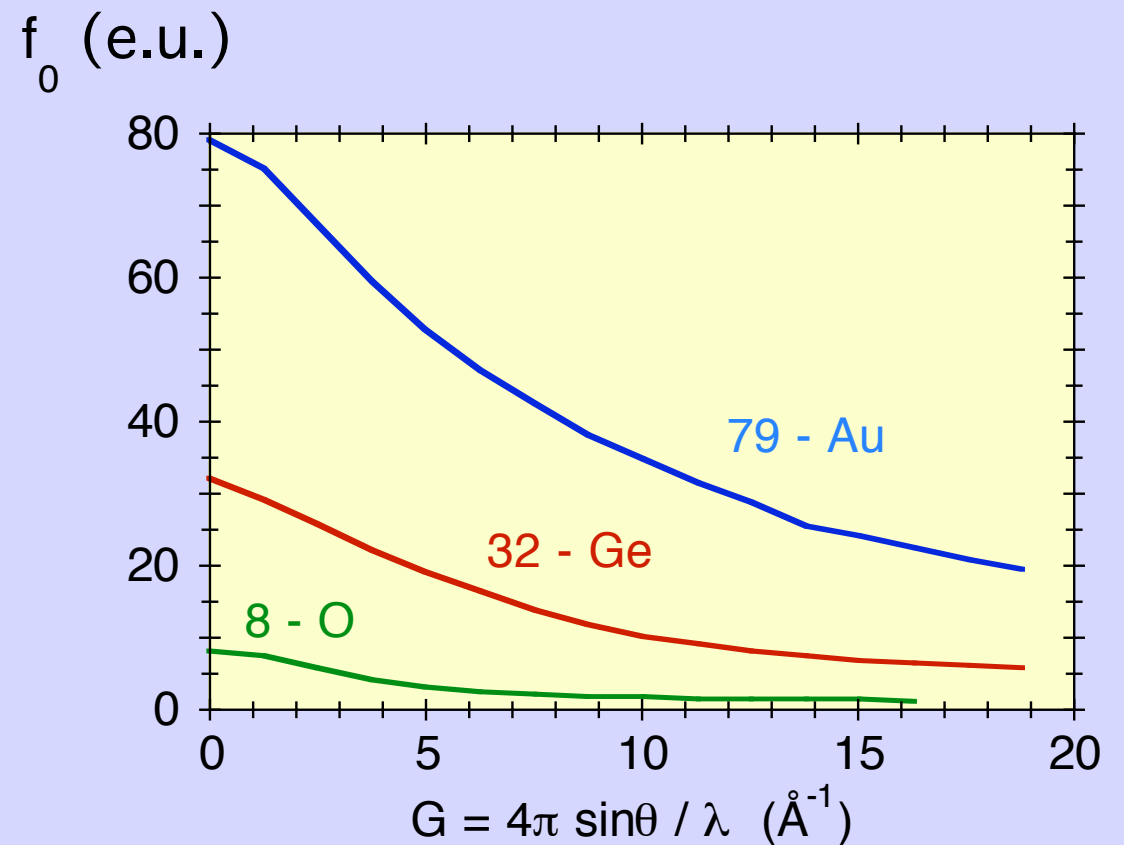
total  
electronic  
density

for spherical symmetry

# Atomic scattering factor (b)

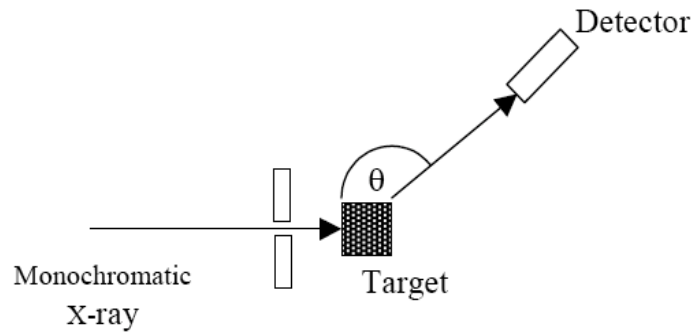


$$f_0(\vec{K}) = \int \rho(\vec{r}) e^{i\vec{K} \cdot \vec{r}} dV$$



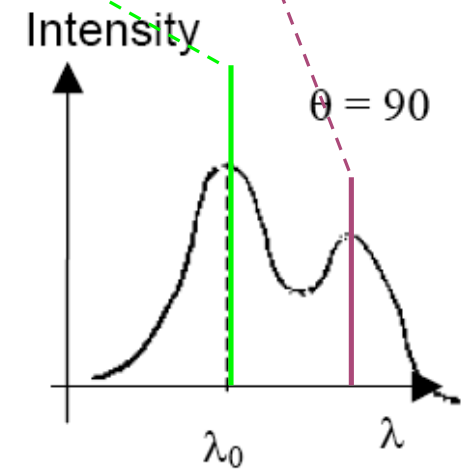
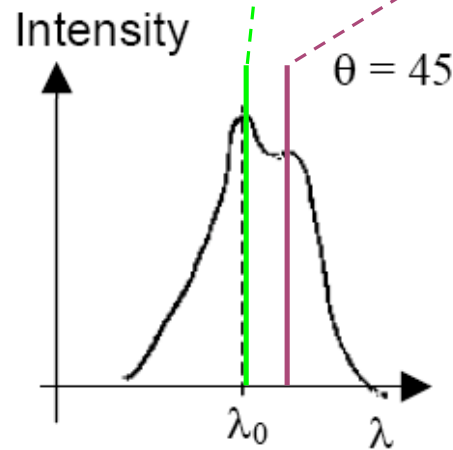
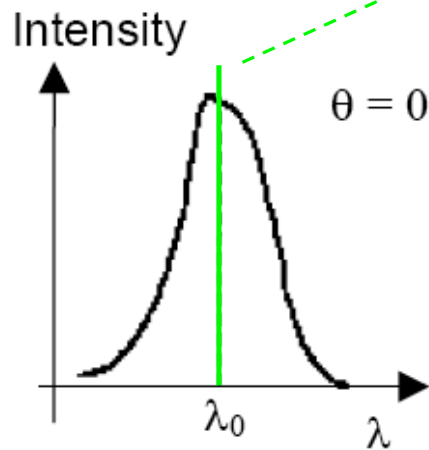
- ♣ Deviations from classical treatment
  - b) Compton effect

# Compton experiment (1922)

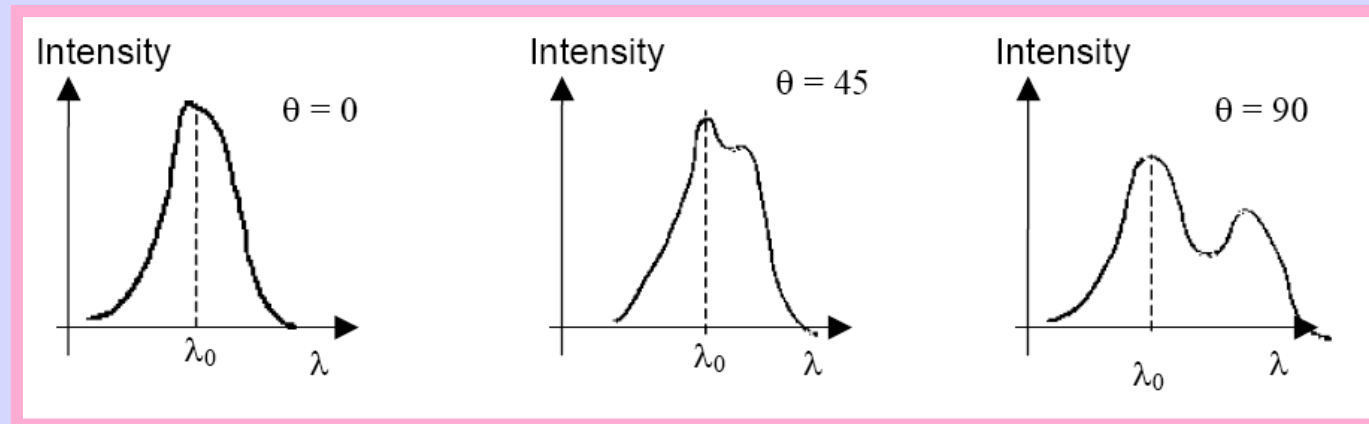


Unmodified (elastic)

Modified (inelastic)



# Compton effect



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

0.002426 Å  
(Compton wavelength)

$$E' [keV] = \frac{E [keV]}{1 + 0.001957 E (1 - \cos \theta)}$$

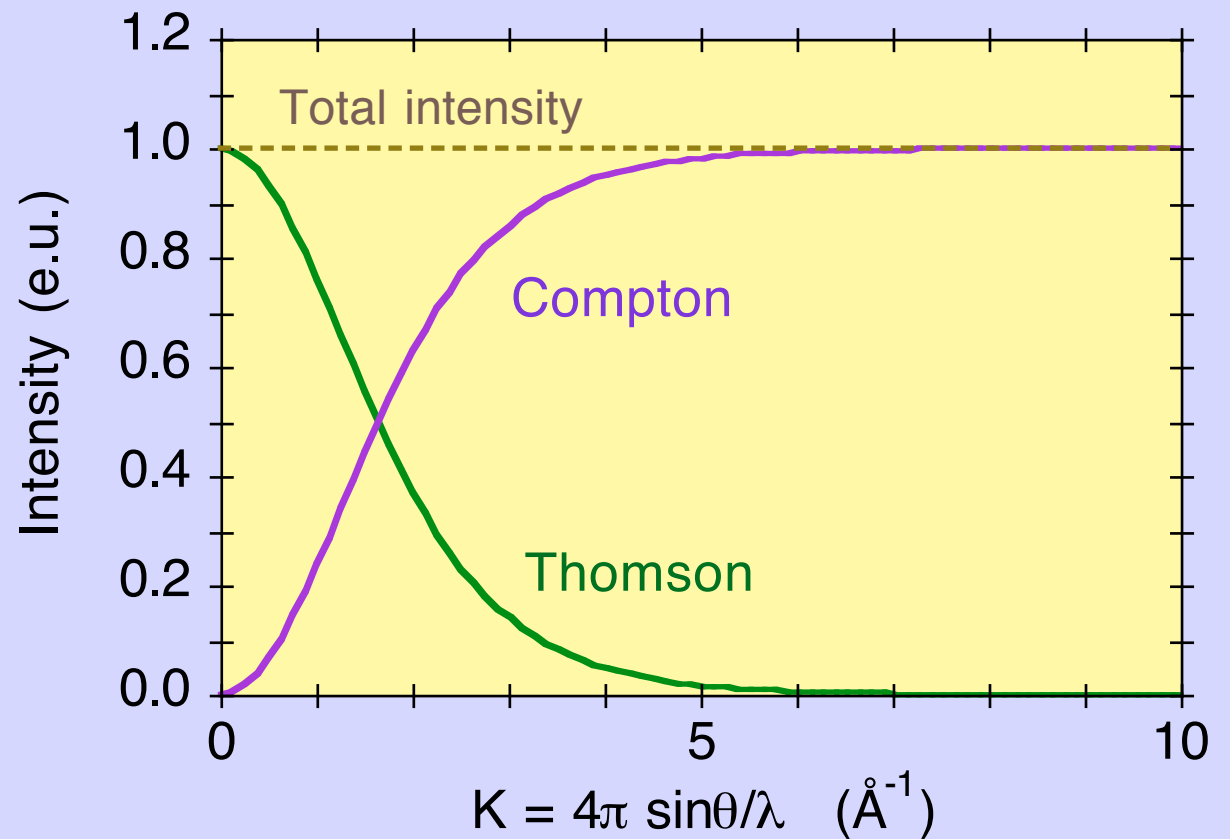
# Modified scattering - 1 electron

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

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

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

Hydrogen



## Thomson

$$I_{\text{unmod}} = \left| \sum_{n=1}^Z f_{e,n} \right|^2 \quad \leq Z^2$$

coherent scattering  
(sum of amplitudes)

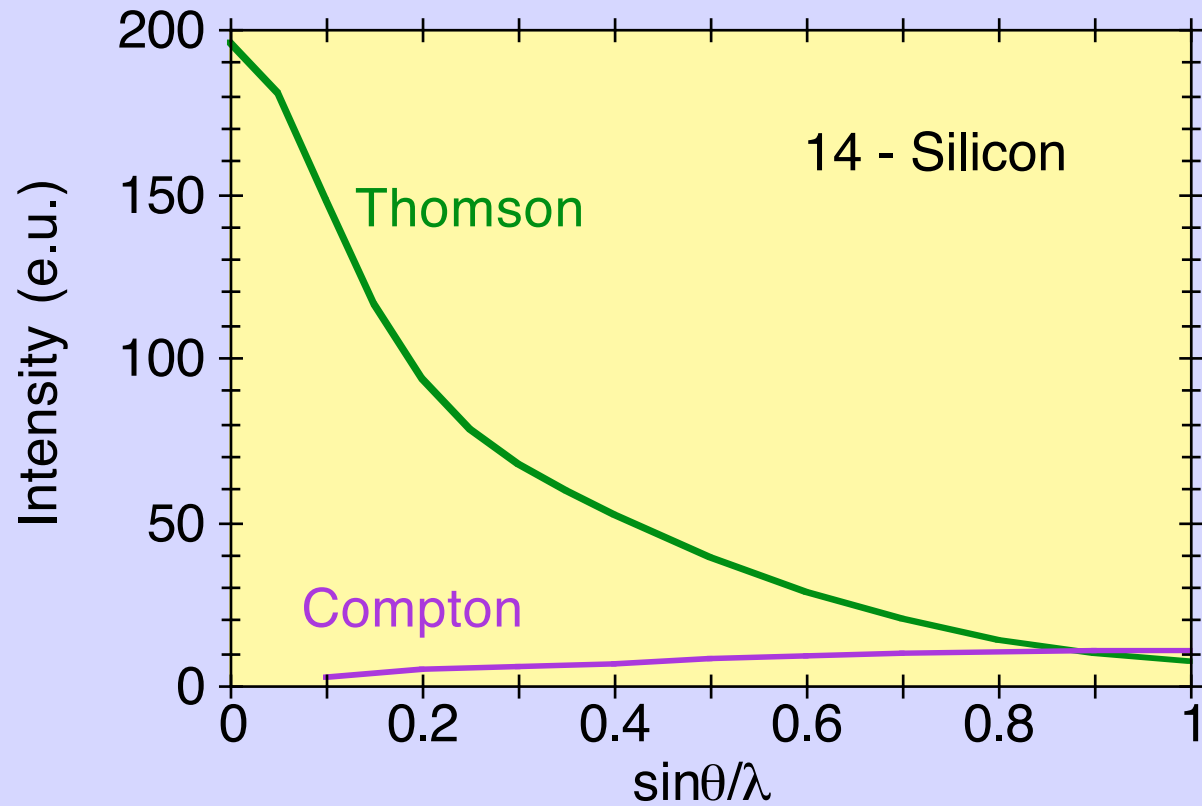
## Compton

$$\begin{aligned} I_{\text{mod}} &= \sum (I_{e,\text{mod}})_n \\ &= \sum (1 - f_{e,n}^2) \\ &= Z - \sum_{n=1}^Z f_{e,n}^2 \quad \leq Z \end{aligned}$$

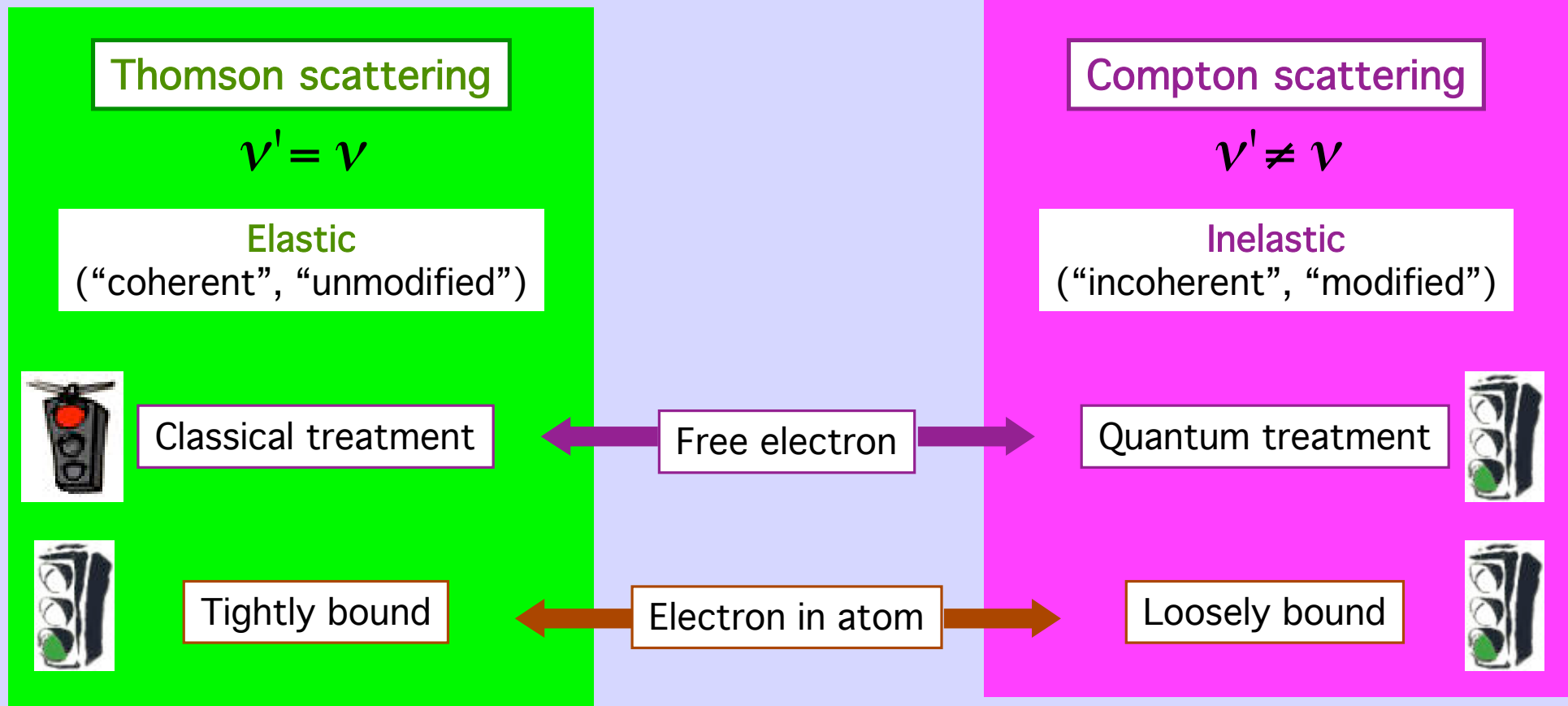
incoherent scattering  
(sum of intensities)



# Thomson .vs. Compton

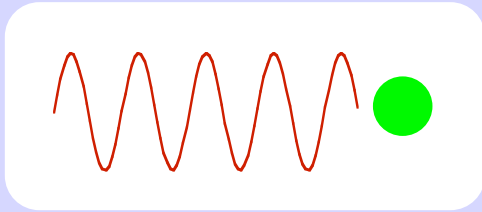


# Scattering of X-rays from an electron



- Deviations from classical treatment
  - c) Electron bonding

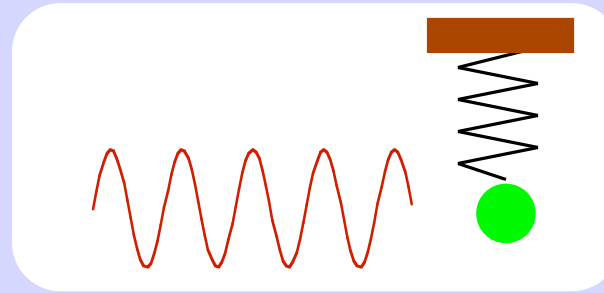
# Effect of electron bonding (a)



Free electron

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

E field



Bound electron

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

Damping  
force

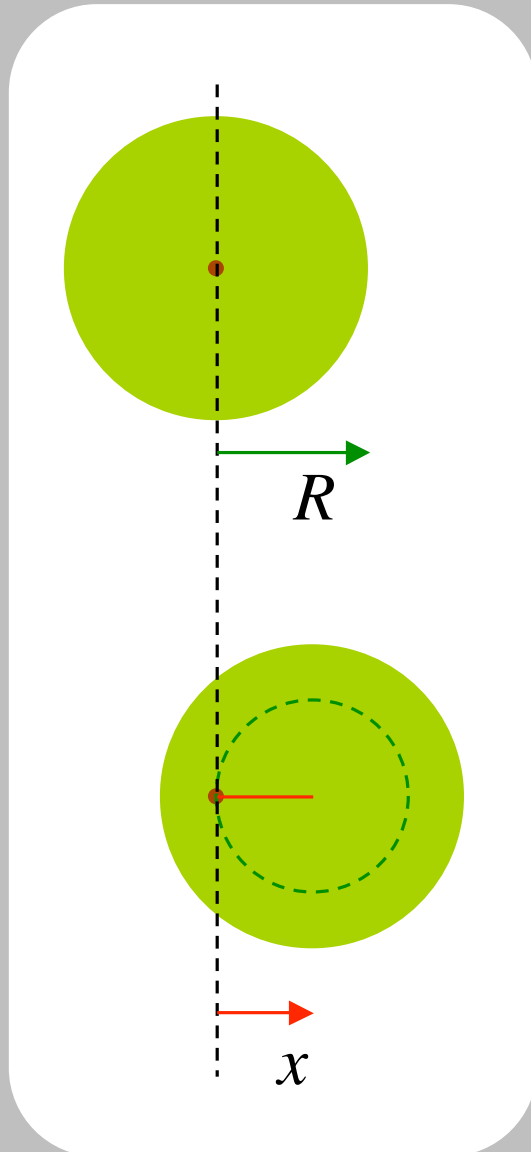
Elastic  
force

E field

Complex  
notation

Damped oscillator model

# Model of bound electron



Spherical distribution of negative charge centered on the positive nucleus

Displacement  $x$

Restoring force

$$|F| = \frac{1}{4\pi\epsilon_0} \frac{Qq_x}{x^2} \approx \frac{1}{4\pi\epsilon_0} \frac{Q^2}{x^2} \frac{x^3}{R^3}$$

$$|F| \propto x$$

# Effect of electron bonding (b)

## Free electron

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

## Bound electron:

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

Oscillating solution

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

Complex notation

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

Amplitude of oscillation

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

# Effect of electron bonding (c)

Free electron

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

Amplitude  
of  
oscillation

Bound electron:

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

Complex  
notation

spatial  
distribution

$$A(\vec{K}) = A_{\text{el}} f_e(\vec{K})$$

Amplitude  
of  
scattering

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

Scattering  
factor

Anomalous  
scattering factor

# “Anomalous” terms (1 electron)

$$\begin{aligned}
 A(\vec{K}) &= E_{\text{free}}^{\text{out}} f_e(\vec{K}) \left[ \frac{\omega^2}{\omega^2 - \omega_0^2 - i\gamma\omega} \right] \\
 &= E_{\text{free}}^{\text{out}} \left[ f_e(\vec{K}) \frac{\omega^2(\omega^2 - \omega_0^2)}{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2} + i f_e(\vec{K}) \frac{\gamma\omega^3}{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2} \right] \\
 &= E_{\text{free}}^{\text{out}} \left[ f_e(\vec{K}) + f_e(\vec{K}) \frac{\omega_0^2(\omega^2 - \omega_0^2) - \gamma\omega^2}{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2} + i f_e(\vec{K}) \frac{\gamma\omega^3}{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2} \right]
 \end{aligned}$$

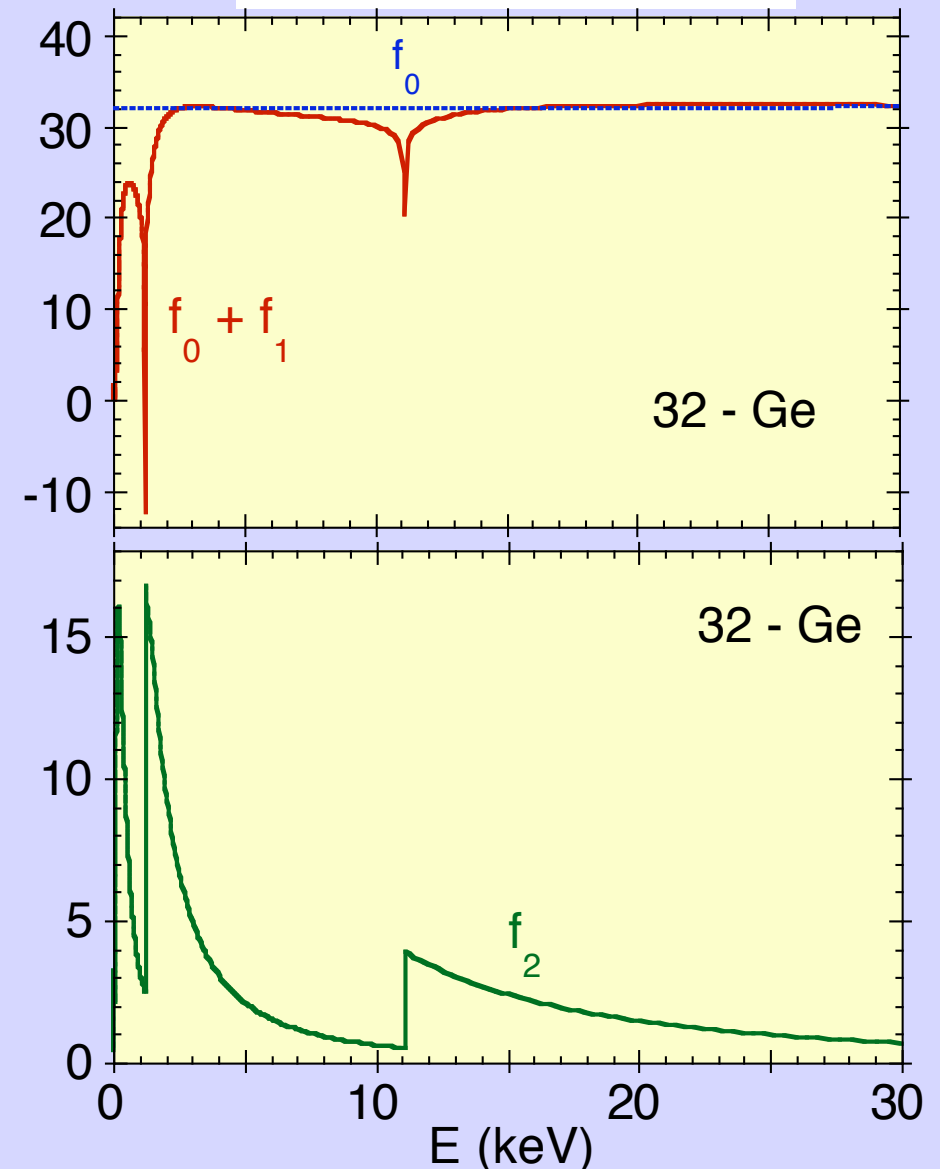
$$A(\vec{K}) = A_{\text{el}} \left[ f_e(\vec{K}) + \underbrace{f'_e + if_e''}_{\text{“Anomalous” terms}} \right]$$

“Anomalous” terms



# “Anomalous” scattering factor (atoms)

(for forward scattering)



Real part

$$f(\vec{K}) = f_0(\vec{K}) + f_1 + i f_2$$

anomalous terms  
(~ indep. from  $K$ )

Imaginary part

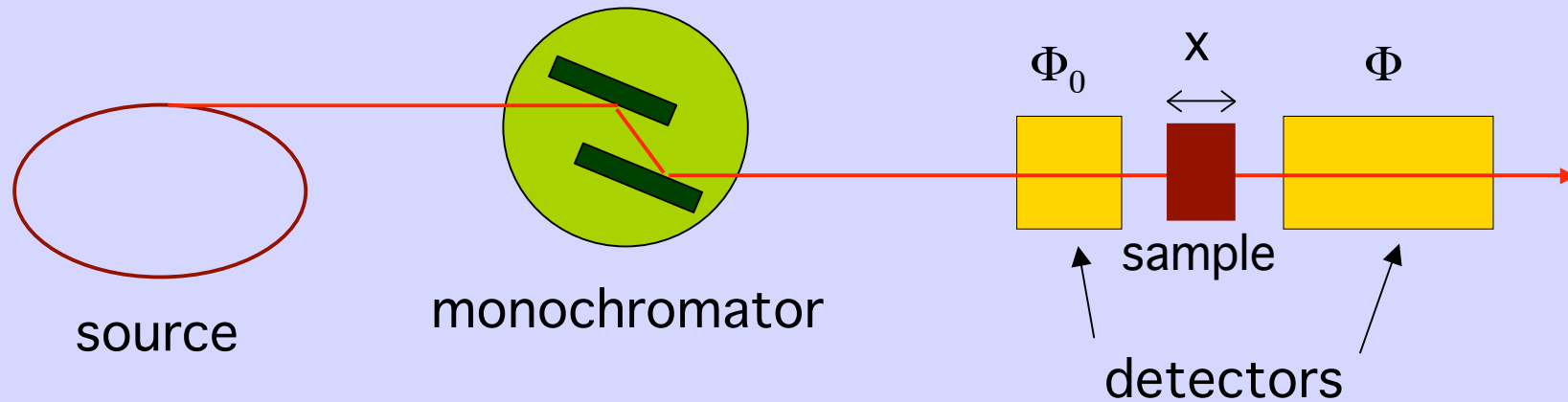
Absorption



Photo-electric absorption

a) Phenomenology

# Attenuation of X-rays



Exponential attenuation

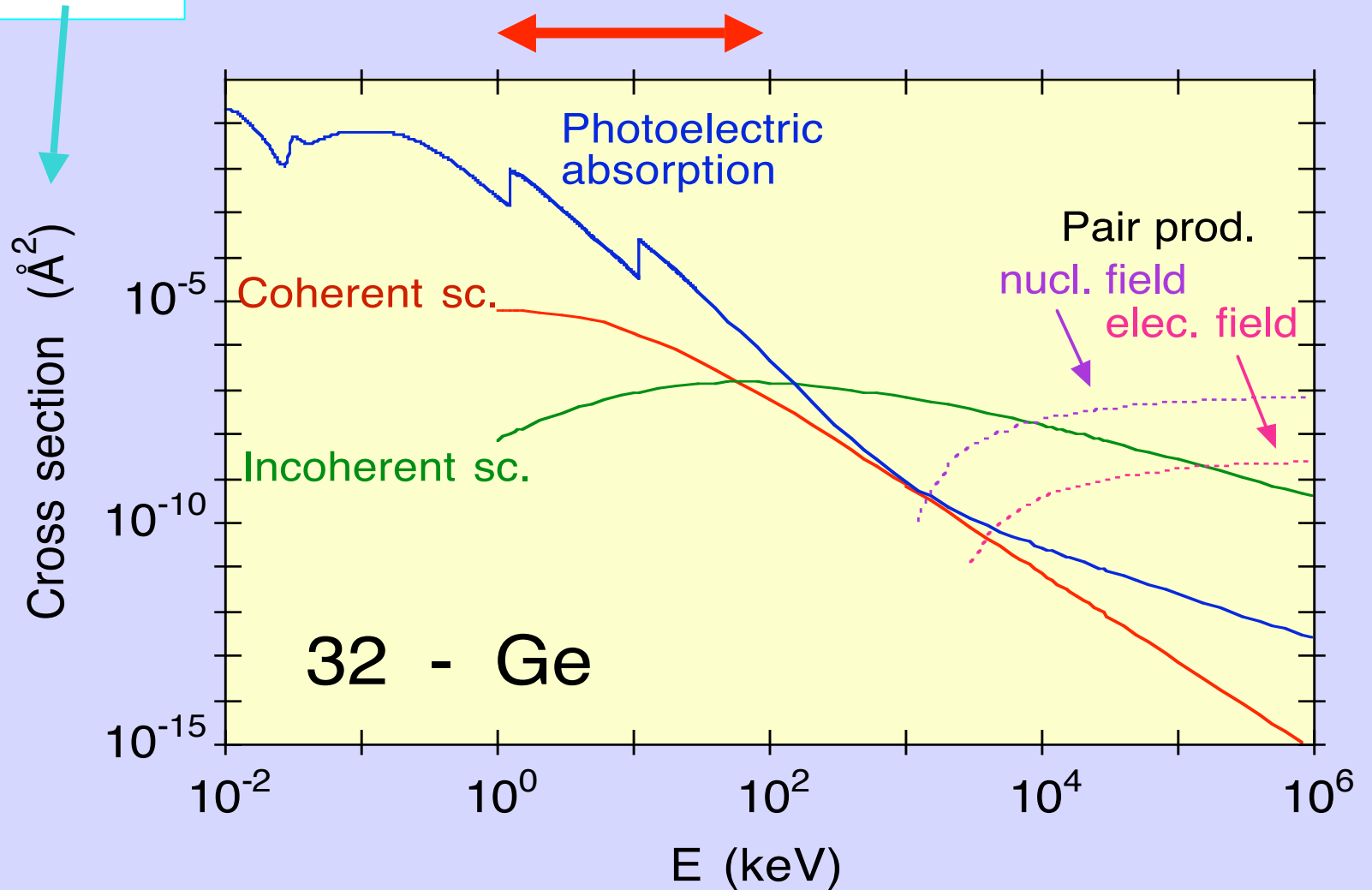
$$\Phi = \Phi_0 \exp[-\mu(\omega) x]$$

Attenuation coefficient

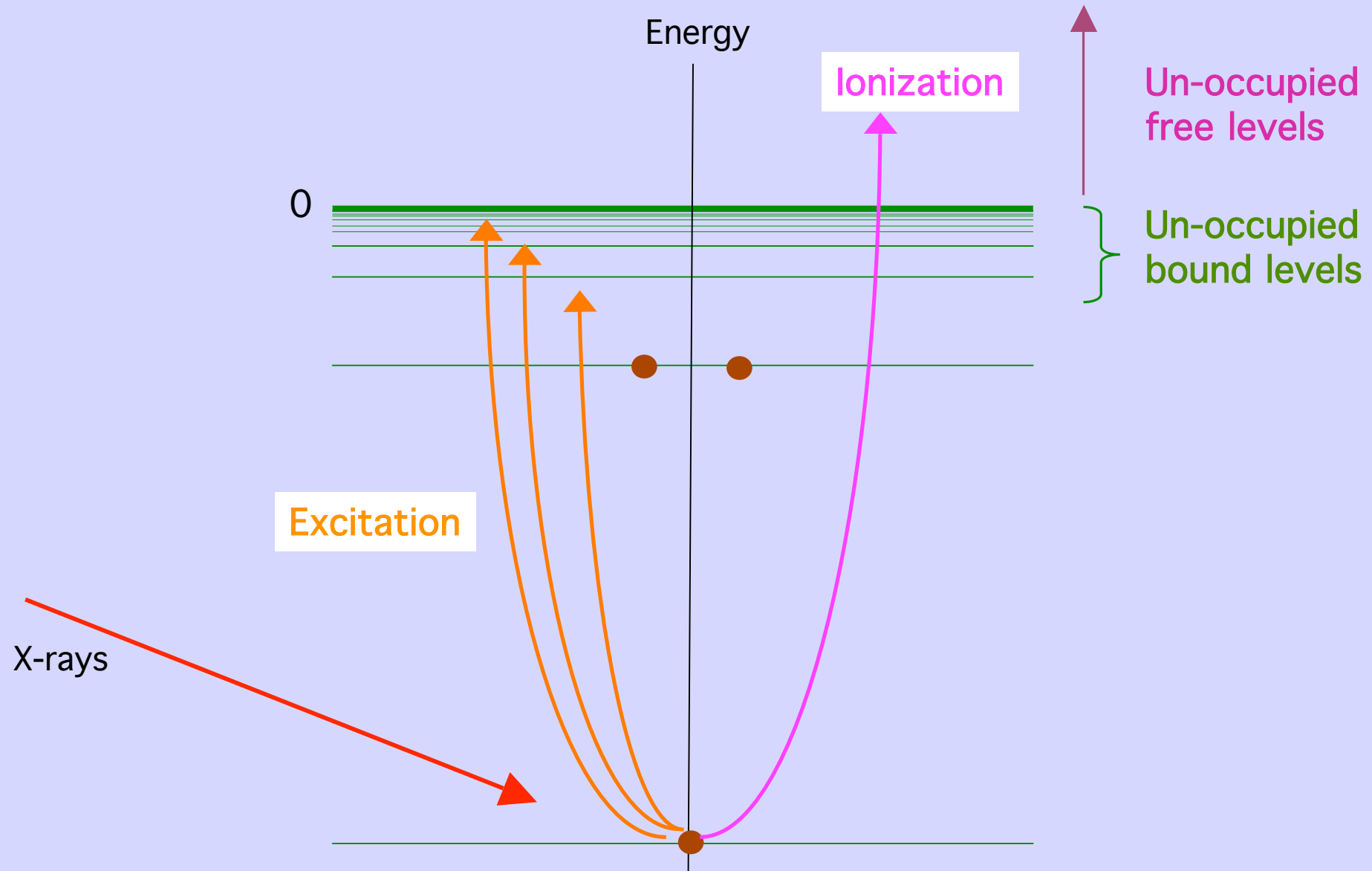
$$\mu(\omega) = \frac{1}{x} \ln \frac{\Phi_0}{\Phi}$$

# Atomic cross sections

$$\mu(\omega) = \frac{N_a \rho}{A} \mu_a(\omega)$$

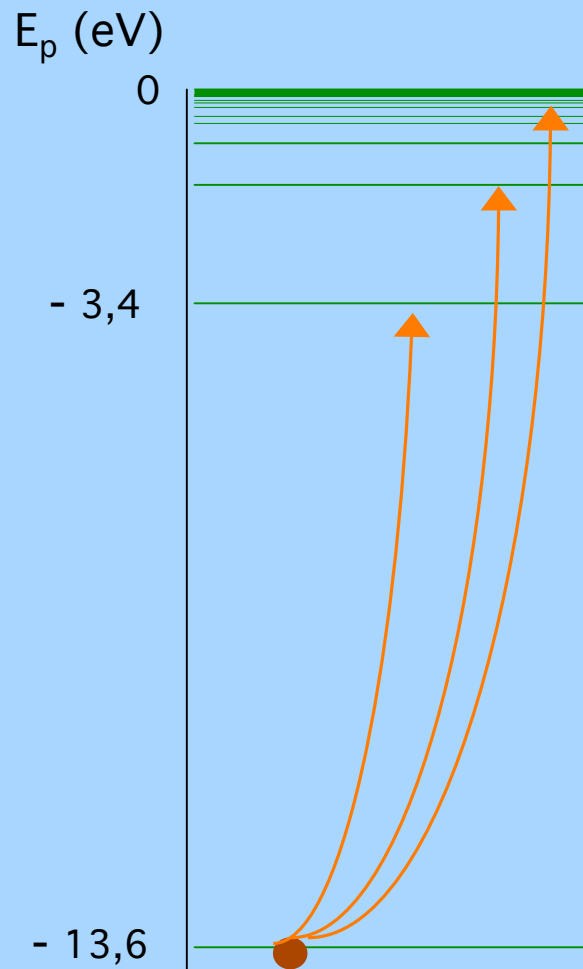


# Excitation and ionization

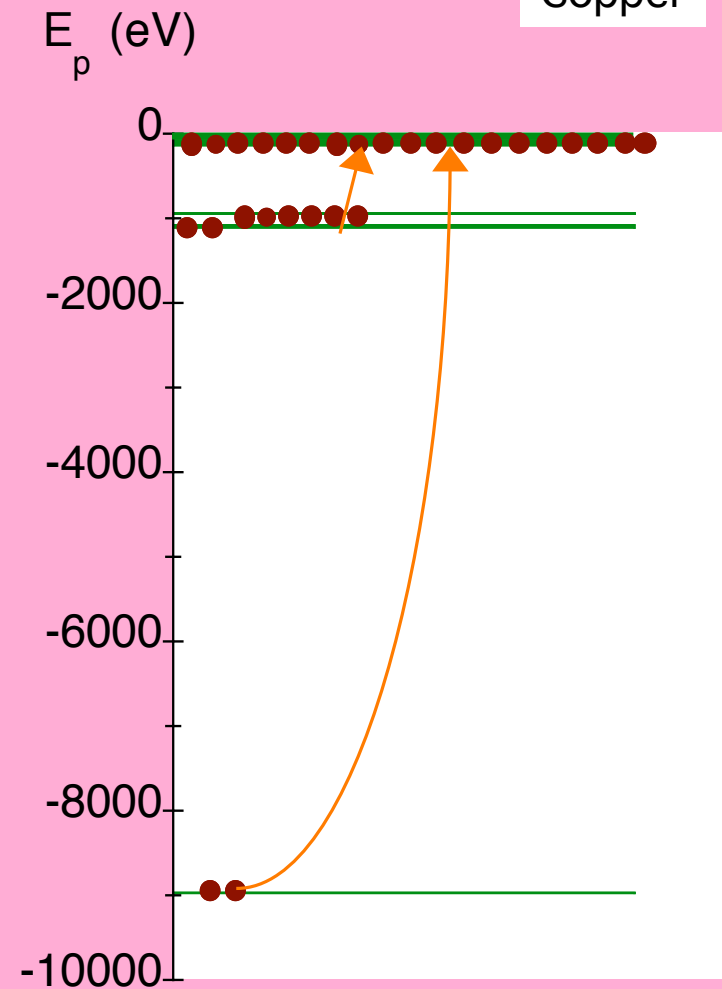


# Photoelectric absorption (a)

## Hydrogen

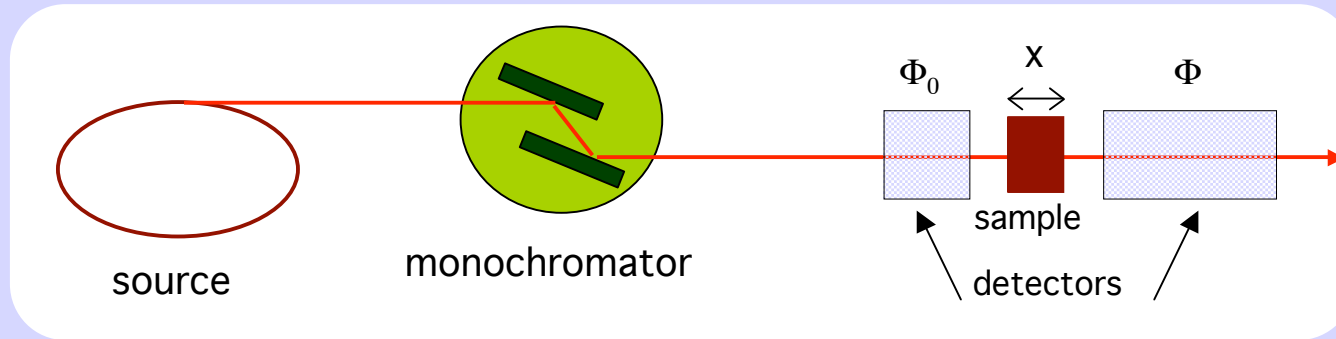


## Copper



# X-ray absorption spectroscopy

Paolo Fornasini  
Univ. Trento

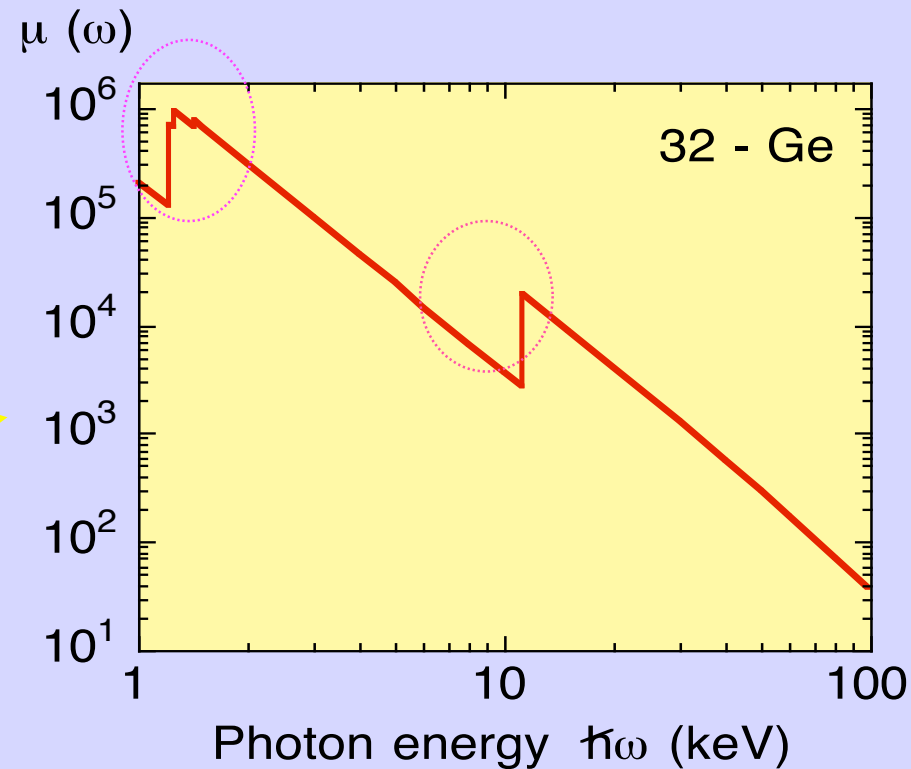


- Exponential attenuation

$$\Phi = \Phi_0 \exp[-\mu(\omega) x]$$

- Attenuation coefficient

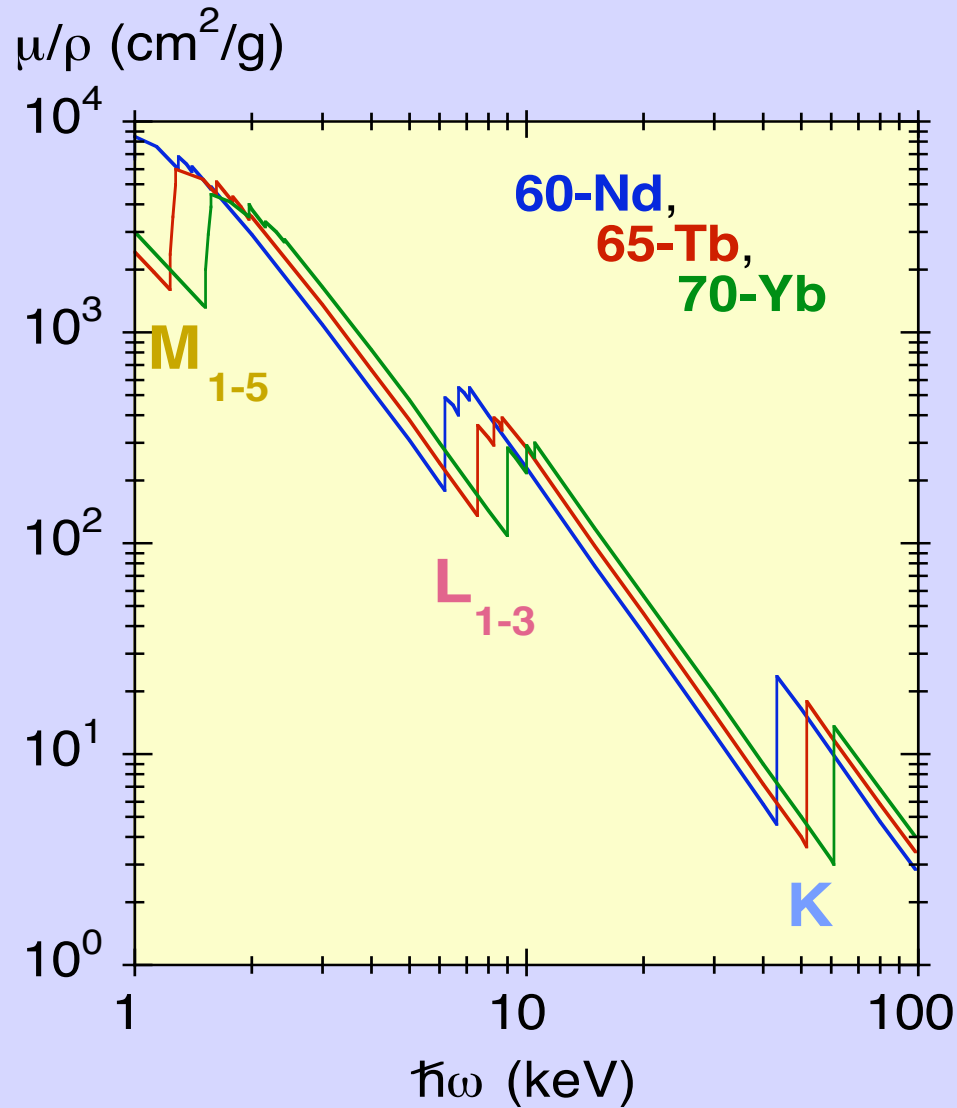
$$\mu(\omega) = \frac{1}{x} \ln \frac{\Phi_0}{\Phi}$$



$$\mu(\omega) \propto \frac{Z^4}{(\hbar\omega)^3}$$

+  
Edges

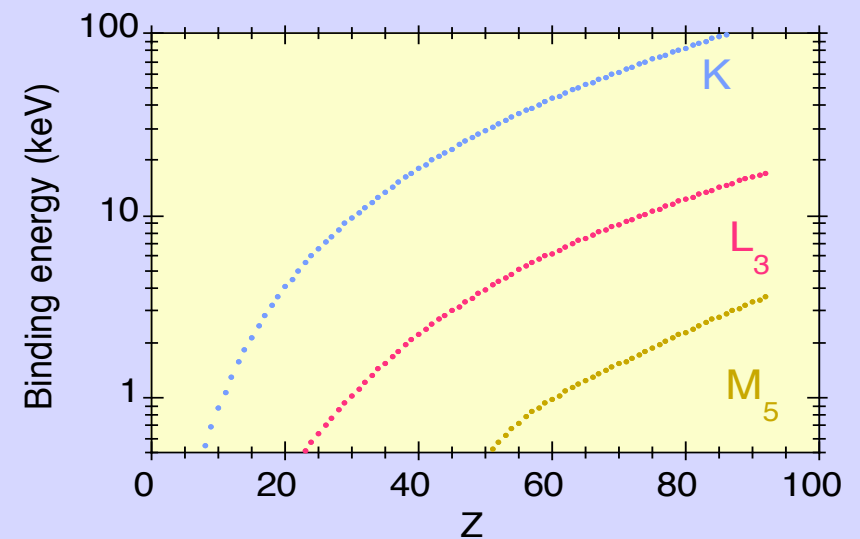
# X-ray absorption edges



K	1s
L <sub>1</sub>	2s
L <sub>2</sub>	2p <sub>1/2</sub>
L <sub>3</sub>	2p <sub>3/2</sub>
M <sub>1</sub>	3s
M <sub>2</sub>	3p <sub>1/2</sub>
M <sub>3</sub>	3p <sub>3/2</sub>
M <sub>4</sub>	3d <sub>3/2</sub>
M <sub>5</sub>	3d <sub>5/2</sub>
.....	

$Z > 9$

$Z > 29$



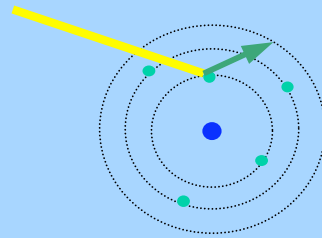


# Fine Structure: Atoms

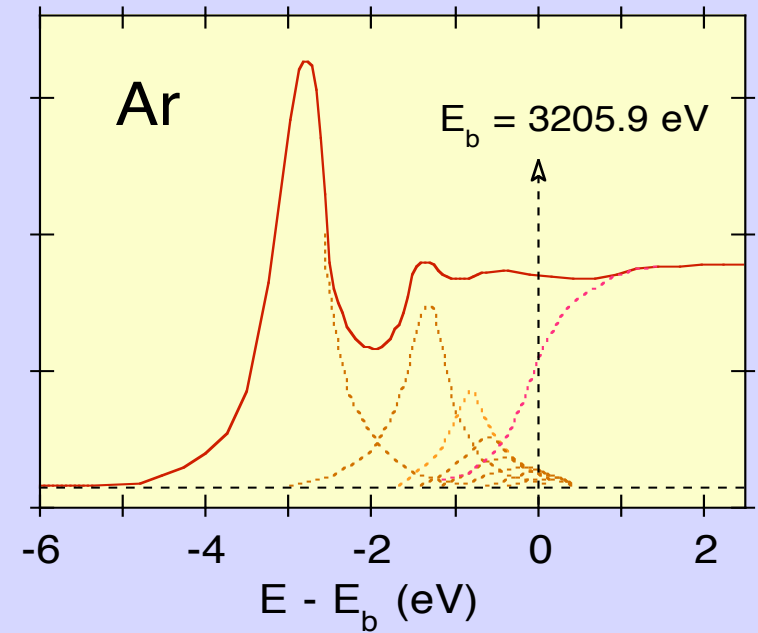
$h\nu < \text{binding energy}$

Core electron

unoccupied levels



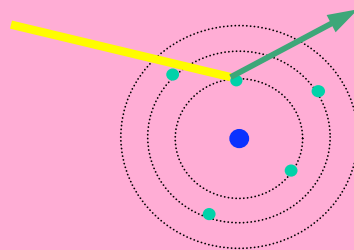
⇒ Edge Fine Structure



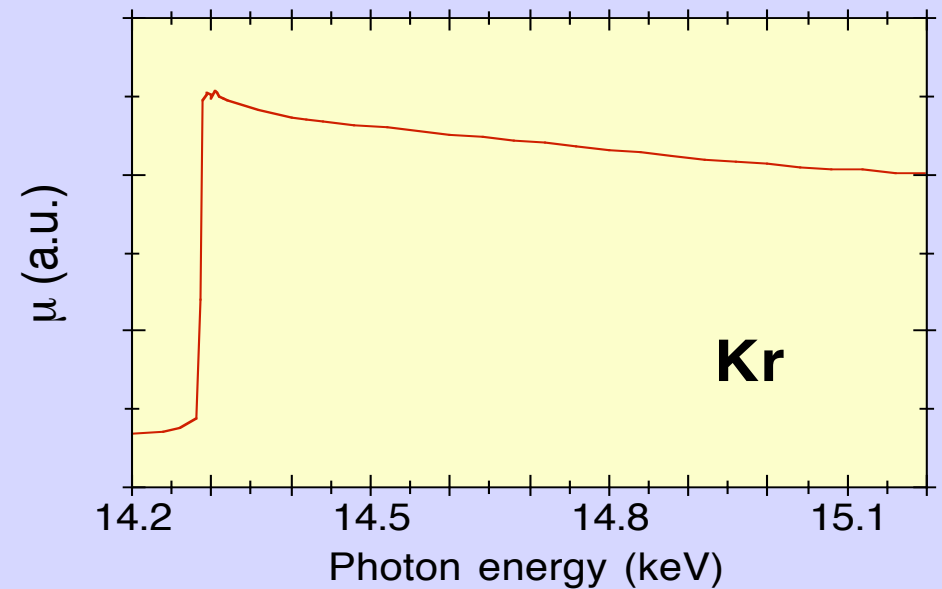
$h\nu > \text{binding energy}$

Core electron

continuum



⇒ Smooth  $\mu$

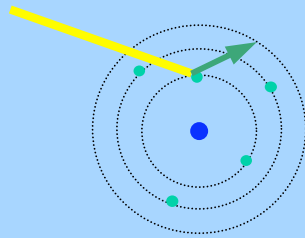


# Fine Structure: Molecules and Condensed systems

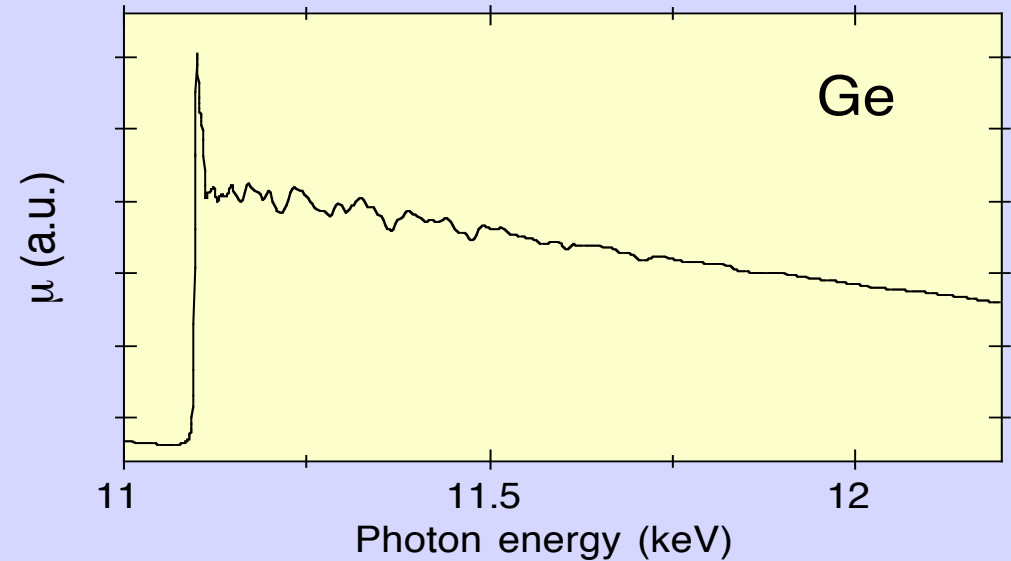
$h\nu \approx \text{binding energy}$

Core electron

unoccupied levels



⇒ Edge Fine Structure



$h\nu > \text{binding energy}$

Core electron

continuum

Outgoing wave-function

Back-scattering  
from  
neighbouring atoms

Incoming wave-function

INTERFERENCE

Extended  
Fine  
Structure



# XAFS: X-ray Absorption Fine Structure

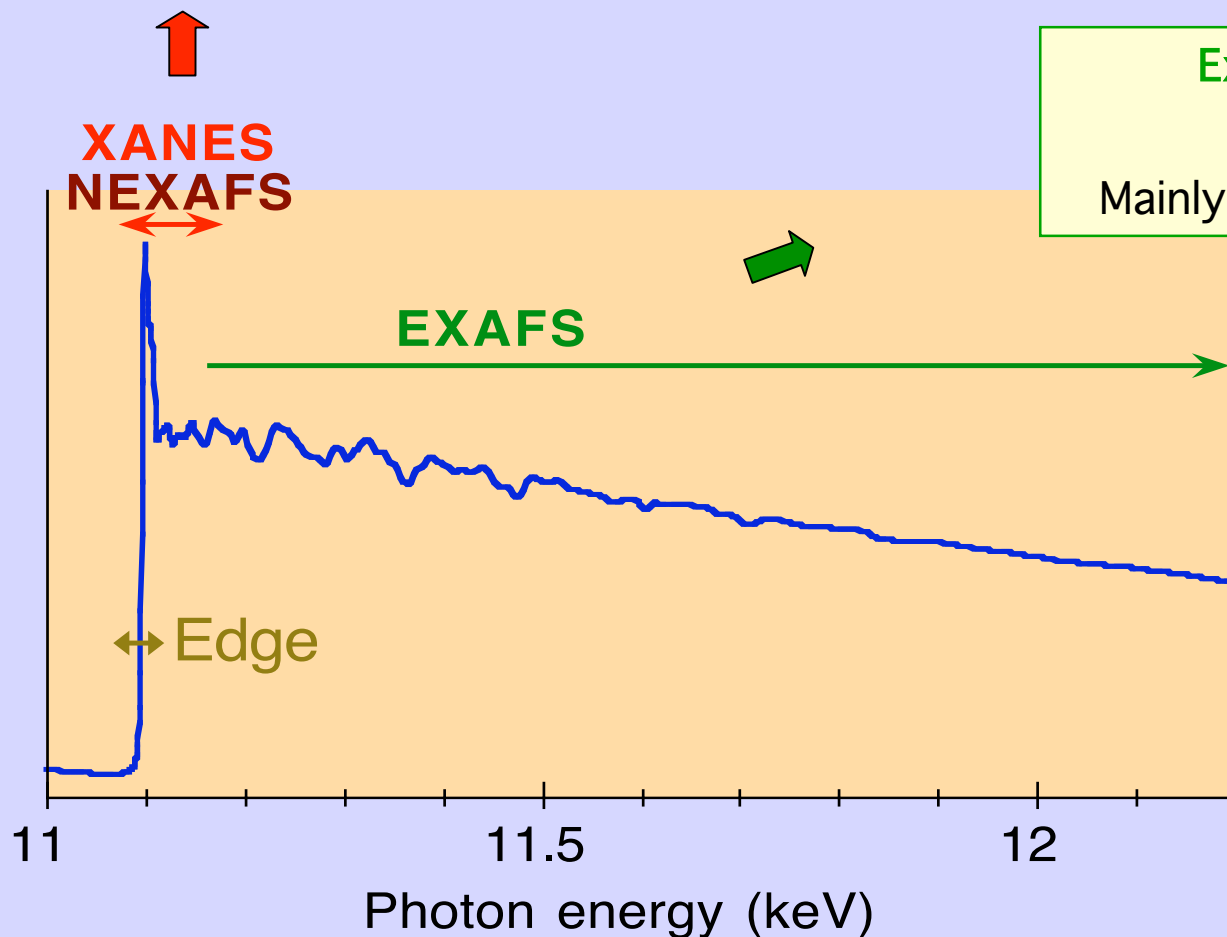
Paolo  
Fornasini  
Univ. Trento

X-ray Absorption Near Edge Structure  
Near Edge X-ray Absorption Fine Structure

Electronic transitions  
Photo-electron multiple scattering

Extended X-ray Absorption  
Fine Structure

Mainly photo-electron single scattering





# Photo-electric absorption

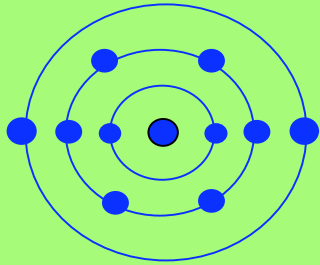
## b) Theory

# Transition probability $W_{if}$

$$\mu(\omega) = \frac{2\hbar}{\epsilon_0 \omega A_0^2} n \sum_f W_{if}$$

$n$  = atomic density  
 $A_0$  = vector potential amplit.

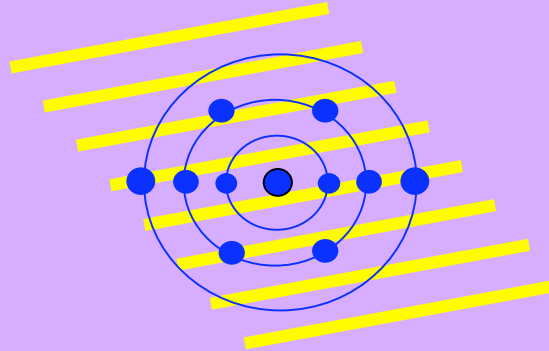
Initial atomic state



$|\Psi_i\rangle$

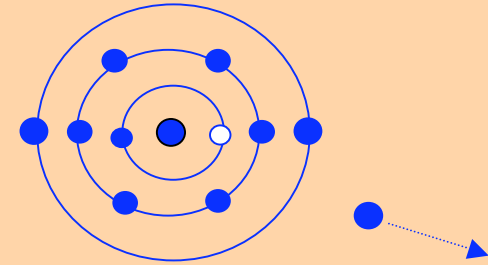
Stationary ground state

Interaction



$|\Psi(t)\rangle$

Final atomic state



$|\Psi_f\rangle$

Stationary excited state

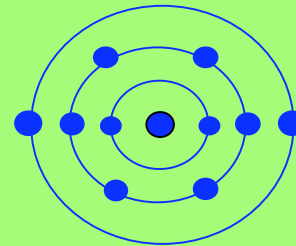
$W_{if} = ?$

# Approximations

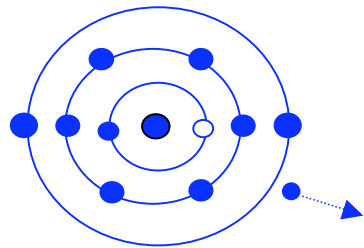
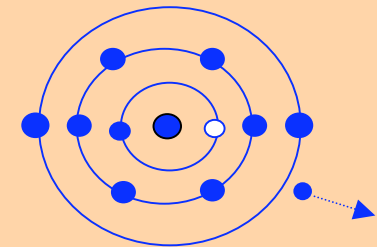
Weak interaction

Time-dependent perturbation theory  
1st order

Initial state

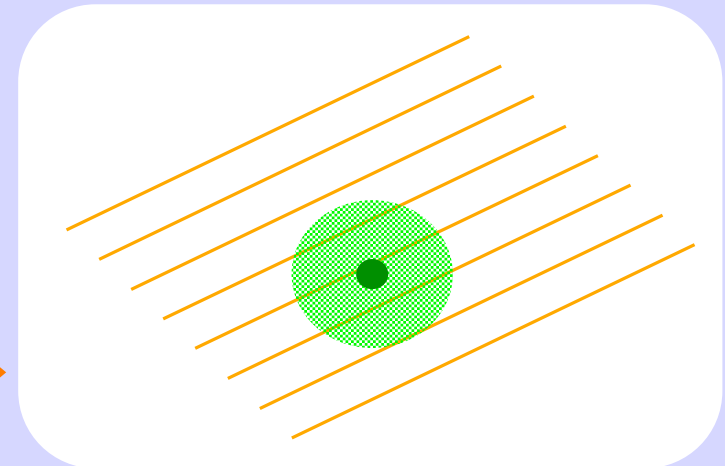


Final state



One electron

Electric dipole approximation



# Absorption coefficient

1 active electron

passive electrons

$$\mu_{\text{el}}(\omega) \propto \left| \langle \psi_i | \hat{n} \cdot \vec{r} | \psi_f \rangle \right|^2 \delta(E_i + \hbar\omega - E_f) \left| \langle \Psi_i^{N-1} | \Psi_f^{N-1} \rangle \right|^2$$

Energy conservation

Superposition integral

X-ray  
polarization

Electron  
position

$$\left| \langle \psi_i | \hat{n} \cdot \vec{r} | \psi_f \rangle \right|^2$$

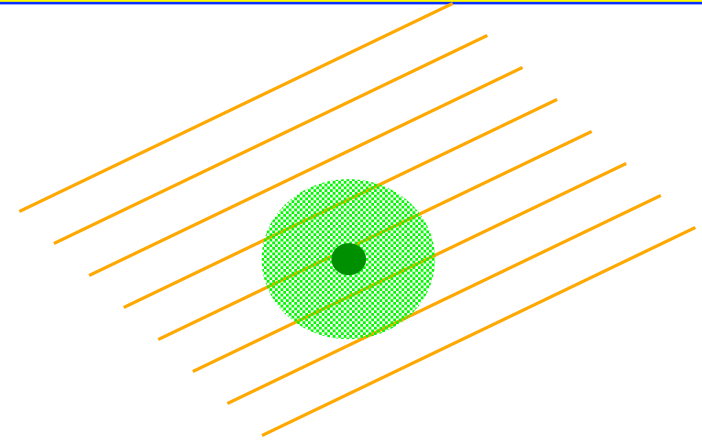
Initial  
state

Final  
state

$$\left| \int \psi_i^*(\vec{r}) \hat{n} \cdot \vec{r} \psi_f(\vec{r}) d\vec{r} \right|^2$$

# Electric dipole approximation

$$e^{i\vec{k}\cdot\vec{r}} = 1 + i\vec{k}\cdot\vec{r} - \dots \approx 1$$



$$H_I \propto e^{i\vec{k}\cdot\vec{r}} \hat{\eta} \cdot \vec{p} \approx \hat{\eta} \cdot \vec{p} = \omega^2 \hat{\eta} \cdot \vec{r}$$

Dipole selection rules:

$$\begin{aligned} \Delta\ell &= \pm 1 & \Delta s &= 0 \\ \Delta j &= \pm 1, 0 & \Delta m &= 0 \end{aligned}$$

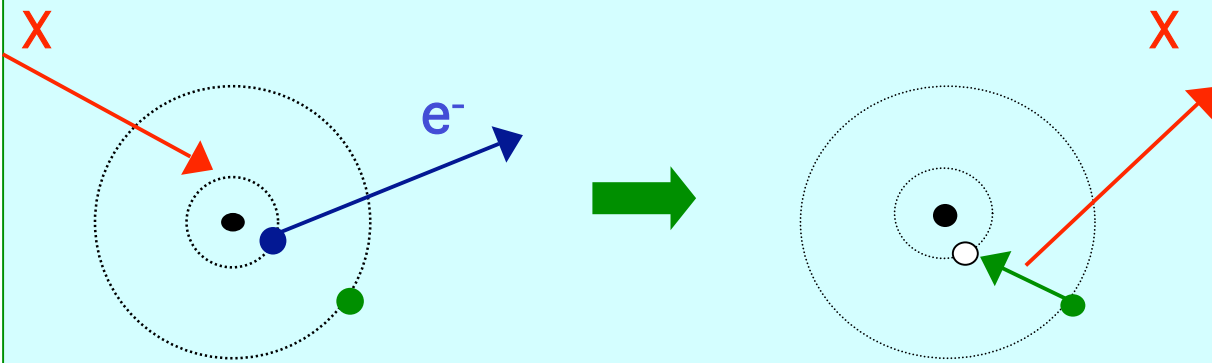
$$\mu_{\text{el}}(\omega) \propto \left| \langle \Psi_i^{N-1} \psi_i | \hat{\eta} \cdot \vec{r} | \psi_f \Psi_f^{N-1} \rangle \right|^2$$



# De-excitation mechanisms

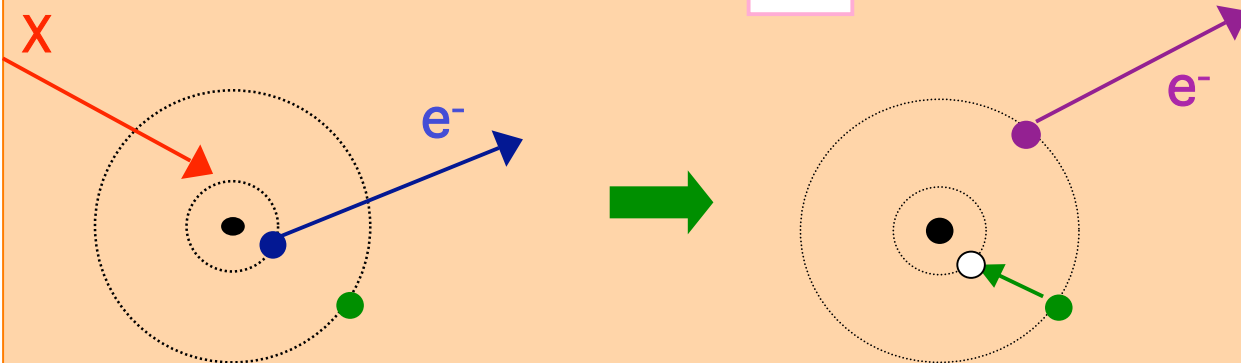
## Radiative: fluorescence

X



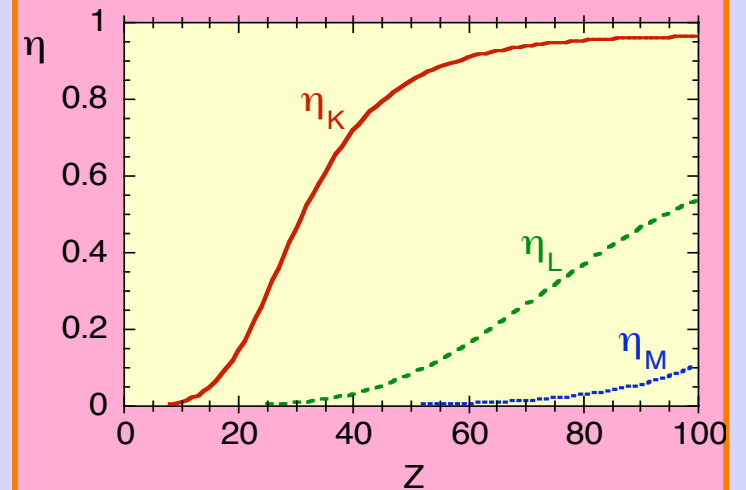
## Non-radiative: Auger

A



## Fluorescence yield

$$\eta = \frac{X}{X + A}$$

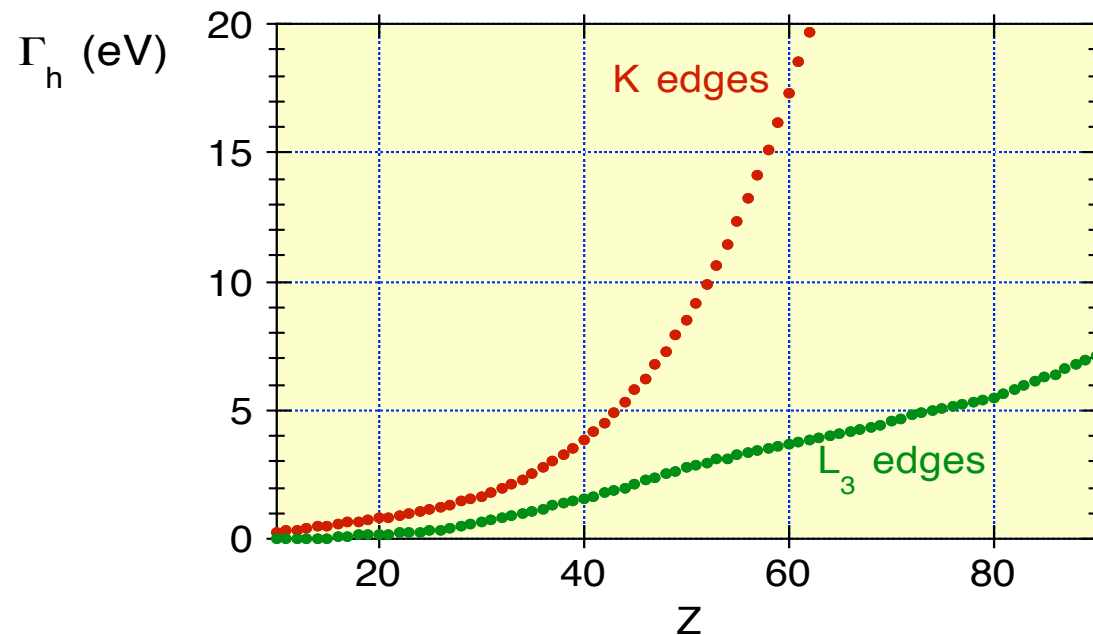


# Core-hole lifetime

Lifetime  
of the excited state  
 $\tau_h \sim 10^{-16} - 10^{-15} \text{ s}$

$$\tau_h \approx 1/\Gamma_h$$

Energy width  
of the excited state  
 $\Gamma_h$



$\tau_h$

Contribution to  
photo-electron life-time

$\Gamma_h$

Energy resolution  
of XAFS spectra



# Summary

- ❑ Attenuation: scattering and absorption
  - Thomson scattering from a free electron (classical)
  - Limits of the classical treatment
  - Basic interference phenomenon
  - Electronic and atomic structure factors
  - Compton effect
  - Anomalous (or 'resonant') scattering
  - ❖ Absorption coefficient and absorption edges
  - ❖ Fine structure at absorption edges
  - ❖ Introduction to theory of photoelectric absorption



Dolomite mountains at sunset (near Trento, Italy)