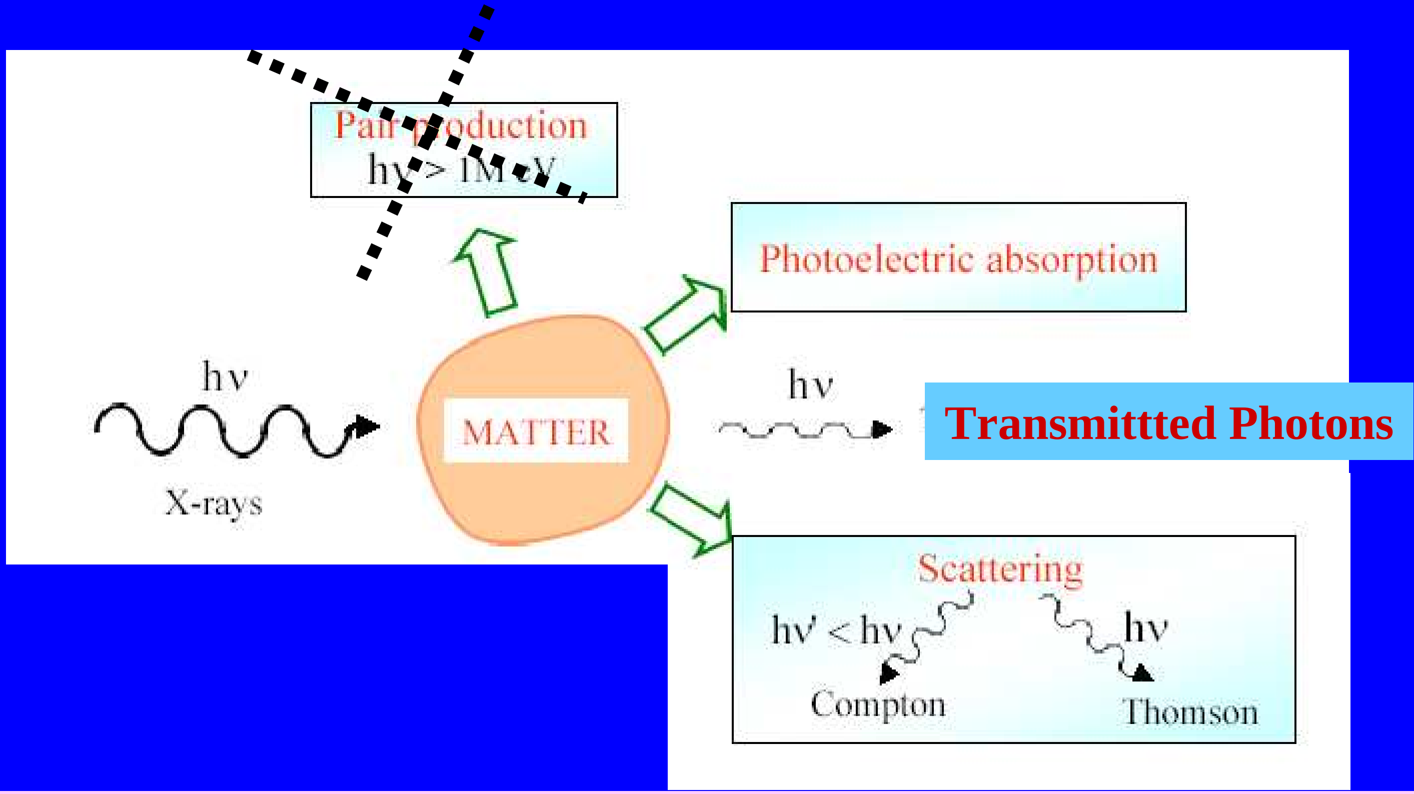
Interaction between matter and radiation: an introduction

Overview of the basic processes
Classical approach
Semi-classical approach

Basic elements to follows lectures

Relativistic effects

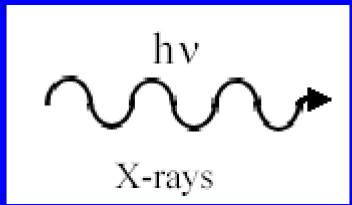
Main interactions



Photon absorption: excitation
with or without emission of electrons

Photon scattering: elastic → Thompson (Magnetic)
inelastic → Compton (Raman)
Resonant (elastic and inelastic)

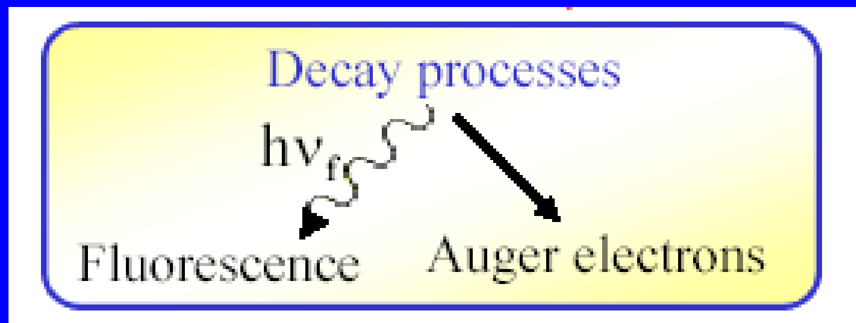
Indirect effects: decay processes



MATTER

Matter is excited by the radiation

It loose energy through decay processes



Experimental techniques

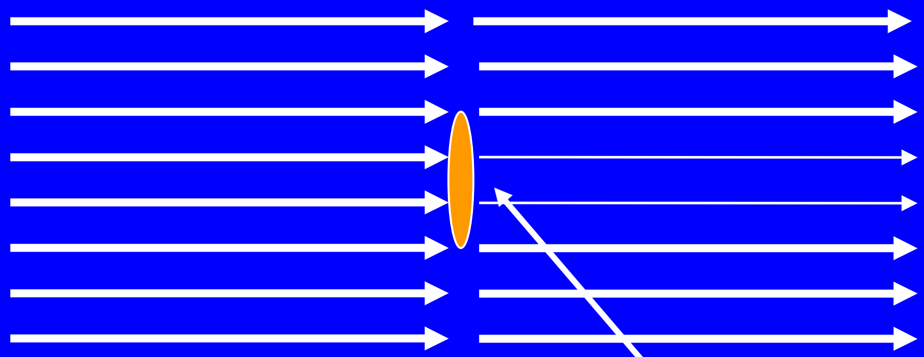
Absorption
Photoemission

Fluorescence Yield
Auger spectroscopy

Scattering:
Elastic Scattering: Diffraction, SAXS
Inelastic Scattering: Compton, IXS
Resonant scattering: RIXS

Imaging

The cross section σ



σ

$$N_{out} = N_{in}\frac{(\Delta S - \sigma)}{\Delta S}$$

$$I_{out} = I_{in}\frac{(\Delta S - \sigma)}{\Delta S}$$

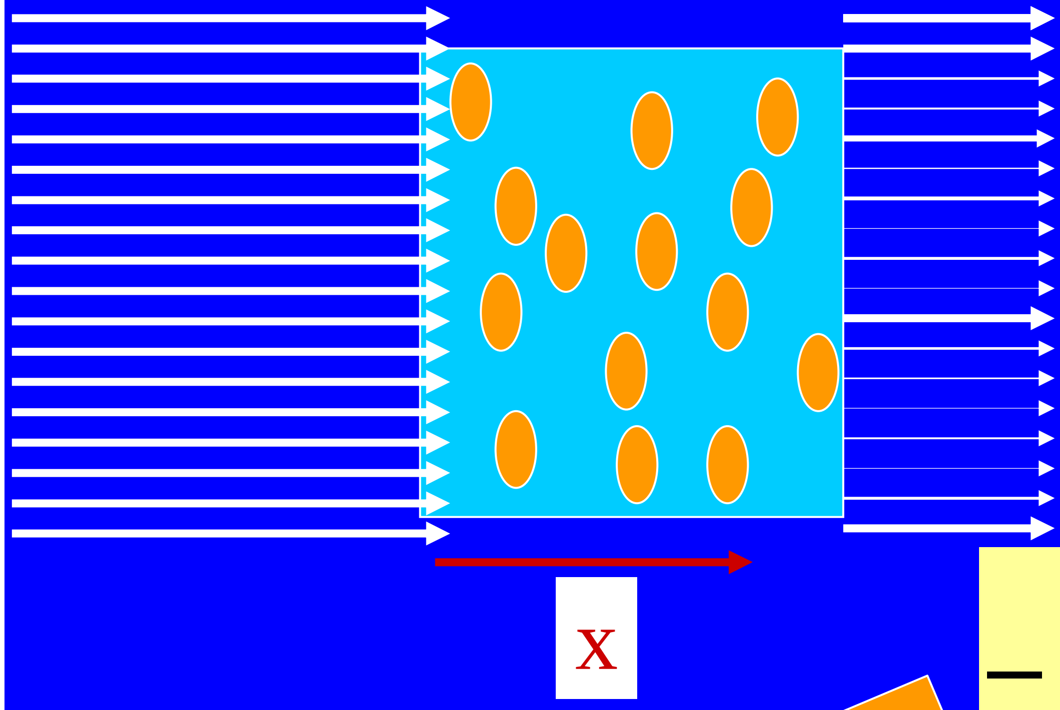
$$I_{in} = \frac{N_{in}}{\Delta S \Delta t}$$

$$\frac{\Delta I}{I_{in}} = -\frac{\sigma}{\Delta S}$$

σ has no geometrical meaning:
it is a measure of the interaction
It is called "cross section"

1 barn = 10^{-24} cm^2

The cross section σ – II



ρ is the density of the objects

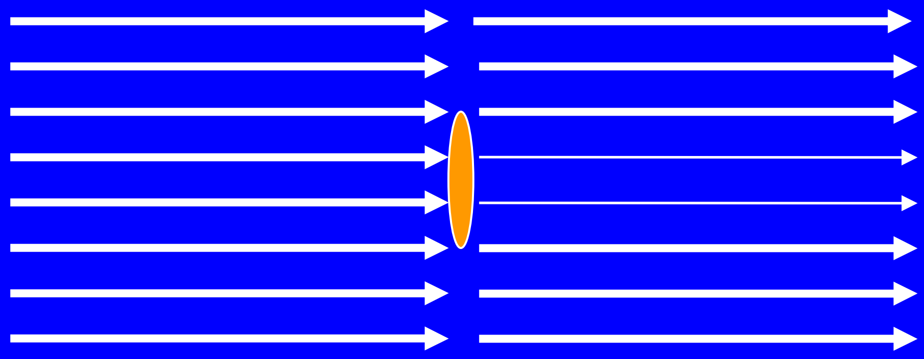
$$\sigma_{tot} = \sigma\rho\Delta S\Delta x$$

$$-\frac{\Delta I}{I_{in}} = \frac{\sigma_{tot}}{\Delta S} = \sigma\rho\Delta x$$

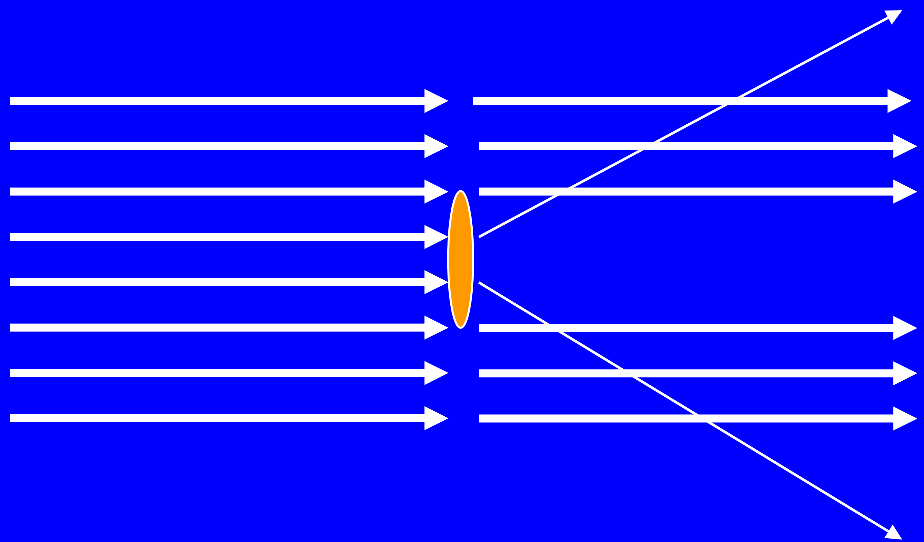
$$\frac{dI}{I_{in}} = -\sigma\rho dx$$

$$I(x) = I_{in} e^{-\sigma\rho}$$

Origin of the cross section



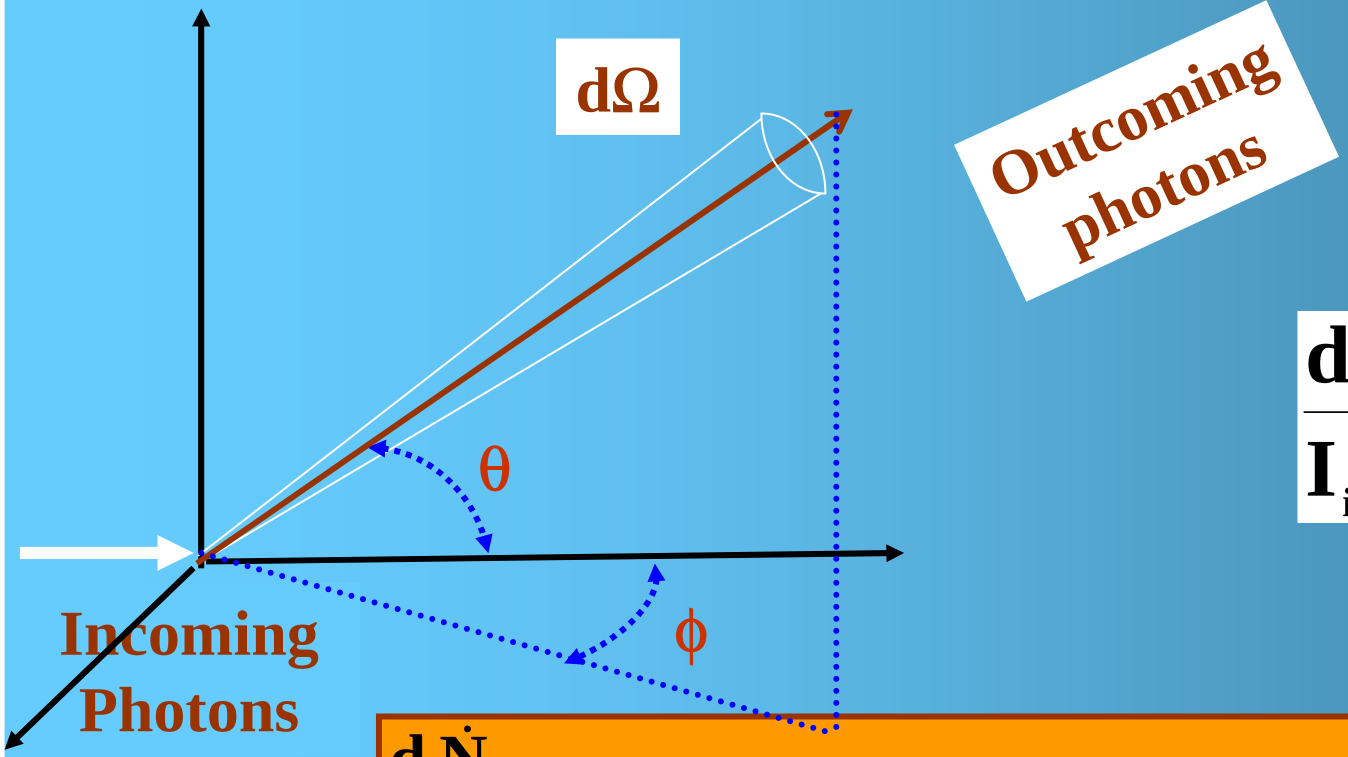
Absorption
Photons are removed from the beam
$\sigma_{abs.}$



Scattering
Photons are scattered into a different direction
$\sigma_{scatt.}$

Total cross section $\sigma = \sigma_{abs.} + \sigma_{scatt.}$

Differential Cross Section dσ/dΩ



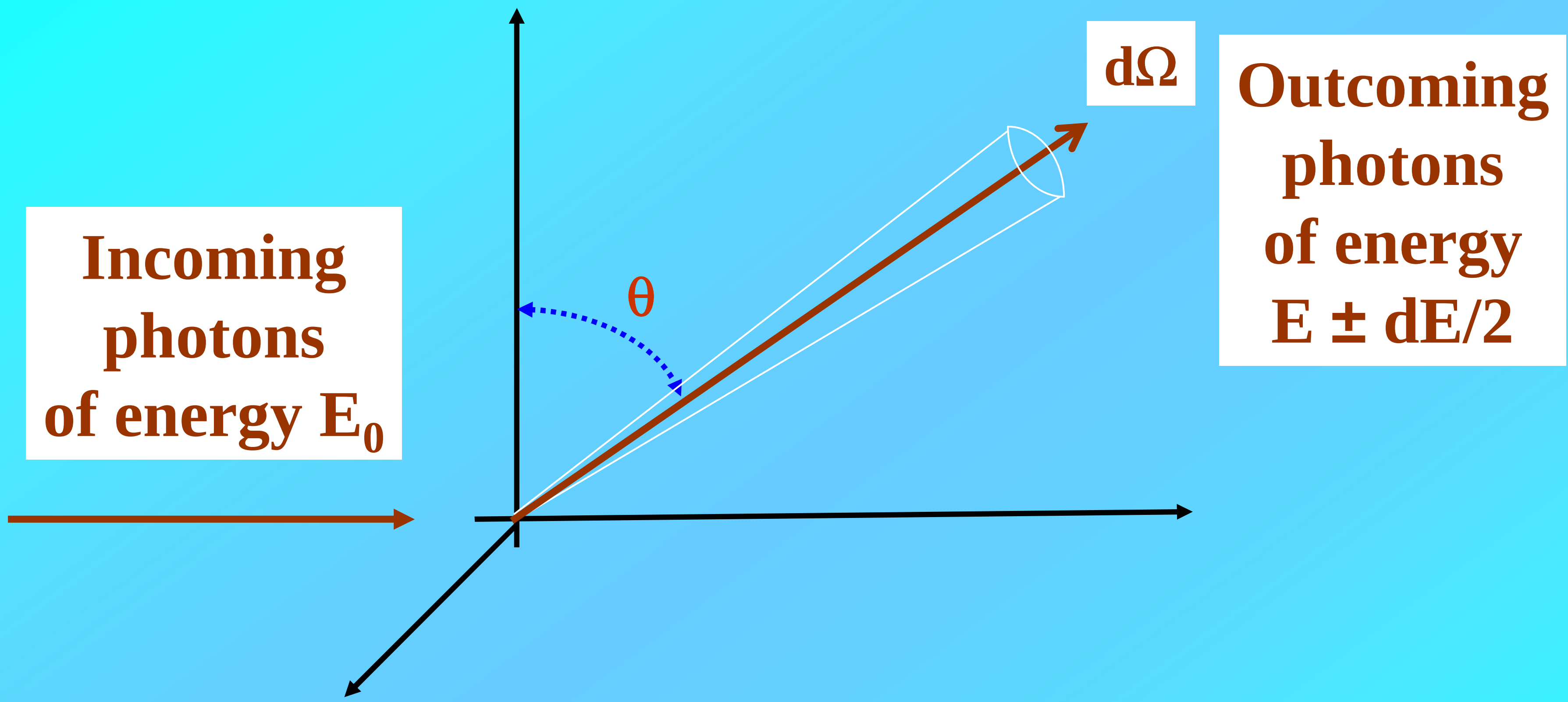
$$\frac{dI}{I_{in}} = -\sigma \rho dx$$

$$\frac{d\dot{N}_{scattered\ photons}}{\dot{N}_{incoming\ photons}} = \left(\frac{d\sigma}{d\Omega}\right) d\Omega \times (\rho dx)$$

$$\frac{d\sigma}{d\Omega} = \frac{d\sigma(\theta,\phi)}{d\Omega}$$

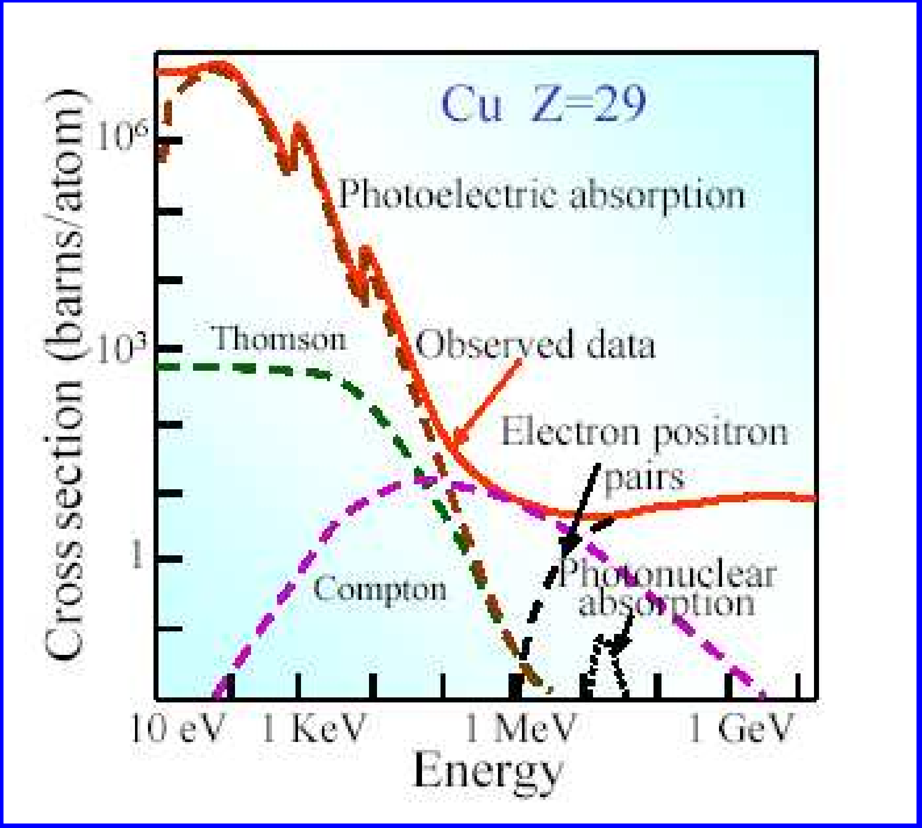
$$\sigma_{scatt} = \int \frac{d\sigma(\theta,\phi)}{d\Omega} d\Omega$$

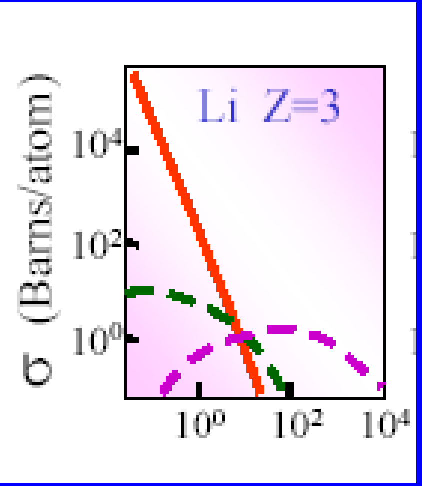
Double Differential Cross Section $d^2\sigma/d\Omega dE$

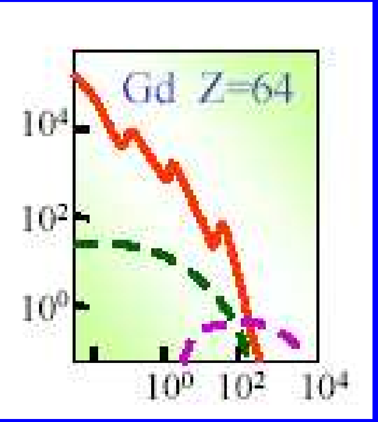


$$\frac{d^2\dot{N}_{events}}{d\Omega dE} = \dot{N}_{photons} \times [\rho dx] \times \left(\frac{d^2\sigma}{d\Omega dE}\right)$$

Total cross section σ of atoms

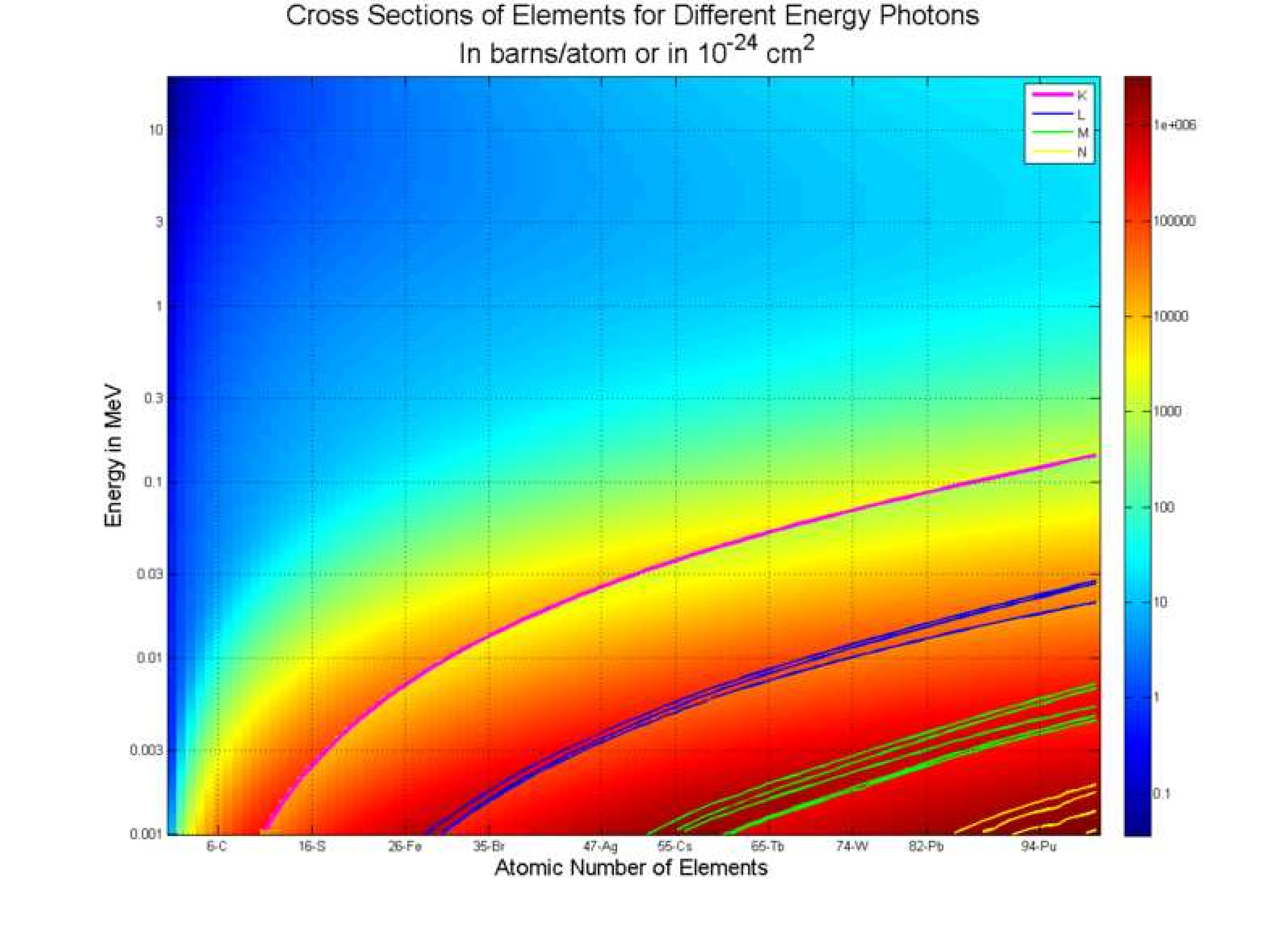




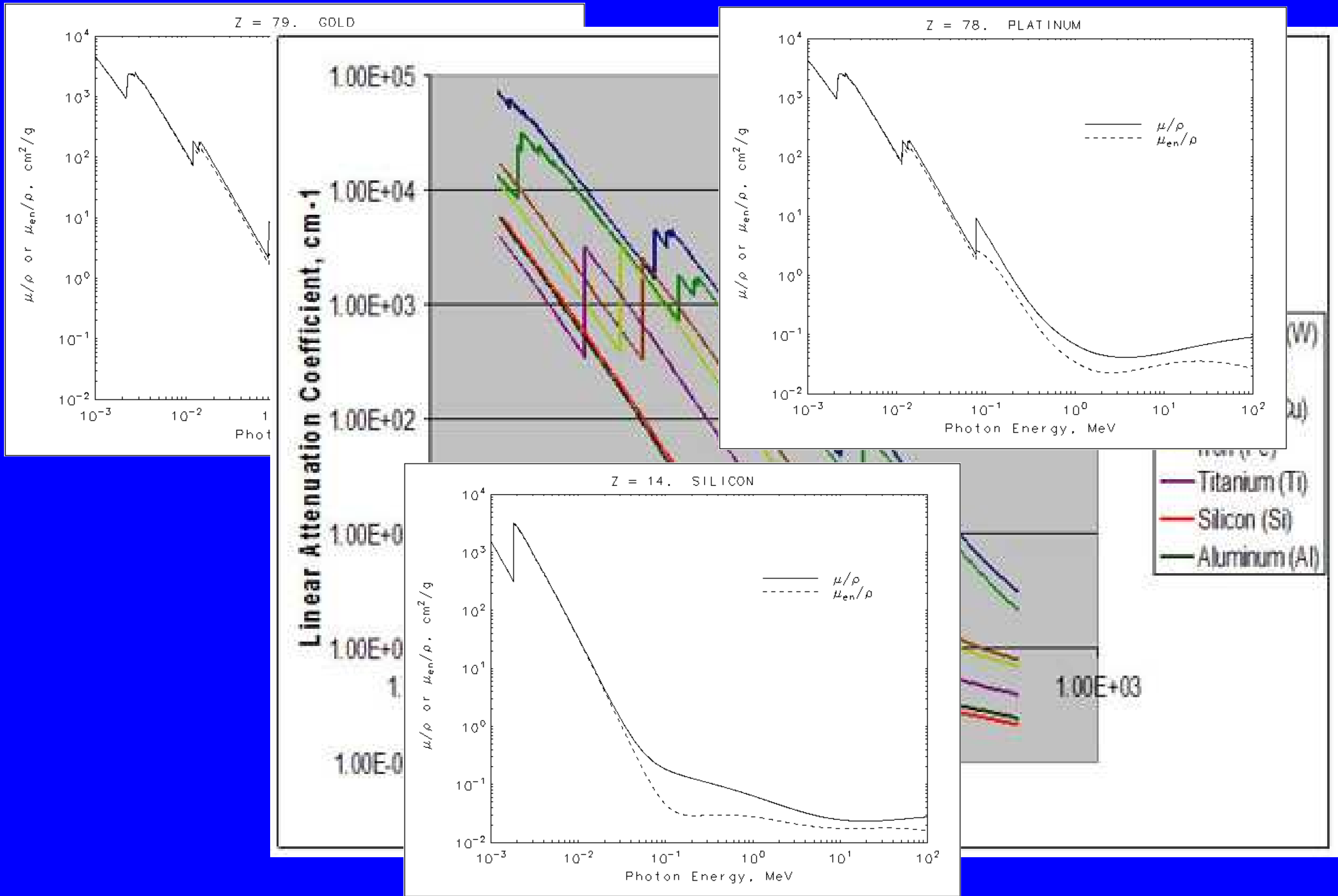


1 Barn = 10^{-24} cm^2

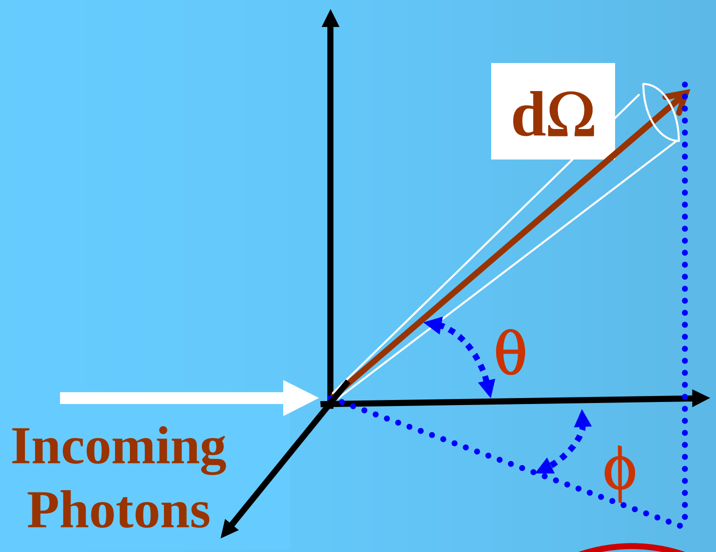
Absorption cross section σ of atoms



Absorption cross section σ of atoms



Cross section & Probability



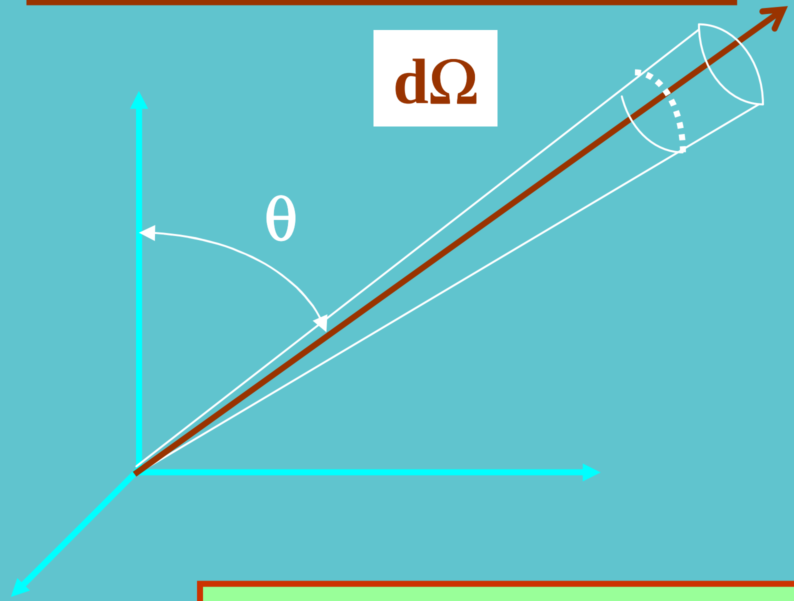
$$\frac{d\dot{N}_{photons}}{\dot{N}_{photons}} = \left(\frac{d\sigma}{d\Omega}\right) d\Omega \times \left(\rho dx \right)$$

Probability

Cross Sections: Classical definition

$$\frac{d\dot{N}_{sc.}}{\dot{N}_{in}} = \left(\frac{d\sigma}{d\Omega}\right) d\Omega \times (\rho dx)$$

$$\frac{dI}{d\Omega} = I_0 \times \left(\frac{d\sigma}{d\Omega}\right) \times (\rho dx)$$



Differential cross section:
it is the differential power scattered in dΩ normalized to the incoming power and to the scattering objects

σ is the intensity lost for absorption normalized to the incoming power and to the absorption object

$$\frac{dI}{I_{in}} = -\sigma \rho dx$$

Matter ←Interaction→ Radiation I

Classical approach

Radiation:

Electromagnetic waves described by Maxwell equations

Matter:

Macroscopic optical constants

Deeper:

microscopic description of the matter as an ensemble of classical oscillator

Classical Approach

•Radiation: Electromagnetic wave composed of E and B

•Matter: Optical constant

Refraction index: $n(\lambda)$

Absorption coefficient: $\mu(\lambda)$

Interaction: Lorentz force $\vec{F} = q\left(\vec{E} + \vec{v} \times \vec{B}\right)$

Measurement: gives $n(\lambda)$ and $\mu(\lambda)$

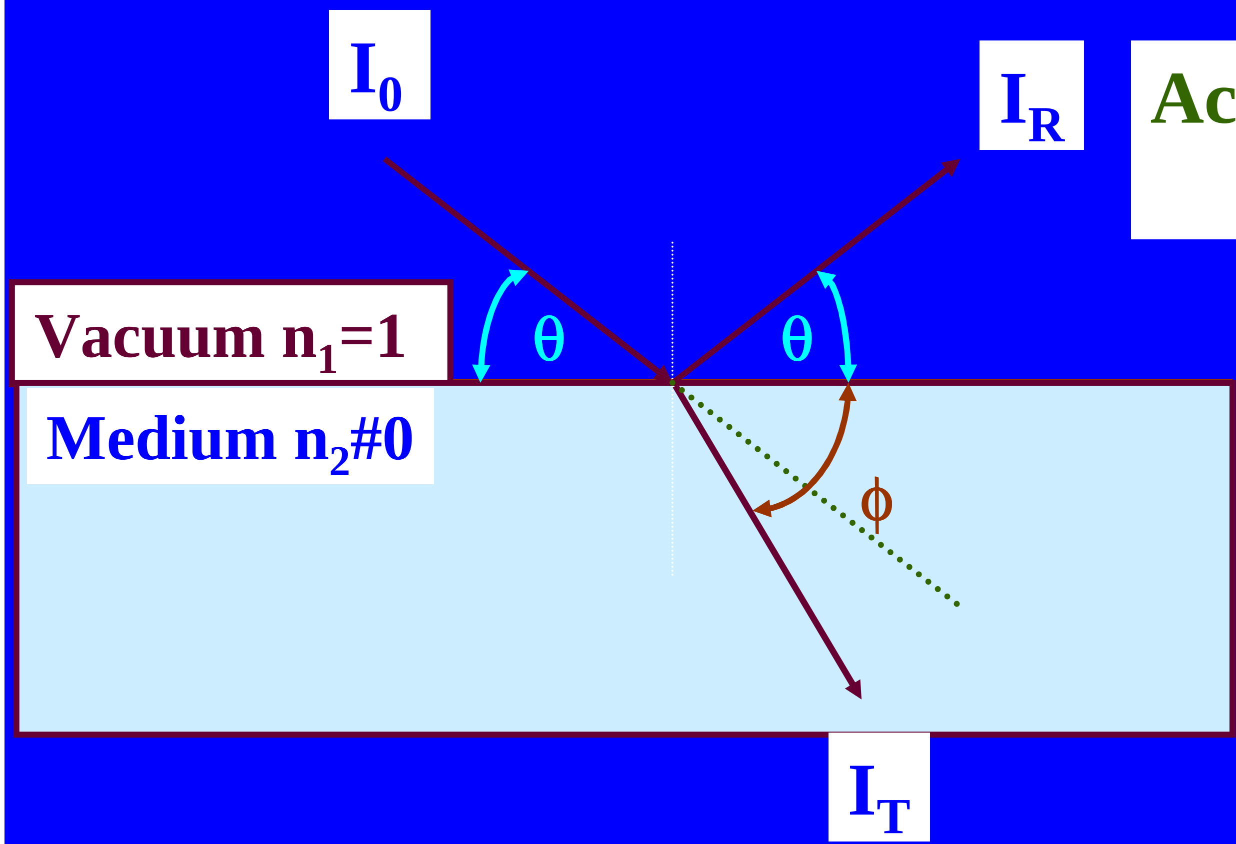
Microscopic model of the charge in motion ➔ $n(\lambda)$ and $\mu(\lambda)$

Reflection and refraction

n_i is the index of refraction

Snell law of refraction

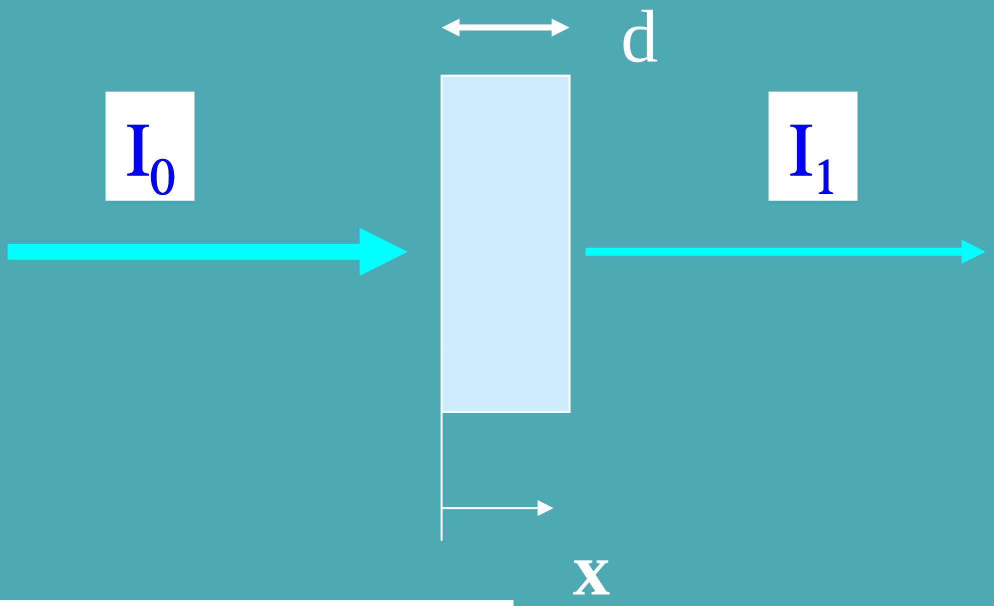
$n_1\cos(\theta)=n_2\cos(\phi)$



According to Newton n_i is ~ to $1/v$

$$R_{\theta\approx\pi/2}=\frac{I_R}{I_0}=\frac{\left|n_2-n_1\right|^2}{\left|n_2+n_1\right|^2}$$

Absorption coefficient



$$I(x) = I_0 e^{-\mu x}$$

$$I_1 = I_0 e^{-\mu d}$$

$$\mu = \frac{1}{d} \ln \frac{I_0}{I_1} = \rho\ \sigma_{tot}$$

Plane Wave in vacuum

$$\vec{E} = \vec{E}_0 e^{i\vec{k}\vec{r}-\omega t}$$

$$\vec{B} = \vec{B}_0 e^{i\vec{k}\vec{r}-\omega t}$$

$\vec{k}$ is the wavevector; it gives
- the direction of the propagation
- the wavelength of the radiation

$$\left|\vec{k}\right| = \frac{2\pi}{\lambda_0}$$

$$\vec{k} = \frac{2\pi}{\lambda_0}\hat{k} = \frac{\omega}{c}\hat{k}$$

The radiation moves with a speed equal to c

$$c = \frac{1}{\sqrt{\mu_0 \varepsilon_0}}$$

Associated to the radiation there is an energy density w equal to:

$$w = \frac{1}{2}\varepsilon_0 E_0^2$$

The intensity I of the beam is equal to I= wc= $c \times \frac{1}{2}\varepsilon_0 E_0^2$

Plane Wave in matter

$$\vec{E} = \vec{E}_0 e^{i\vec{k}\vec{r}-\omega t}$$

$$\vec{B} = \vec{B}_0 e^{i\vec{k}\vec{r}-\omega t}$$

$\vec{k}$ is the wavevector

$$\left|\vec{k}\right| = \frac{2\pi}{\lambda}$$

$$\nabla^2\vec{E} - \mu\varepsilon\frac{\partial^2\vec{E}}{\partial t^2}$$

$$v = \frac{1}{\sqrt{\mu\ \varepsilon}} = \frac{1}{\sqrt{\mu_0\mu_r\varepsilon_0\varepsilon_r}} = \frac{c}{\sqrt{\mu_r\varepsilon_r}} = \frac{c}{n}$$

Dispersion relation:

$$k^2 - \mu\varepsilon\omega^2 = 0 \Rightarrow k^2 - \frac{1}{v^2}\omega^2 = 0 \Rightarrow \frac{2\pi}{\lambda^2} - \frac{\omega^2}{v^2} = 0$$

$$\lambda\omega = 2\pi v$$

E.M. Waves in matter

$n=(\varepsilon_r \mu_r)^{1/2}$
refraction index

$$|\vec{v}| = \frac{1}{\sqrt{\mu_0 \mu_r \varepsilon_0 \varepsilon_r}} = \frac{c}{\sqrt{\mu_r \varepsilon_r}} = \frac{c}{n}$$

Non magnetic medium: $\mu_r = 1$
Generally: $\varepsilon_r > 1 \rightarrow n > 1$

$$|\vec{v}| = \frac{c}{n} < c$$

In the matter the light is slower than in the vacuum

$$\lambda = \frac{\lambda_0}{n}$$

In the matter the wavelength is shorter than in the vacuum

$$|\vec{k}| = \frac{2\pi}{\lambda_0} \times n$$

Origin of the dielectric function (qualitative)

The electric field of the radiation cause a motion of the microscopic charges

Electrons and nuclei moves in opposite directions giving rise to fluctuating microscopic electric dipoles

Dipoles generate additional electric fields that adds to the radiation ones

The dielectric function describe the relation between the e.m. field and the induced dipoles: it is a complex quantity

Real part → amplitude relation

Imaginary part → phase relation

Complex dielectric function

$$\varepsilon = \varepsilon_0 \varepsilon_r = \varepsilon_0 (\varepsilon_1 + i\varepsilon_2)$$

$n^2 = \varepsilon_r = \varepsilon_1 + i\varepsilon_2$ → n is complex $n = n_r + i\beta$

$$n_r = \left[\frac{\varepsilon_1 + \left(\varepsilon_1^2 + \varepsilon_2^2\right)^{1/2}}{2} \right]^{1/2} \cong \sqrt{\varepsilon_1}$$

$$\beta = \left[\frac{-\varepsilon_1 + \left(\varepsilon_1^2 + \varepsilon_2^2\right)^{1/2}}{2} \right]^{1/2} \cong \frac{1}{2} \frac{\varepsilon_2}{n_r}$$

Complex wavevector

$$\vec{k} = \frac{2\pi}{\lambda}\hat{k} = \frac{2\pi}{\lambda_0}n\hat{k} = \frac{\omega}{c}n\hat{k} \quad \text{is complex}$$

$$\vec{k} = \vec{k}_r + i\vec{k}_i = (k_r + ik_i)\,\hat{k}$$

$$\vec{k}_r = \frac{\omega n_r}{c}\hat{k}$$

$$\vec{k}_i = \frac{\omega\beta}{c}\hat{k}$$

$$\vec{k} = (k_r + ik_i)\,\hat{k} = \frac{\omega}{c}(n_r + i\beta)\hat{k} = \frac{\omega n}{c}\hat{k}$$

Wave-damping: Absorption coefficient

$$\vec{k} = \vec{k}_r + i\vec{k}_i = \frac{\omega}{c}(n_r + i\beta)\,\hat{k}$$

$$\vec{E} = \vec{E}_0 e^{i(\vec{k}\vec{r}-\omega t)} = \vec{E}_0 e^{i(\vec{k}_r\vec{r}-\omega t)} e^{-\vec{k}_i\vec{r}}$$

Standard plane wave as in vacuum with $\lambda = \lambda_0 / n$

Amplitude reduction

$$\vec{k}_i = \frac{\omega\beta}{c}\hat{k}$$

Intensity $I \propto E^2$

Absorption coefficient μ

$$I(r) = I_0 e^{-2\vec{k}_i\vec{r}} = I_0 e^{-\mu x}$$

$$\mu = 2k_i = \frac{2\omega\beta}{c} \cong \frac{\omega\varepsilon_2}{2c}$$

Kramers-Kronig Relation

The real and imaginary parts of the dielectric function depend one on the other

$$\varepsilon_1(\omega) - 1 = \frac{2}{\pi}\int_0^{\infty} \frac{\overline{\omega}\,\varepsilon_2(\overline{\omega})}{\overline{\omega}^2 - \omega^2}\, d\overline{\omega}$$

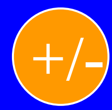
$$\varepsilon_2(\omega) = \frac{2\omega}{\pi}\int_0^{\infty} \frac{\varepsilon_1(\overline{\omega}) - 1}{\overline{\omega}^2 - \omega^2}\, d\overline{\omega}$$

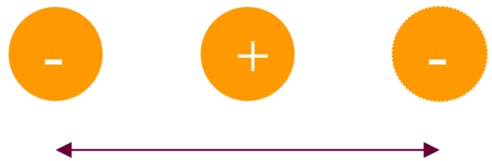
Causality: the dipole moment P(t) at time t is determined only by the values of the electric field at time t'≤ t

Microscopic model

The matter is composed of positive and negative charges

At equilibrium the positive and negative charges do not give rise to any dipole moment





Oscillating negative charge
Damped oscillator

$$\frac{d^2\vec{r}}{dt^2} + \gamma \frac{d\vec{r}}{dt} + \omega_0^2 \vec{r} = \frac{e}{m} E_0 e^{i\omega t}$$

Induced dipole moment

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

In stationary condition

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

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

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

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

Dielectric function

$\vec{P} = \varepsilon_0 \chi \vec{E}$

$\varepsilon_r = 1 + \chi$

N = number of atoms per unit volume

$$\vec{P}(t) = N\vec{p} = \frac{NZe^2\vec{E}_0}{m}\frac{1}{\left(-\omega^2 + i\gamma\omega + \omega_0^2\right)}e^{i\omega t}$$

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

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

Real and imaginary part of the dielectric function

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

$$\varepsilon_1 = 1 + \frac{NZe^2}{\varepsilon_0 m} \frac{\omega_0^2 - \omega^2}{\left(\omega_0^2 - \omega^2\right)^2 + \left(\gamma\omega\right)^2}$$

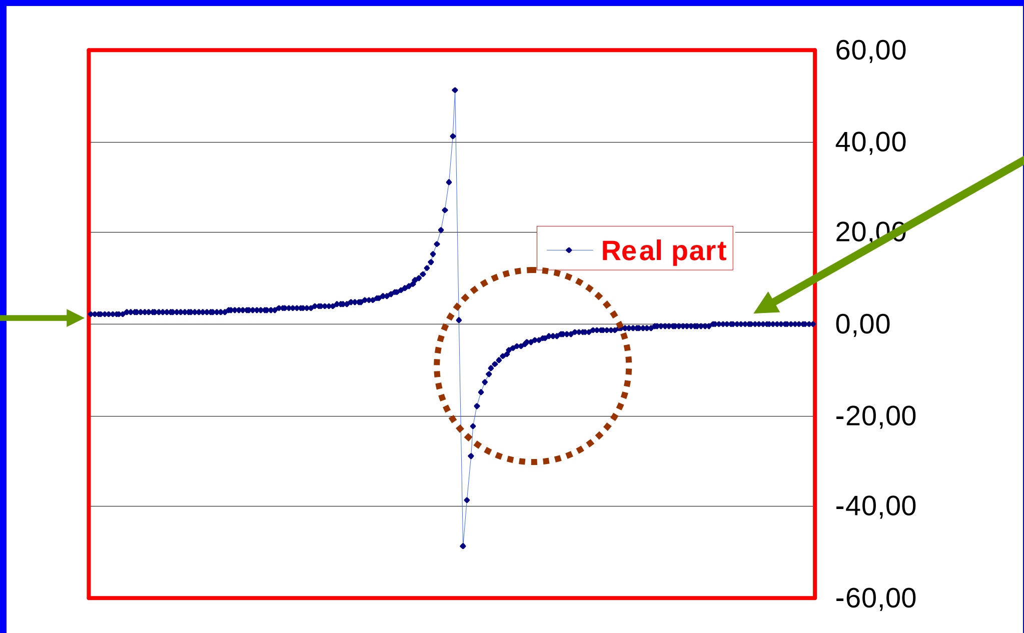
$$\varepsilon_2 = \frac{NZe^2}{\varepsilon_0 m} \frac{\gamma\omega}{\left(\omega_0^2 - \omega^2\right)^2 + \left(\gamma\omega\right)^2}$$

General behavior of the real part of the dielectric function

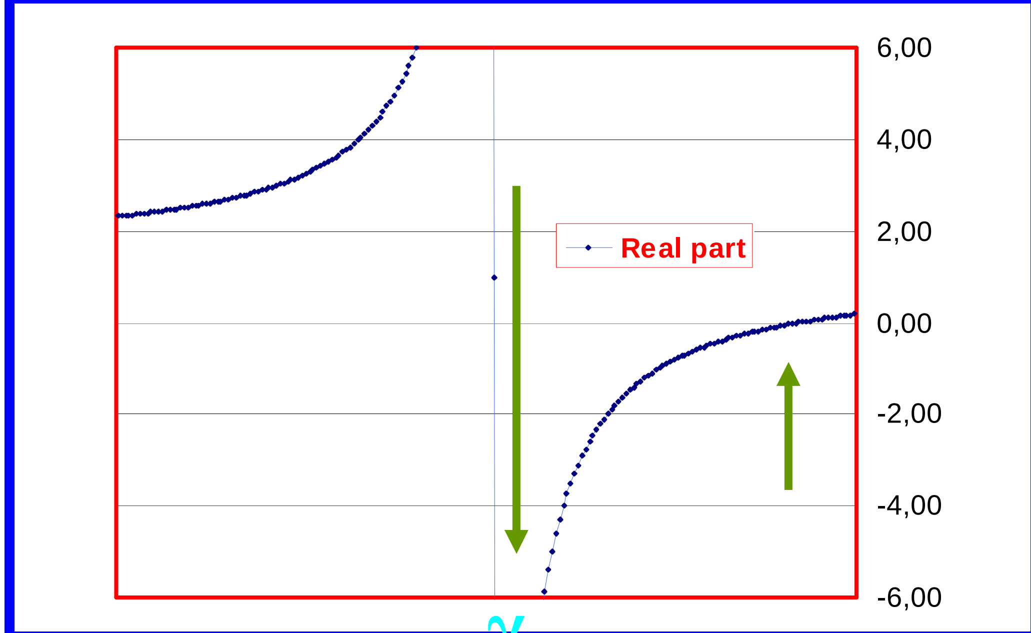
$$\varepsilon_1 = 1 + \frac{NZe^2}{\varepsilon_0 m} \frac{\omega_0^2 - \omega^2}{\left(\omega_0^2 - \omega^2\right)^2 + (\gamma\omega)^2}$$

$$\varepsilon_1(0) = 1 + \frac{NZe^2}{\varepsilon_0 m \omega_0^2}$$

$$\varepsilon_2(\omega >> \omega_0) = 1 - \frac{NZe^2}{\varepsilon_0 m \omega^2}$$



Behavior of the real part above ω_0



$\varepsilon_1 < 0$
$\varepsilon_2 = 0$

$\beta = 0$

$$n_r = \sqrt{\varepsilon_r} = i\sqrt{|\varepsilon_r|}$$

$$\vec{k} = i\frac{\omega|n_r|}{c}\hat{k}$$

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

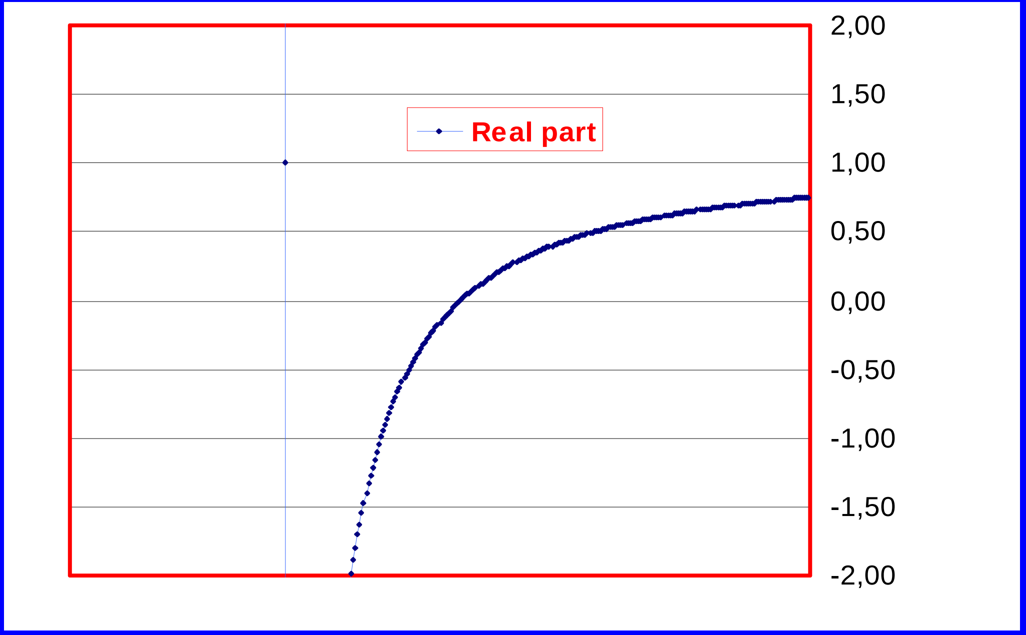
There is no propagation into the matter
no energy exchange

$$\frac{1}{|k|} = \frac{c}{\omega|n_r|}$$

is called "extinction length"

Behavior of the real part at high energy

$$\varepsilon_1(\omega >> \omega_0) = 1 - \frac{N\mathbf{Ze}^2}{\varepsilon_0 \mathbf{m}\boldsymbol{\omega}^2}$$



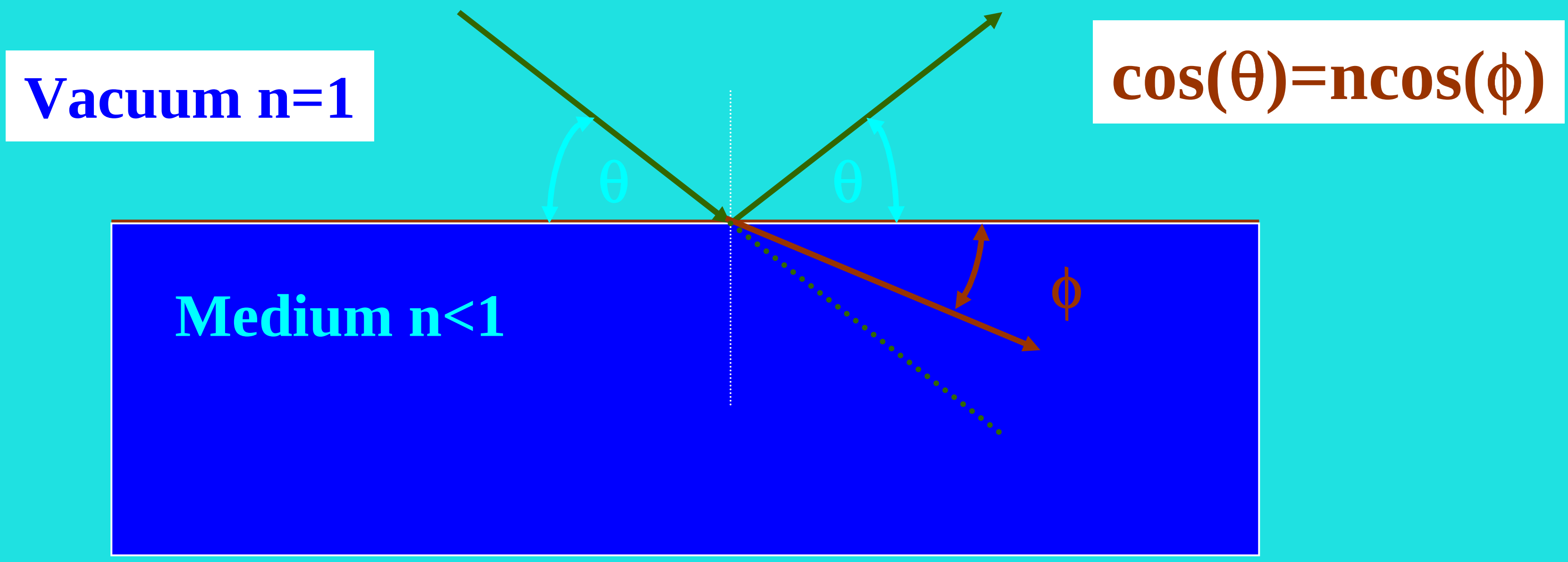
$$\varepsilon_1(\omega >> \omega_0) < 1$$

Refraction index at high energy

$$n_r = \sqrt{1 - \frac{NZe^2}{\varepsilon_0 m \omega^2}} \cong 1 - \frac{1}{2}\frac{NZe^2}{\varepsilon_0 m \omega^2} = 1 - \delta$$

$$\delta = \frac{1}{2}\frac{NZe^2}{\varepsilon_0 m \omega^2} \cong 10^{-5} - 10^{-6}$$

Total Reflection



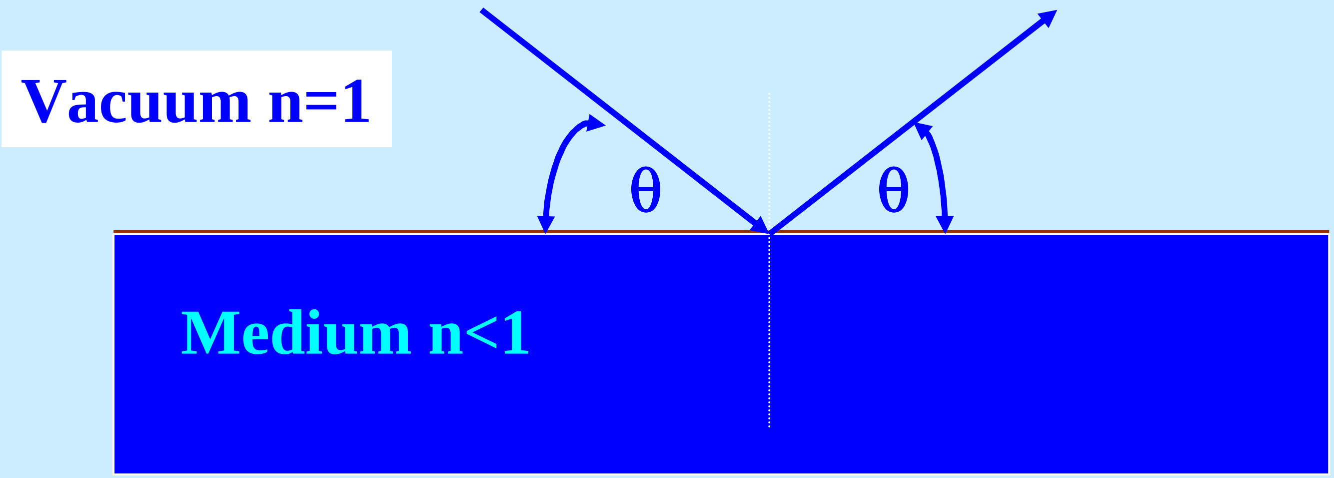
The critical angle θ_c is defined by cos(ϕ)=1

→

$\cos(\theta_c)=n$

$$1-\frac{\theta_c^2}{2}=n=1-\delta \Rightarrow \theta_c=\sqrt{2\delta}\cong \text{few } 10^{-3}$$

Use of Total Reflection

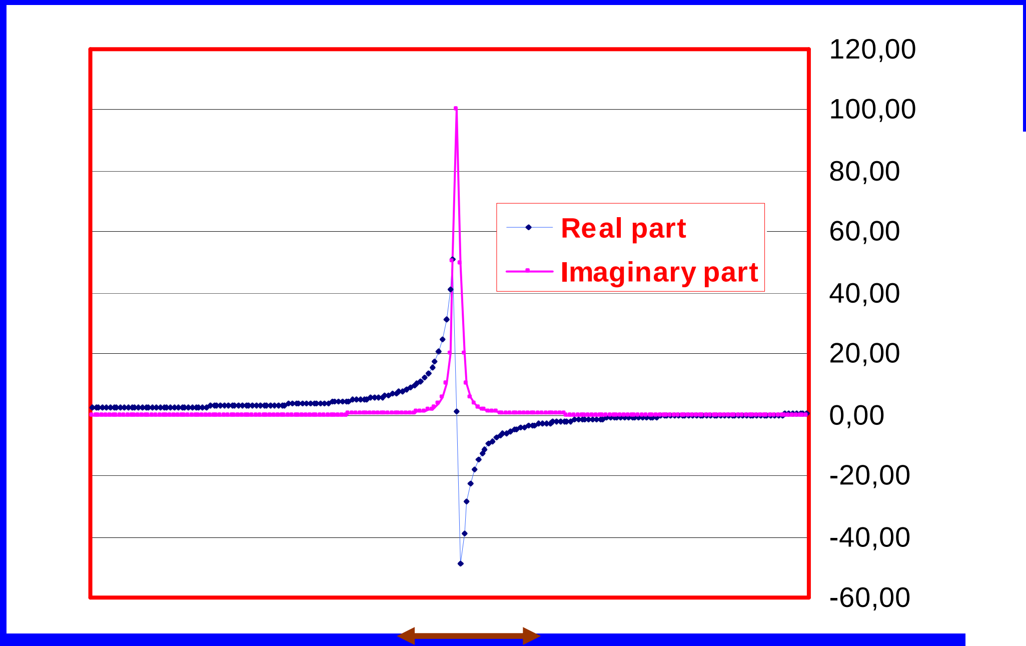


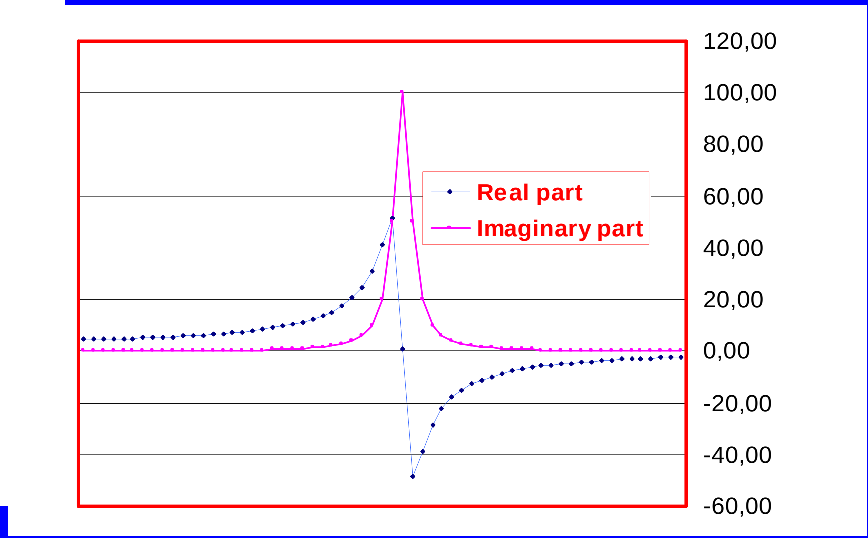
$$\theta_c = \sqrt{2\delta} \cong \textbf{few } 10^{-3}$$

- X-ray Mirrors
- Surface Diffraction
- REFLEXAFS

Behavior of the imaginary part

$$\varepsilon_2 = \frac{NZe^2}{\varepsilon_0 m} \frac{\gamma\omega}{(\omega_0^2 - \omega^2)^2 + (\gamma\omega)^2}$$

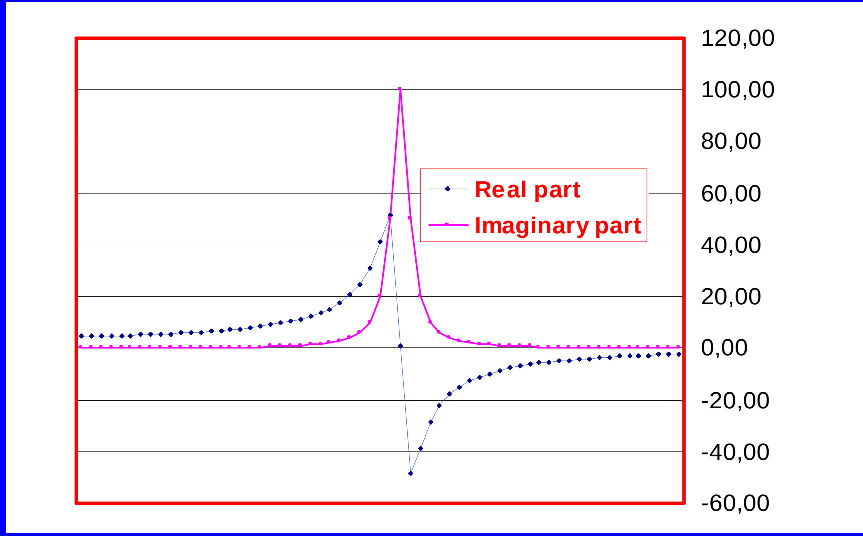


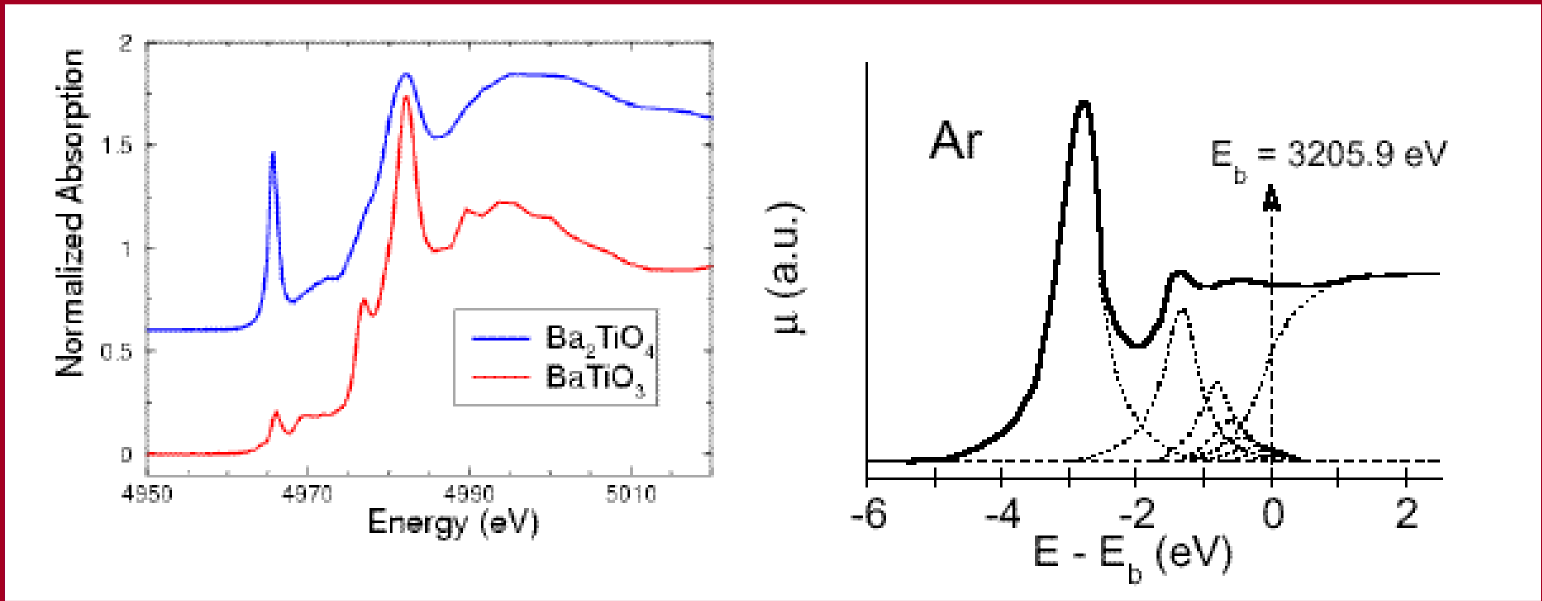


Absorption coefficient

$$\mu = 2k_i = \frac{2\omega\beta}{c} \cong \frac{\omega\varepsilon_2}{2c}$$

$$I(r) = I_0 e^{-2\vec{k}_i \cdot \vec{r}} = I_0 e^{-\mu x}$$

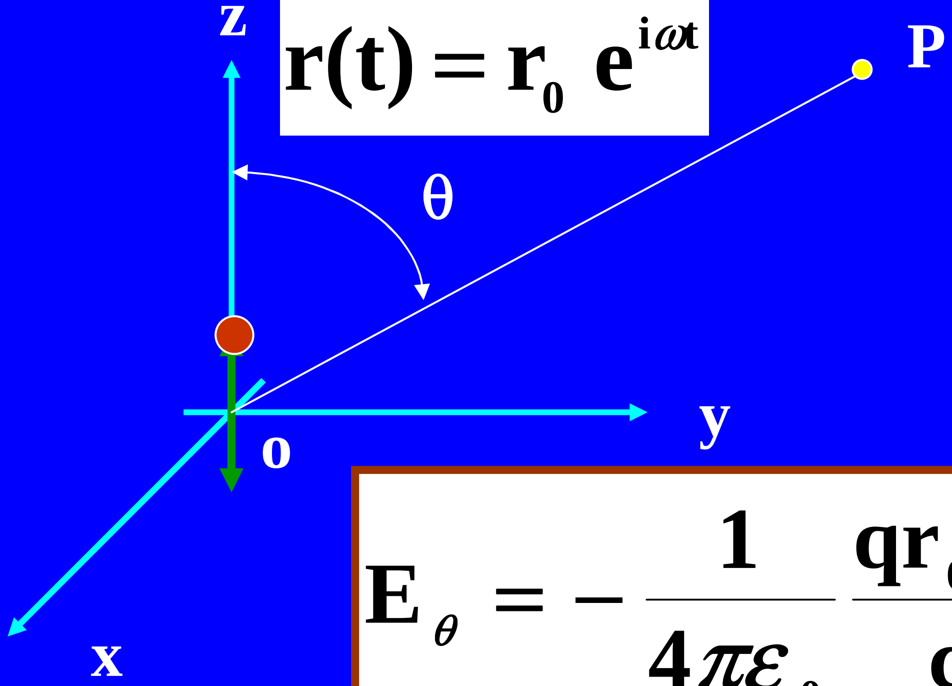




Scattering

Electric field generated by an oscillating point electric charge q
The charge is oscillating under the action of the electric field of the incoming radiation

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



$$E_\theta = -\frac{1}{4\pi\varepsilon_0}\,\frac{q r_0 \omega^2}{c^2}\,\frac{e^{i\left(\vec{k}_{out}\vec{r} - \omega t\right)}}{|\mathbf{r}|}\sin\theta$$

The electric field is in the plane (OzP)

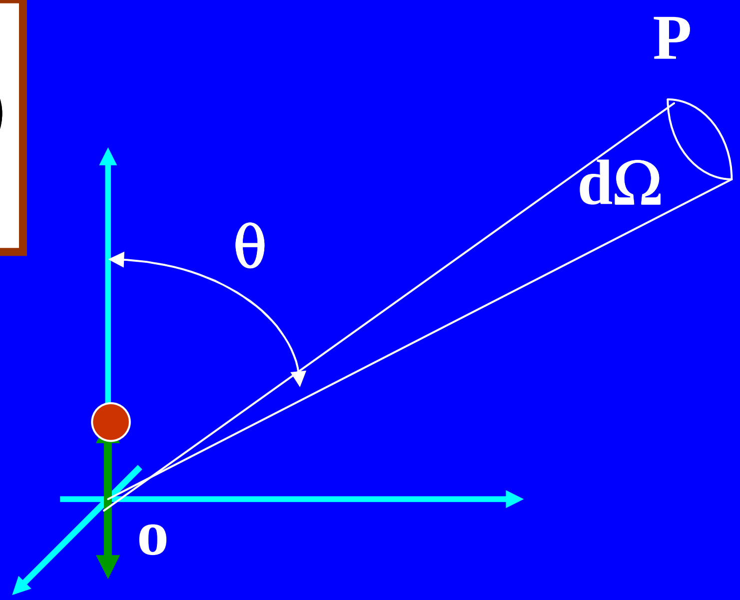
Scattering by a free electron

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

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

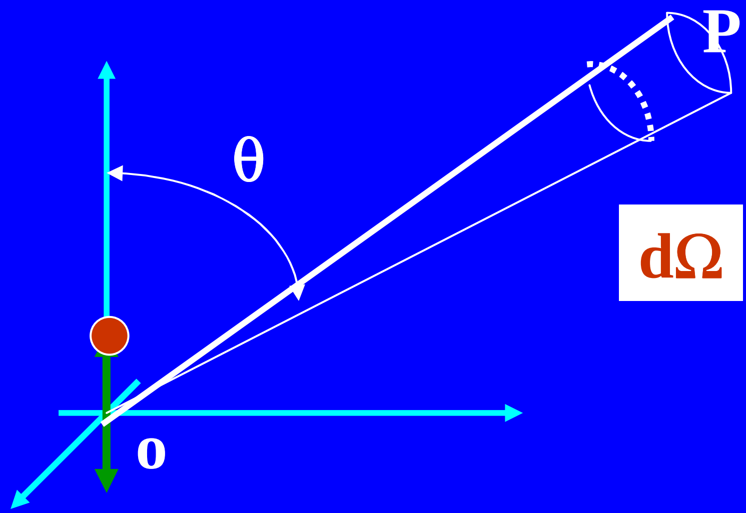
$$\vec{r}_0 = -\frac{e}{m\omega^2}\vec{E}_0$$

$$E_\theta = \frac{1}{4\pi\varepsilon_0}\frac{e^2 E_0}{mc^2}\frac{e^{i\left(\vec{k}_{out}\vec{r}-\omega t\right)}}{|r|}\sin\theta$$



Differential cross section

Differential cross section (normalized differential scattered power)



$$I = \frac{dW}{dS} = \left(\frac{1}{2}\varepsilon_0 E^2\right) c\,dS$$

$$dW = I_\theta c\,dS = \left(\frac{1}{2}\varepsilon_0 E_\theta^2\right) c\,r^2 d\Omega = \frac{1}{2}\frac{cE_0^2}{(4\pi)^2\varepsilon_0}\left(\frac{e^2}{mc^2}\right)^2 \sin^2\theta\, d\Omega$$

$$\frac{d\sigma}{d\Omega} = \frac{1}{I_0}\frac{dW}{d\Omega} = \frac{1}{\frac{1}{2}\varepsilon_0 c E_0^2}\frac{dW}{d\Omega} = \left(\frac{1}{4\pi\varepsilon_0}\frac{e^2}{mc^2}\right)^2 \sin^2\theta$$

Electron classical radius

Electron classical radius

$$\frac{d\sigma}{d\Omega} = \left(\frac{1}{4\pi\varepsilon_0}\frac{e^2}{mc^2}\right)^2 \sin^2\theta = r_e^2 \sin^2\theta$$

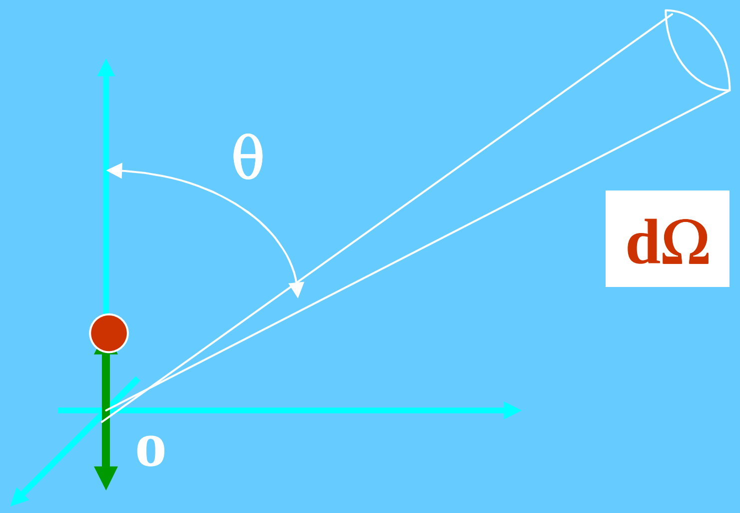
r_e is called the electron classical radius=2.818 10^{-15} m

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

In Gauss system $$r_e = \frac{e^2}{mc^2}$$

Total scattering cross section: polarized radiation

$$\sigma = \int \frac{d\sigma}{d\Omega} = \int r_e^2 \sin^2\theta d\Omega$$



Linear Polarization

$$\sigma = \int r_e^2 \sin^2\theta d\Omega = r_e^2 \int_0^{\pi} \sin^2\theta\, 2\pi \sin\theta d\theta =$$

$$= r_e^2\, 2\pi \int_0^{\pi} \sin^3\theta d\theta = \frac{8\pi}{3} r_e^2 = 6.7\text{x}10^{-29}\, m^2 / \text{electron}$$

Thomson cross section

Scattering Plane

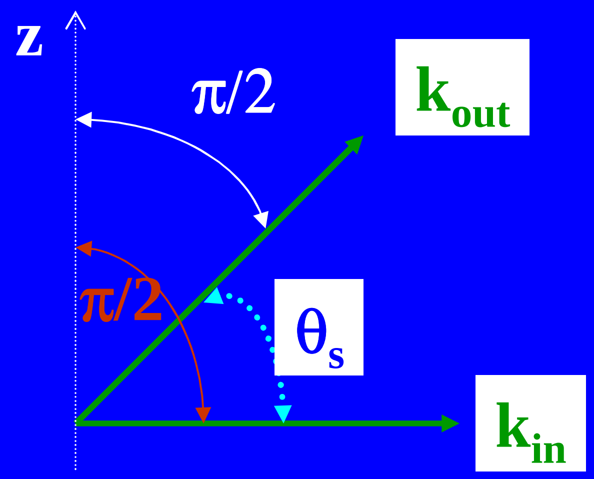
The plane formed by the direction of the incoming and outcoming radiation is called is scattering angle

It is the plane formed by k_{in} and k_{out}

The angle θ_s is called the scattering angle

(Sometimes the scattering angle is indicated with 2 θ_s

Incoming Radiation polarized perpendicular to the Scattering Plane



Incoming radiation polarized perpendicular to the scattering plane π_s

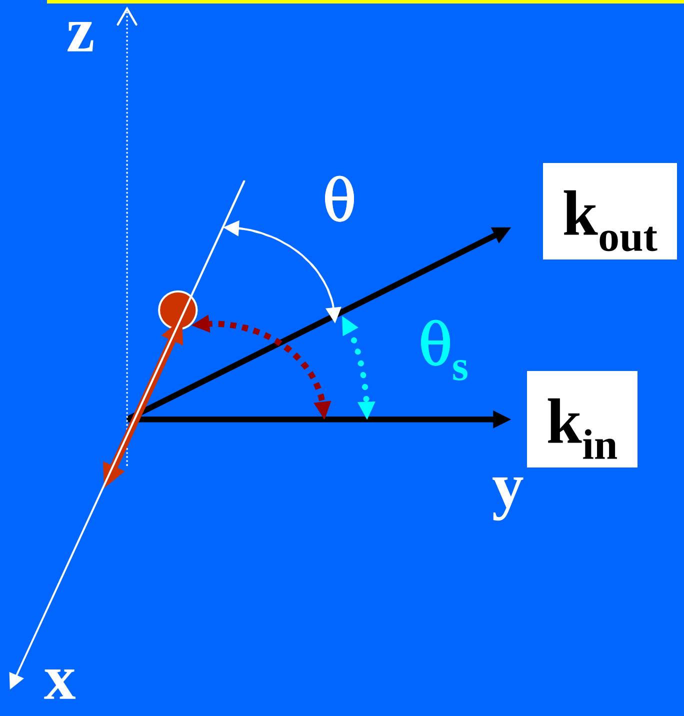
$\rightarrow \theta = \pi/2 \rightarrow \sin\theta = 1$

Scattering radiation perpendicular to the scattering plane

$$\left(\hat{\mathbf{e}}_{in} \bullet \hat{\mathbf{e}}_{out}\right) = 1 = \sin\theta$$

$$\frac{d\sigma}{d\Omega} = \sin^2\theta \; r_e^2 = r_e^2 = \left(\hat{\mathbf{e}}_{in} \bullet \hat{\mathbf{e}}_{out}\right)^2 r_e^2$$

Incoming radiation polarized in the Scattering Plane



Incoming radiation polarized in the scattering plane π_s
It is also perpendicular to k_{in}

Scattering radiation is polarized in the scattering plane

$$\theta + \theta_s = \frac{\pi}{2}$$

$$\left(\hat{e}_{in} \bullet \hat{e}_{out}\right) = \left(\hat{k}_{in} \bullet \hat{k}_{out}\right) = \cos\theta_s = \sin\theta$$

$$\frac{d\sigma}{d\Omega} = \left(\hat{e}_{in} \bullet \hat{e}_{out}\right)^2 r_e^2$$

Differential scattering cross section for un-polarized radiation

At any θ the radiation can be decomposed into two component of equal intensity

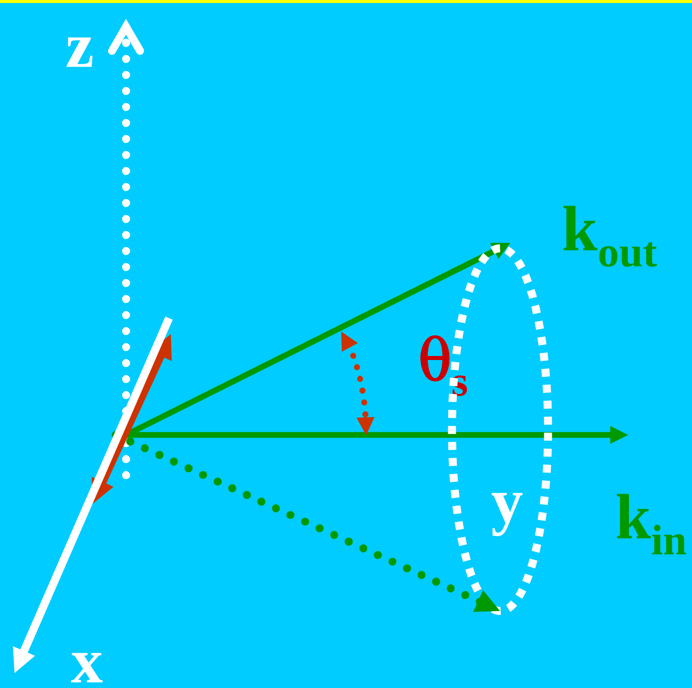
- The first one is polarized perpendicular to the scattering plane
- The second one is polarized in the scattering plane

$$\frac{d\sigma}{d\Omega} = \frac{1}{2}\left[\left(\hat{e}_{in} \bullet \hat{e}_{out}\right)^2\right]_{\perp} r_e^2 + \frac{1}{2}\left[\left(\hat{e}_{in} \bullet \hat{e}_{out}\right)^2\right]_{//} r_e^2$$

$$\frac{d\sigma}{d\Omega} = r_e^2 \frac{1 + \cos^2\theta_s}{2}$$

Total scattering cross section for un-polarized radiation

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \int r_e^2 \frac{1 + \cos^2\theta_s}{2} d\Omega$$



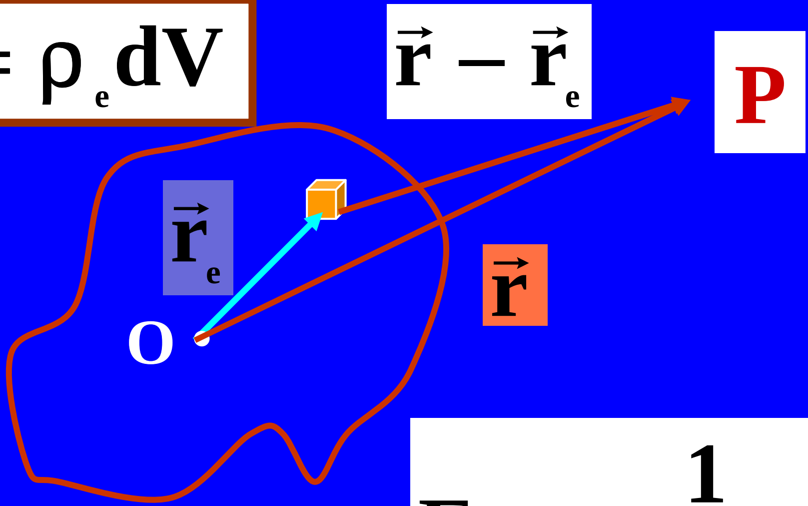
$$\sigma = \frac{1}{2} 4\pi r_e^2 + \frac{r_e^2}{2} \int \cos^2\theta_s \sin\theta_s d\Omega = 2\pi r_e^2 + \frac{2\pi}{3} r_e^2 =$$

$$\frac{8\pi}{3} r_e^2 = 6.7x10^{-29} m^2 / \text{electron}$$

Thompson cross section

Charge distributions: Scattering Factor

$$dN_e = \rho_e dV$$



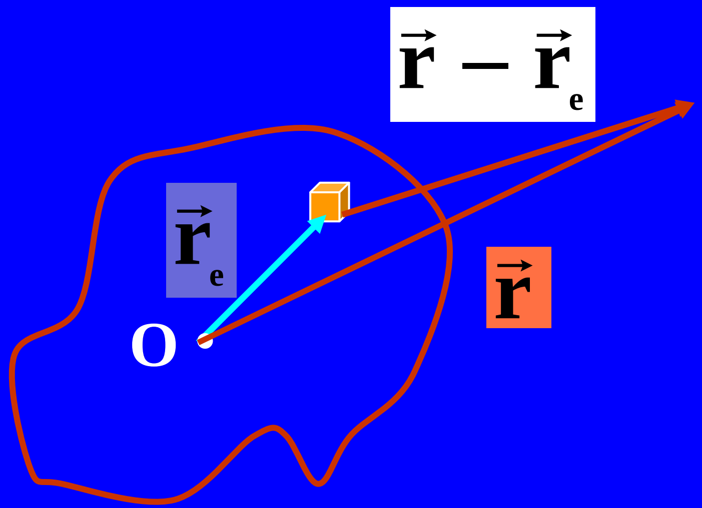
$$E_{in} = E_0 e^{i\left(\vec{k}_{in}\vec{r} - \omega t\right)}$$

$$E_\theta = \frac{1}{4\pi\varepsilon_0}\frac{e^2 E_0}{mc^2}\frac{e^{i\left(\vec{k}_{out}\vec{r} - \omega t\right)}}{|\vec{r}|}\left(\hat{e}_{in} \bullet \hat{e}_{out}\right)$$

$$\left|\vec{r} - \vec{r}_e\right|$$

$$dE_\theta = \frac{1}{4\pi\varepsilon_0}\frac{e^2 E_0 e^{i\vec{k}_{in}\vec{r}_e}}{mc^2}\frac{e^{i\left(\vec{k}_{out}(\vec{r} - \vec{r}_e) - \omega t\right)}}{\left|\vec{r} - \vec{r}_e\right|}\left(\hat{e}_{in} \bullet \hat{e}_{out}\right)\rho_e dV$$

Scattering Factor II

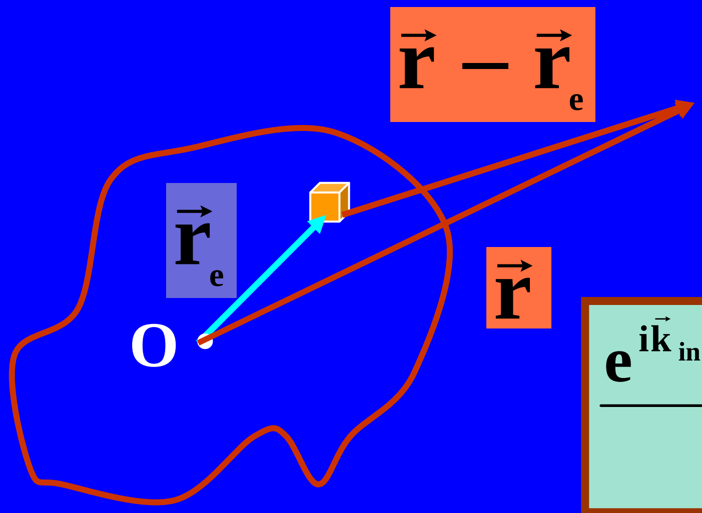


$$dE_\theta = \frac{1}{4\pi\varepsilon_0}\frac{e^2 E_0 e^{i\vec{k}_{in}\vec{r}_e}}{mc^2}\frac{e^{i\left(\vec{k}_{out}(\vec{r}-\vec{r}_e)-\omega t\right)}}{\left|\vec{r}-\vec{r}_e\right|}\left(\hat{e}_{in}\bullet\hat{e}_{out}\right)\rho_e dV$$

$$dE_\theta = \frac{1}{4\pi\varepsilon_0}\frac{e^2 E_0}{mc^2}\left(\hat{e}_{in}\bullet\hat{e}_{out}\right)\frac{e^{i\vec{k}_{in}\vec{r}_e}e^{i\left(\vec{k}_{out}(\vec{r}-\vec{r}_e)-\omega t\right)}}{\left|\vec{r}-\vec{r}_e\right|}\rho_e dV$$

$$\frac{e^{i\left(\vec{k}_{out}\vec{r}-\omega t\right)}}{\left|\vec{r}\right|}$$

Scattering Factor III



$$|\vec{r} - \vec{r}_e| \gg |\vec{r}_e|$$

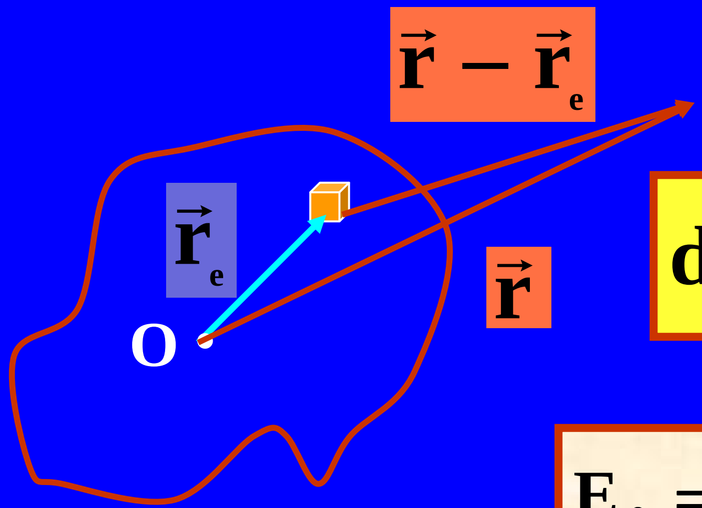
$$\frac{e^{i(\vec{k}_{out}\vec{r} - \omega t)}}{|\vec{r}|}$$

$$\frac{e^{i\vec{k}_{in}\vec{r}_e}\, e^{i(\vec{k}_{out}(\vec{r}-\vec{r}_e) - \omega t)}}{|\vec{r} - \vec{r}_e|} \cong e^{-i(\vec{k}_{out} - \vec{k}_{in})\vec{r}_e}\, \frac{e^{i(\vec{k}_{out}\vec{r} - \omega t)}}{|\vec{r}|}$$

$$dE_\theta = \frac{1}{4\pi\varepsilon_0}\frac{e^2 E_0}{mc^2}\left(\hat{e}_{in} \bullet \hat{e}_{out}\right)\frac{e^{i(\vec{k}_{out}\vec{r} - \omega t)}}{|\vec{r}|}\, e^{-i(\vec{k}_{out} - \vec{k}_{in})\vec{r}_e}\, \rho_e dV$$

$$dE_\theta = E_{SinglePointElectron}\, e^{-i(\vec{k}_{out} - \vec{k}_{in})\vec{r}_e}\, \rho_e dV$$

Scattering Factor IV



$$dE_\theta = E_{Single}\, e^{-i\left(\vec{k}_{out} - \vec{k}_{in}\right)\vec{r}_e} \rho_e dV$$

$$E_\theta = \int dE_\theta = E_{Single} \int e^{-i\left(\vec{k}_{out} - \vec{k}_{in}\right)\vec{r}_e} \rho_e dV$$

$$\vec{q} = \vec{k}_{out} - \vec{k}_{in}$$

$$E_\theta = \int dE_\theta = E_{Single} \int e^{-i\vec{q}\vec{r}_e} \rho_e dV = E_{Single}\, f(\vec{q})$$

f is called the scattering factor
f is the Fourier Transform of the charge density (in e.u.)

Scattering Factor V

$$E_{\theta} = E_{\text{Single}}\, f(\vec{q})$$

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

f is called the scattering factor

$$f(\vec{q}) = \int e^{-i\vec{q}\vec{r}_e} \rho_e \, dV$$

Number of electrons per unit volume

Scattering amplitude ∝ to:
Fourier Transform of the charge density (in electron units)
For atoms, molecules, crystals …

$$\frac{d\sigma}{d\Omega} = r_e^2 \left(\hat{e}_{\text{in}} \bullet \hat{e}_{\text{out}}\right)^2 \left|f(\vec{q})\right|^2$$

→ **Phase Problem**

Scattering Factor of electrons

Single electron: quantum case

$$\rho_e = |\psi|^2$$

$$f(\vec{q}) = \int e^{-i\vec{q}\vec{r}_e} \rho_e \, dV$$

$$f(\vec{q}) = \int e^{-i\vec{q}\vec{r}_e} |\psi|^2 \, dV$$

Scattering Factor of atoms

Atomic case

$$\rho_e = \sum_j \left|\psi_j\right|^2$$

$$\rho_e(\vec{r}) = \rho_e(|\vec{r}|) \rightarrow f(\vec{q}) = f(|\vec{q}|) = f(q)$$

$$f(\vec{q}) = \int e^{-i\vec{q}\,\vec{r}} \rho \, dV =$$

$$\int e^{-iqr\cos\theta} \rho \, 2\pi \sin\theta \, r^2 \, d\vartheta \, dr =$$

$$\frac{2\pi}{iq} \int \left[e^{-iqr\cos\theta} \right]_0^\pi \rho \, r \, dr =$$

$$\frac{4\pi}{q} \int \sin(qr) \rho(r) \, r \, dr$$

Scattering Factor atoms

$$f(q) = \frac{4\pi}{q}\int \rho(r)\sin(qr)\ rdr$$

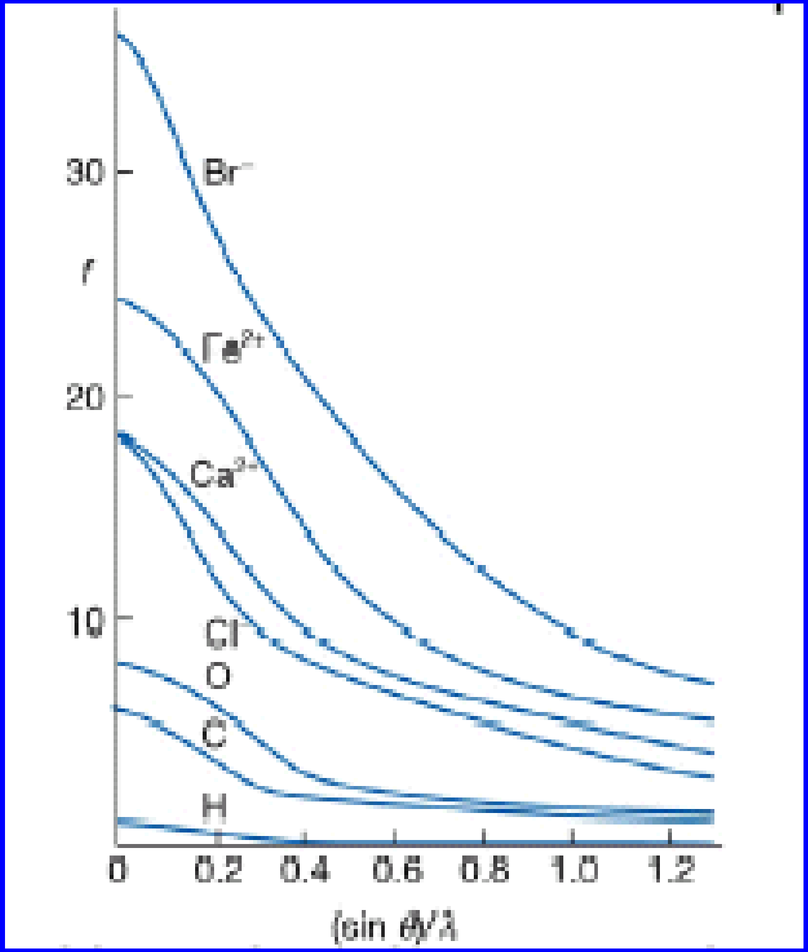
For small q $\sin(qr) \cong qr$

$$f(q) \cong \frac{4\pi}{q}\int \rho(r)\ (qr)\ rdr \cong 4\pi\int \rho(r)\ r^2 dr = Z$$

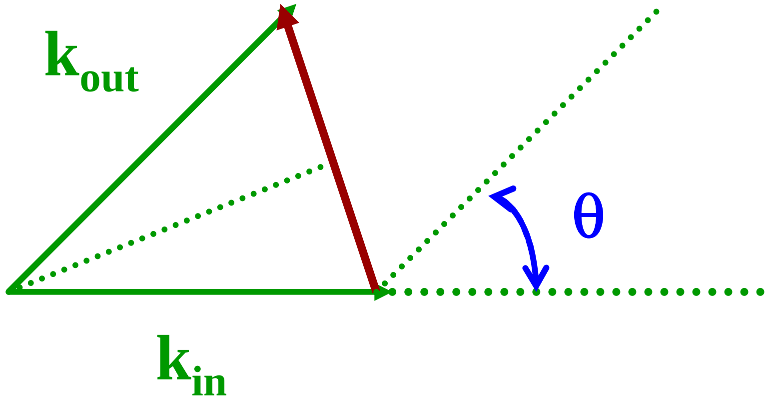
For high q because ρ(r) is a slowly decreasing function rρ(r) can be assumed as a constant in the integral →

$$f(q) \to 0$$

Behavior of the Atomic Scattering Factor

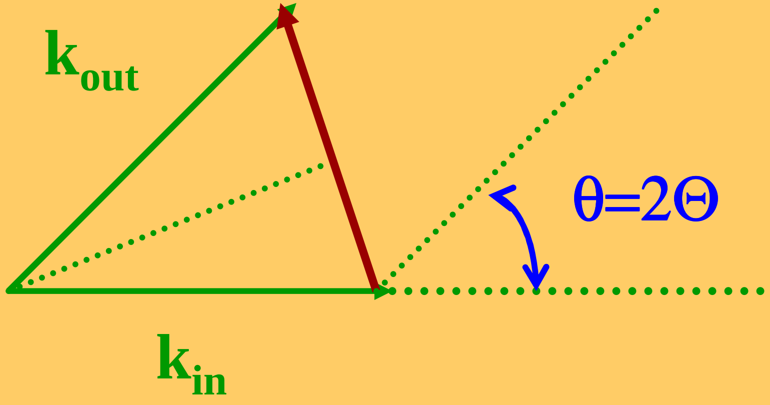


Scattering vector



$$\vec{q} = \vec{k}_{out} - \vec{k}_{in}$$

$$\left|\vec{q}\right| = 2\left|\vec{k}\right| \sin\frac{\theta}{2} = \frac{4\pi}{\lambda}\sin\frac{\theta}{2}$$



$$\vec{q} = \vec{k}_{out} - \vec{k}_{in}$$

$$\left|\vec{q}\right| = 2\left|\vec{k}\right| \sin\Theta = \frac{4\pi}{\lambda}\sin\Theta$$

Overview

$$E_\theta = \frac{1}{4\pi\pi_0}\frac{e^2}{mc^2}\left(\hat{e}_{in}\bullet\hat{e}_{out}\right)\frac{e^{i\left(\vec{k}_{out}\vec{r}-\omega t\right)}}{\left|\vec{r}\right|}E_0 = r_e\left(\hat{e}_{in}\bullet\hat{e}_{out}\right)\frac{e^{i\left(\vec{k}_{out}\vec{r}-\omega t\right)}}{\left|\vec{r}\right|}E_0$$

$$\frac{d\sigma}{d\Omega} = r_e^2\left(\hat{e}_{in}\bullet\hat{e}_{out}\right)^2$$

$$E_\theta = \int dE_\theta = E_{Single}\int e^{i\left(\vec{k}_{out}-\vec{k}_{in}\right)\vec{r}_e}\rho_e dV = E_{Single}f(\vec{q})$$

$$\frac{d\sigma}{d\Omega} = r_e^2\left(\hat{e}_{in}\bullet\hat{e}_{out}\right)^2\left|f\left(\vec{q}\right)\right|^2$$

$$d\dot{N}_{scattered} = \left(\frac{d\dot{N}_0}{dS}\right)\left(\frac{d\sigma}{d\Omega}\right)d\Omega$$

Anomalous correction

$$\frac{d^2\vec{r}}{dt^2} + \gamma \frac{d\vec{r}}{dt} + \omega_0^2 \vec{r} = \frac{e}{m} E_0 e^{i\omega t}$$

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

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

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

Anomalous correction

$$f_i = f_i^{free}\left[1 - \frac{\omega_0^2 - i\gamma\omega}{(\omega_0^2 - \omega^2) - i\gamma\omega}\right]$$

$\omega << \omega_0$

$$f_i = 0$$

At low frequency electron do not Contribute to the scattering

$\omega >> \omega_0$

$$f_i = f_i^{free}$$

At high frequency the electron behaves like free electrons

Anomalous correction

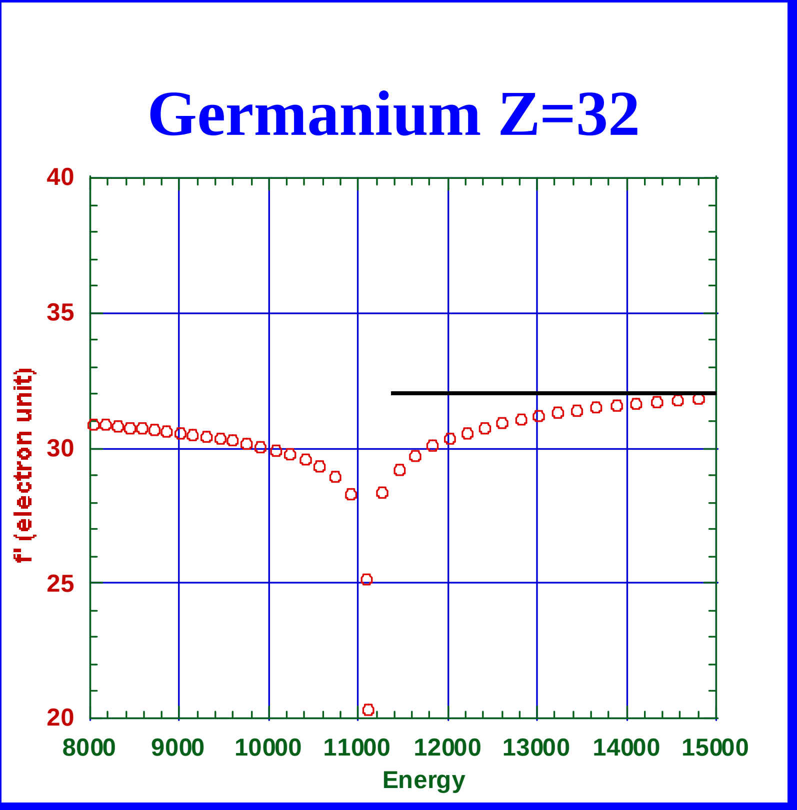
$$f_i = f_i^{free}\left[1 - \frac{\omega_0^2 - i\gamma\omega}{\left(\omega_0^2 - \omega^2\right) - i\gamma\omega}\right] = f_i^{free} + \delta f_i$$

$$\delta f_i' = -f_i^{free}\frac{\omega_0^2\left(\omega_0^2 - \omega^2\right) + \gamma^2\omega^2}{\left(\omega_0^2 - \omega^2\right)^2 + \gamma^2\omega^2}$$

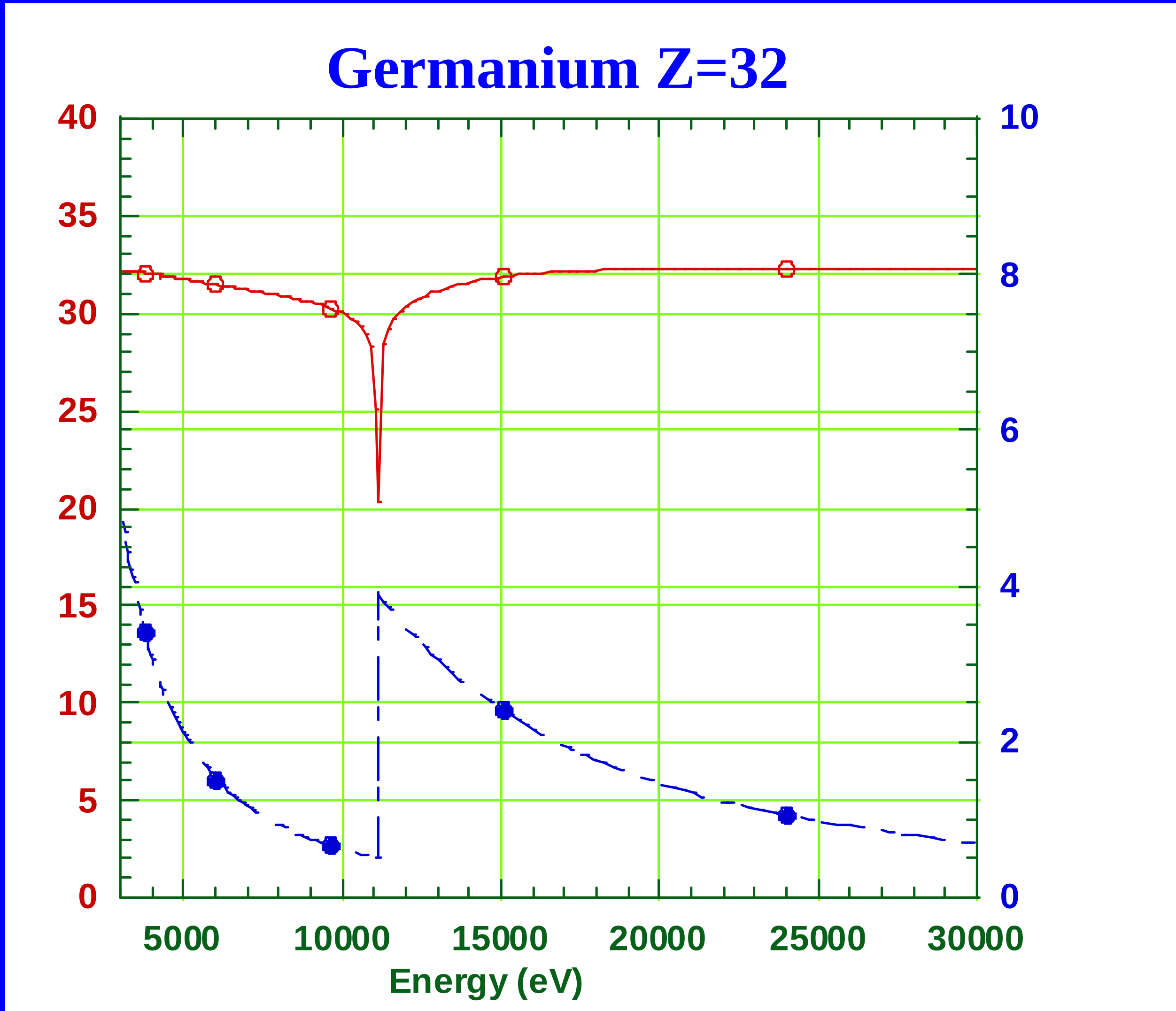
$$\delta f_i'' = f_i^{free}\frac{\gamma\omega^3}{\left(\omega_0^2 - \omega^2\right)^2 + \gamma^2\omega^2}$$

Anomalous correction for atoms

$$\mathbf{f} = \mathbf{f}^{\text{free}} + \Delta\mathbf{f} = \sum_j \mathbf{f}_j^{\text{free}} - \sum_j \mathbf{f}_j^{\text{free}} \frac{\omega_{0j}^2 - i\gamma\omega}{\left(\omega_{0j}^2 - \omega^2\right) - i\gamma\omega}$$



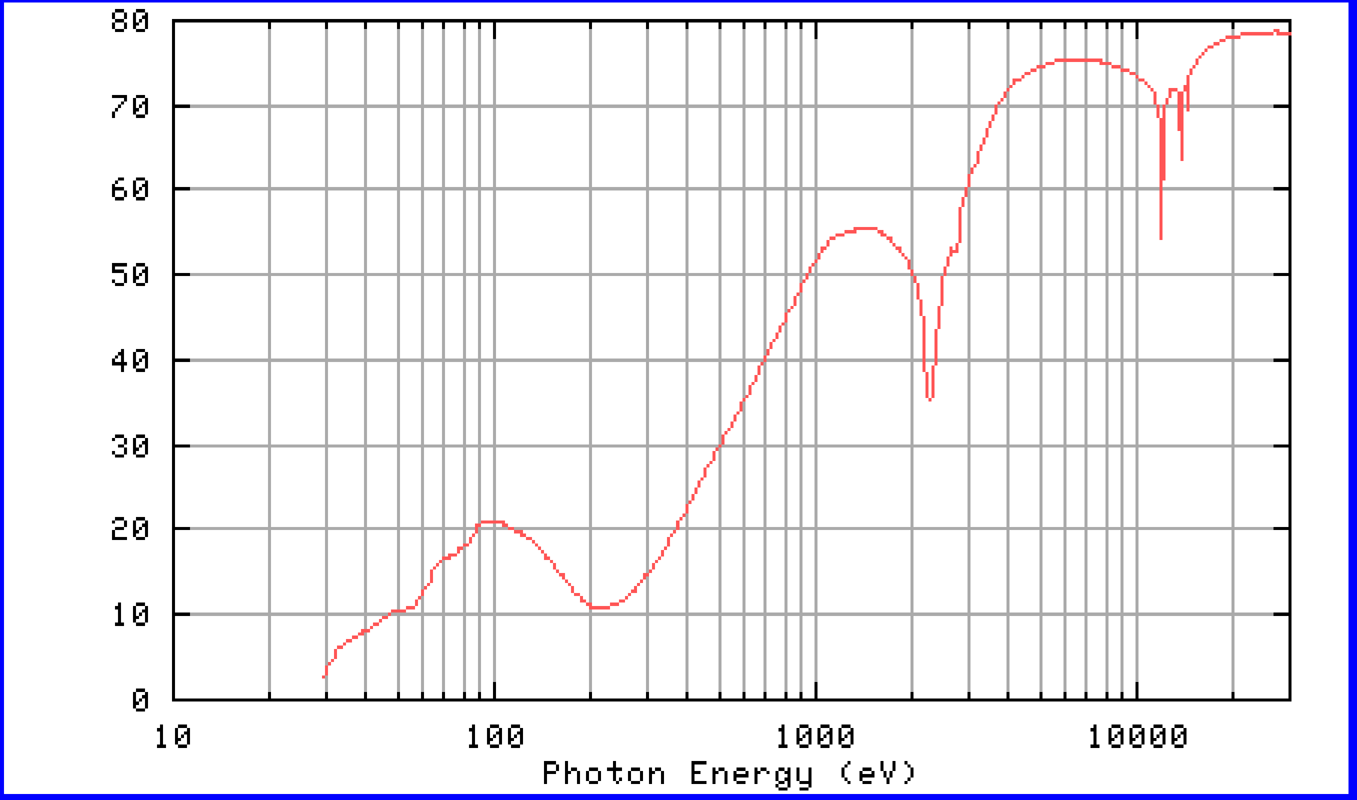
Anomalous correction for atoms: f’ and f” of Ge



Anomalous correction for Au

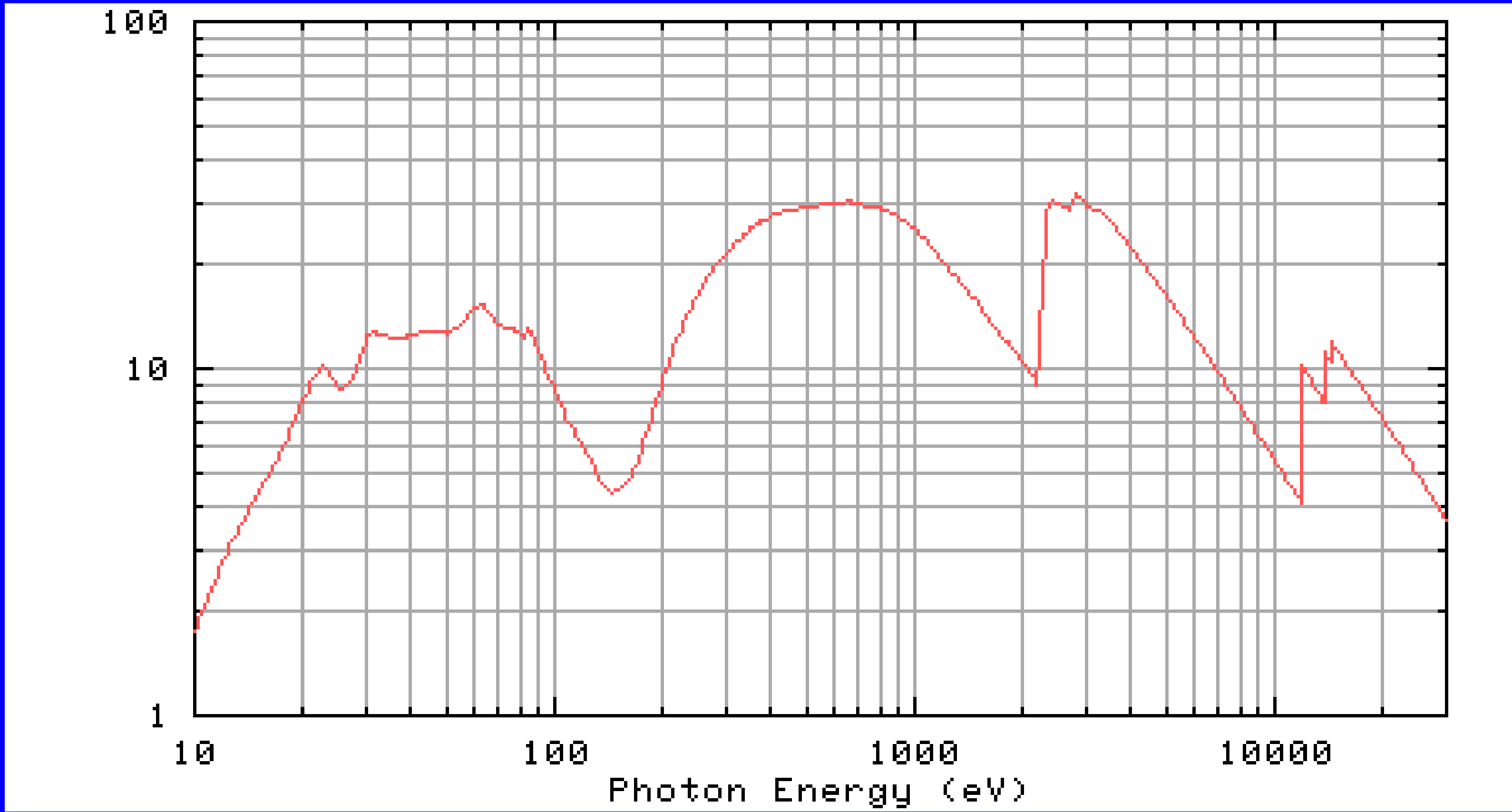
$$f = f^{free} + \Delta f = \sum_j f_j^{free} + \sum_j f_j^{free} \frac{\omega_{0j}^2 - i\gamma\omega}{\left(\omega_{0j}^2 - \omega^2\right) - i\gamma\omega}$$

Gold Z=



Anomalous correction: f” of Ge

Germanium Z=32



Angular dependence of the Anomalous corrections

$$f = f^{free} + \Delta f = \sum_j f_j^{free} + \sum_j f_j^{free} \frac{\omega_{0j}^2 - i\gamma\omega}{\left(\omega_{0j}^2 - \omega^2\right) - i\gamma\omega}$$

For each electron the anomalous correction has the same q dependence as the free term

In the X-ray regime the only electron to consider are the inner shell electron,which origin a spherically symmetric charge distribution

Anomalous corrections do not depend on the angle

KK & Optical theorem

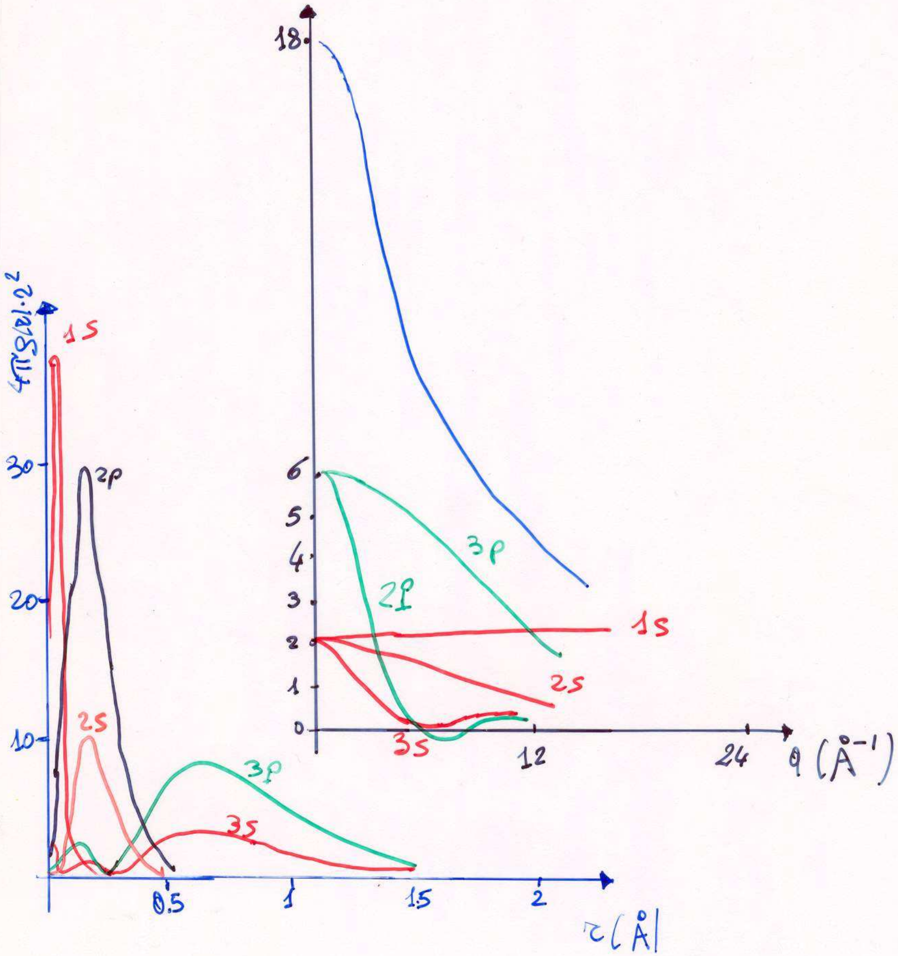
$$f'' = \frac{mc^2}{2Ne^2\lambda}\mu \propto \mu$$

$$f' = \frac{2}{\pi}\int_0^\infty \overline{\omega} f''(\overline{\omega}) d\overline{\omega} + \frac{5E_{tot}}{3mc^2}$$

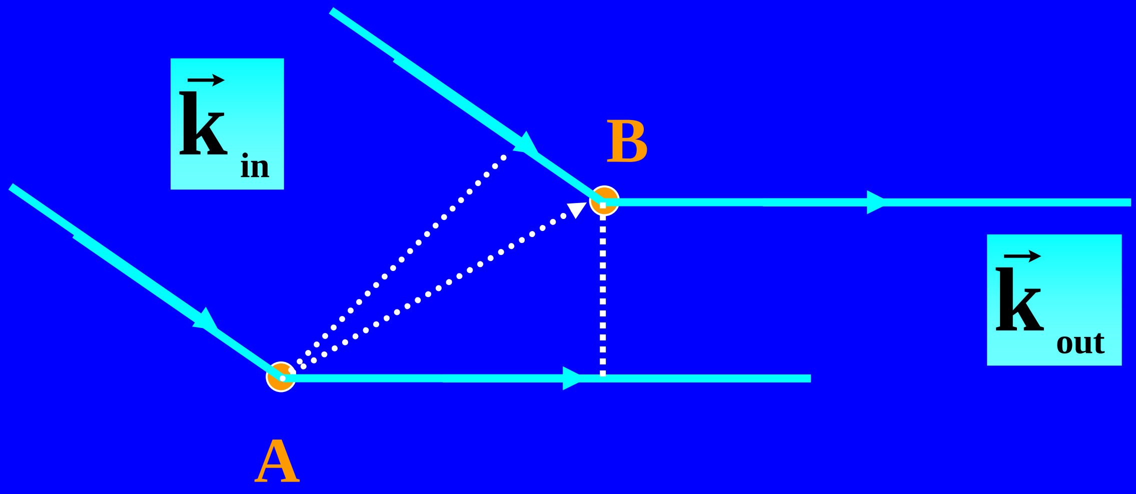
$$f'' = -\frac{2\omega}{\pi}\int_0^\infty \frac{f'(\overline{\omega})}{\omega^2 - \overline{\omega}^2} d\overline{\omega}$$

K+ scattering factors

$K^+ \equiv (1s)^2 (2s)^2 (2p)^6 (3s)^2 (3p)^6$



Anomalous scattering to solve the phase problem



$$E_{sc.} \propto E_0 e^{i\vec{k}_{in}\vec{r}_A} f_A e^{i\vec{k}_{out}(\vec{r}-\vec{r}_A)} + E_0 e^{i\vec{k}_{in}\vec{r}_B} f_B e^{i\vec{k}_{out}(\vec{r}-\vec{r}_B)}$$

$$\propto E_0 e^{i\vec{k}_{in}\vec{r}_A} e^{i\vec{k}_{out}(\vec{r}-\vec{r}_A)} \left(f_A + f_B e^{i\vec{k}_{in}(\vec{r}_B-\vec{r}_A)} e^{i\vec{k}_{out}(\vec{r}_A-\vec{r}_B)}\right) \propto$$

$$E_0 e^{i\vec{k}_{in}\vec{r}_A} e^{i\vec{k}_{out}(\vec{r}-\vec{r}_A)} \left(f_A + f_B e^{i\vec{q}(\vec{r}_A-\vec{r}_B)}\right)$$

Friedel law

$$I(q) \propto \left|E_{sc.}\right|^2 \propto \left|\left(f_A + f_B e^{i\vec{q}(\vec{r}_A - \vec{r}_B)}\right)\right|^2$$

When f_A and f_B are real → I(q)=I(-q)

$$\left|\left(f_A + f_B e^{i\vec{q}(\vec{r}_A - \vec{r}_B)}\right)\right|^2 = \left(f_A + f_B e^{i\vec{q}(\vec{r}_A - \vec{r}_B)}\right)\left(f_A + f_B e^{-i\vec{q}(\vec{r}_A - \vec{r}_B)}\right)$$

Friedel law

Friedel law

When f_A and f_B are complex → I(q)≠I(-q)

$$\left|\left(f_A + f_B e^{i\vec{q}(\vec{r}_A-\vec{r}_B)}\right)\right|^2 = \left(f_A + f_B e^{i\vec{q}(\vec{r}_A-\vec{r}_B)}\right)\left(f_A^* + f_B^* e^{-i\vec{q}(\vec{r}_A-\vec{r}_B)}\right)$$

$$\left|\left(f_A + f_B e^{-i\vec{q}(\vec{r}_A-\vec{r}_B)}\right)\right|^2 = \left(f_A + f_B e^{-i\vec{q}(\vec{r}_A-\vec{r}_B)}\right)\left(f_A^* + f_B^* e^{+i\vec{q}(\vec{r}_A-\vec{r}_B)}\right)$$

$$f_A = |f_A|\ e^{i\Phi_A} \qquad f_B = |f_B|\ e^{i\Phi_B}$$

$$I(\vec{q}) - I(-\vec{q}) \propto \mathrm{Re}\left\{e^{i\vec{q}(\vec{r}_A-\vec{r}_B)}\right\}\mathrm{Re}\left\{e^{i(\Phi_A-\Phi_B)}\right\}$$

Matter ←Interaction→ Radiation II

Semi-Classical approach

Radiation:

Electromagnetic waves described by Maxwell equations

Matter:

Quantum system obeying Schrodinger equation (oscillators,…)

Semiclassical approach

Radiation: classical

Electromagnetic field described by the potential vector A

Matter: Quantum system

Matter ←Interaction→ Radiation III

Quantum approach

Radiation
Quantum system composed of mass less particles (Photons)

Matter
Quantum system obeying Schrodinger equation

Semiclassical approach: the radiation

One vector is enough to describe e.m. radiation → **Vector potential A(r,t)**

$$\vec{E} = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t} - \mathrm{grad}V$$

$$\vec{B} = \mathrm{rot}\,\vec{A}$$

$$\nabla^2 V + \frac{1}{c^2}\frac{\partial^2 V}{\partial t^2} = \rho$$

$$-\nabla^2 \vec{A} + \frac{1}{c^2}\frac{\partial^2 \vec{A}}{\partial t^2} = \frac{\mu}{c}\vec{j}$$

$$\nabla^2 V = \rho$$

$$-\nabla^2 \vec{A} = \frac{\mu}{c}\vec{j}$$

$$\nabla^2 \vec{A} - \frac{1}{c^2}\frac{\partial^2 \vec{A}}{\partial t^2} = 0$$

Semiclassical approach: the radiation

$$\vec{A} = \vec{A}_{\vec{k}} e^{i(\vec{k}\vec{r}-\omega t)}$$

$$\vec{E} = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t} - \mathrm{grad}V$$

$$\vec{B} = \mathrm{rot}\,\vec{A}$$

$$\vec{E} = -\vec{A}_k \frac{i\omega}{c} e^{i(\vec{k}\vec{r}-\omega t)}$$

$$\vec{B} = \vec{k} \times \vec{A}_k e^{i(\vec{k}\vec{r}-\omega t)}$$

Semiclassical approach: the matter

Matter: Quantum system

The system is characterized by its Hamiltonian H_0 and by its eigenfunctions ψ_n and energy eigenvalues E_n obtained by solving the Schrodinger equation

$$\hat{H}_0 \psi_n = E_n \psi_n$$

$$\left(\frac{\hat{p}^2}{2m} + V \right) \psi_n = E_n \psi_n$$

Interaction Hamiltonian

$$\hat{p} \rightarrow \left(\hat{p} - \frac{e}{c}\vec{A} \right)$$

$$\hat{H} = \frac{1}{2m}\left(\hat{p} - \frac{e}{c}\vec{A} \right)^2 + V =$$

$$\left(\frac{\hat{p}^2}{2m} - \frac{e}{mc}\vec{A}\hat{p} + \frac{e^2}{2mc^2}A^2 \right) + V$$

$$\hat{H}_0 - \frac{e}{mc}\vec{A}\hat{p} + \frac{e^2}{2mc^2}A^2 = \hat{H}_0 + \hat{H}_{int}$$

Perturbation Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{H}_{int}$$

$$\hat{H}_{int} = -\frac{e}{mc}\vec{A}\hat{p} + \frac{e^2}{2mc^2}A^2$$

Linear in A

Quadratic in A

$$\vec{A} = \vec{A}_{\vec{k}}\, e^{i(\vec{k}\vec{r} - \omega t)}$$

Time dependent terms

Fermi Golden rule

The perturbation due to the e.m. field induce transitions from the ground state ψ_i to excited states ψ_f with a probability per unit time given by

$$\Gamma_{if} = \frac{2\pi}{\hbar}\left|M_{if}\right|^2 \delta(E_f - E_i) = \frac{2\pi}{\hbar}\left|M_{if}\right|^2 g(E_f)$$

$$M_{if} = \left\langle \psi_f \middle| \widehat{H}_{int.} \middle| \psi_i \right\rangle + \sum_n \frac{\left\langle \psi_f \middle| \widehat{H}_{int.} \middle| \psi_n \right\rangle \left\langle \psi_n \middle| \widehat{H}_{int.} \middle| \psi_i \right\rangle}{E_i - E_n \pm \hbar\omega + i\varepsilon}$$

Absorption

$$\hat{H}_{int} = -\frac{e}{mc}\vec{A}\hat{p} + \frac{e^2}{2mc^2}A^2$$

$$\Gamma_{if} = \frac{2\pi}{\hbar}|M_{if}|^2 g(E_f)$$

$$M_{if} = \langle\psi_f|\hat{H}_{int.}|\psi_i\rangle + \sum_n \frac{\langle\psi_f|\hat{H}_{int.}|\psi_n\rangle\langle\psi_n|\hat{H}_{int.}|\psi_i\rangle}{E_i - E_n \pm \hbar\omega + i\varepsilon}$$

$$\Gamma_{if} = \frac{2\pi}{\hbar}\left(\frac{e\,A_k}{m\,c}\right)^2 \left|\langle\psi_f|e^{i\vec{k}\vec{r}}(\hat{e}_k \bullet \hat{p})|\psi_i\rangle\right|^2 \delta(E_f - E_i - \hbar\omega)$$

$$\Gamma_{if} = \frac{2\pi}{\hbar}\left(\frac{e\,E_k}{m\,\omega}\right)^2 \left|\langle\psi_f|e^{i\vec{k}\vec{r}}(\hat{e}_k \bullet \hat{p})|\psi_i\rangle\right|^2 \delta(E_f - E_i - \hbar\omega)$$

Power Absorption

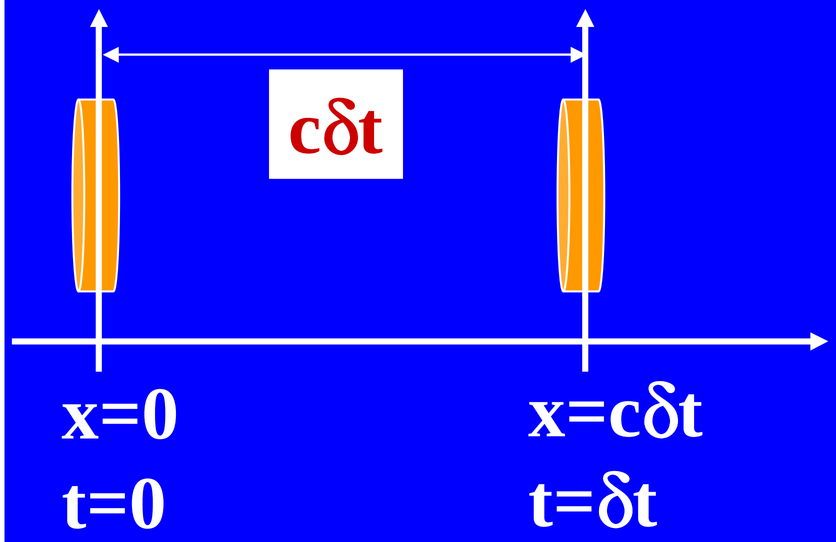
$$\Gamma_{if} = \frac{2\pi}{\hbar}\left(\frac{e\,E_k}{m\,\omega}\right)^2 \left|\left\langle \psi_f \left| e^{i\vec{k}\vec{r}} \left(\hat{e}_k \bullet \hat{p}\right) \right| \psi_i \right\rangle\right|^2 \delta(E_f - E_i - \hbar\omega)$$

Total power absorbed per unit volume

$$\frac{dW}{dt} = \frac{1}{V}\sum_f \hbar\omega\Gamma_{if} =$$

$$\frac{1}{V}\sum_f \frac{2\pi}{\omega}\left(\frac{e\,E_k}{m\,\omega}\right)^2 \left|\left\langle \psi_f \left| e^{i\vec{k}\vec{r}} \left(\hat{e}_k \bullet \hat{p}\right) \right| \psi_i \right\rangle\right|^2 \delta(E_f - E_i - \hbar\omega)$$

Absorption Coefficient



$w(0)\Delta V$

$w(x)\Delta V$

w(r) = Energy density

$$wdV = \langle E^2 \rangle dV = \frac{1}{2} E_0^2 dV$$

$$w(x) = w(0)e^{-\mu x} \cong w(0)(1-\mu x) = \\ = w(0)(1-\mu cdt)$$

$$\frac{dW}{dt} = \frac{\left(w(c\delta t) - U(0)\right)}{dt} = w(0)\mu c$$

Absorption Coefficient

$$\frac{dW}{dt} = \frac{\left(w(cdt) - w_0\right)}{dt} = w(0)\ \mu\ c = \frac{\mu\ c}{2} E_0^2$$

$$\frac{dW}{dt} = \sum_f \hbar\omega \frac{2\pi}{\hbar} \left(\frac{e\ E_k}{m\ \omega} \right)^2 \left| \left\langle \psi_f \left| e^{i\vec{k}\vec{r}} \left(\hat{e}_k \bullet \hat{p} \right) \right| \psi_i \right\rangle \right|^2 \delta(E_f - E_i - \hbar\omega)$$

$$\mu = \frac{4\pi^2 \hbar\alpha}{m^2\omega} \sum_f \left| \left\langle \psi_f \left| e^{i\vec{k}\vec{r}} \left(\hat{e}_k \bullet \hat{p} \right) \right| \psi_i \right\rangle \right|^2 \delta(E_f - E_i - \hbar\omega)$$

$$\alpha = \frac{e^2}{\hbar c} \cong \frac{1}{137}$$

Absorption Coefficient:dipole approximation

$$e^{i\vec{k}\vec{r}} \cong 1 + \vec{k}\vec{r}$$

$$\mu = \frac{4\pi^2\hbar\alpha}{m^2\omega}\sum_f \left| \left\langle \psi_f \left| \left(\hat{e}_k \bullet \hat{p} \right) \right| \psi_i \right\rangle \right|^2 \delta\left(E_f - E_i - \hbar\omega\right)$$

Optical transitions: λ ≈ 5000 Å → always valid

In the case of X-ray, the wavelength is few Å, i.e.
of the same order as the extensions of the atomic orbitals

In general the core states spatial extension reduces as 1/Z with increasing the Z number of the atom with respect to the hydrogen orbitals

the energy of the absorption edges increases as Z^2 and the wavelength of the radiation needed to excite a core level decreases as $1/Z^2$

→

Therefore for high Z elements, deviations from the dipole approximations must be expected and must be taken into account.

Quadrupole approximation

Second term in the expansion of e^{jkr}

$$\mu = N_A 4\pi^2 \alpha \hbar\omega_k \left| \hat{e}_{\vec{k},\lambda} \bullet \left\langle \psi_f \left| \left(1 + i\vec{k}\vec{r}_i\right) \vec{r}_i \right| \psi_i \right\rangle \right|^2 g(E_f) =$$

$$N_A 4\pi^2 \alpha \hbar\omega_k \left| \hat{e}_{\vec{k},\lambda} \bullet \left\langle \psi_f \left| \hat{r}_i \right| \psi_i \right\rangle + \hat{e}_{\vec{k},\lambda} \bullet \left\langle \psi_f \left| \left(i\vec{k}\vec{r}_i\right) \vec{r}_i \right| \psi_i \right\rangle \right|^2$$

Peculiar angular dependance

Important when the dipole term is zero

Quadrupole/dipole term

Atom	K Edge	L_1 Edge	$L_{2,3}$ Edge
Al	0.012	0.004	0.001
Cu	0.058	0.026	0.01
Ag	0.152	0.073	0.03
Yb	0.314	0.194	0.06
Au	0.397	0.270	0.08

Negligible for light elements

Relevant for the K edge of 3d elements

Cannot be neglected for heavy elements

Always negligible far from the edge

Absorption Coefficient: electric dipole

$$\langle \psi_f | \hat{p} | \psi_i \rangle = \langle \psi_f | m \dot{\hat{r}} | \psi_i \rangle = \frac{im}{\hbar} \langle \psi_f | [\hat{H}\hat{r} - \hat{r}\hat{H}] | \psi_i \rangle =$$

$$\frac{im(E_f - E_i)}{\hbar} \langle \psi_f | \hat{r} | \psi_i \rangle = im\omega \langle \psi_f | \hat{r} | \psi_i \rangle$$

$$\mu = 4\pi^2 \hbar\omega\alpha \sum_f \left| \langle \psi_f | (\hat{\mathbf{e}}_k \bullet \hat{\mathbf{r}}) | \psi_i \rangle \right|^2 \delta(E_f - E_i - \hbar\omega)$$

$$\mu = 4\pi^2 \hbar\omega\alpha \left| \langle \psi_f | (\hat{\mathbf{e}}_k \bullet \hat{\mathbf{r}}) | \psi_i \rangle \right|^2 D(E_f)$$

$$D(E_f) = \text{Density of states}$$

Scattering in the semiclassical approach - I

$$\left(\hat{H}_0 + -\frac{e}{mc}\vec{A}\hat{p} + \frac{e^2}{2mc^2}A^2\right)\Psi = -i\hbar\frac{\partial\Psi}{\partial t}$$

$$\Psi_n = \psi_n e^{-i\frac{E_n}{\hbar}t} \quad \Rightarrow \quad \Psi'_n = \psi_n e^{-i\frac{E_n}{\hbar}t} + \text{correction}$$

$$\hat{j} = e\vec{v} = e\frac{\hat{p}}{m} \to \frac{e}{m}\left(\hat{p} - \frac{e}{c}\vec{A}\right)$$

Scattering in the semiclassical approach - II

$$\vec{j}_{nm} = \frac{e}{2m}\left\langle \Psi'_n \middle| \hat{p} \middle| \Psi'_m \right\rangle - \frac{e^2}{mc}\vec{A}\left\langle \Psi'_n \middle\| \Psi'_m \right\rangle$$

Current associated with a moving electron:

$$\vec{r} = \vec{r}_0 \sin \omega t$$

$$\vec{j} = e\vec{v} = ei\omega\vec{r} = -i\frac{\omega e^2}{m\omega^2}\vec{E} = -\frac{e^2}{mc}\vec{A}$$

$$\frac{d\sigma}{d\Omega} = \left(\hat{e}_{in} \bullet \hat{e}_{out}\right)^2 r_e^2$$

Elastic Scattering at high energy - I

$$\Psi_n' = \psi_n e^{-i\frac{E_n}{\hbar}t} + \text{correction}$$

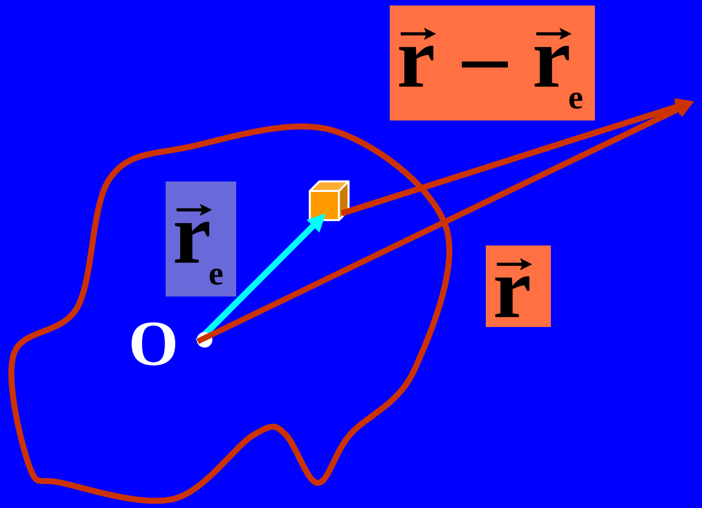
$$\text{correction} \propto \left|\frac{1}{\hbar\omega_{ln} \pm \hbar\omega}\right|^2 \cong 0 \Rightarrow \Psi_n' \cong \psi_n e^{-i\frac{E_n}{\hbar}t}$$

$$\vec{j}_{nn} = \frac{e}{2m}\langle\Psi_n|\hat{p}|\Psi_n\rangle - \frac{e^2}{mc}\vec{A}\langle\Psi_n\|\Psi_n\rangle \cong -\frac{e^2}{mc}\vec{A}|\psi_n|^2$$

Does not depend on time

Depend on time

Elastic Scattering at high energy - II



$$\vec{j}_{nn} \cong -\frac{e^2}{mc}\vec{A}\left|\psi_n\right|^2$$

$$dE_\theta = \frac{1}{4\pi\varepsilon_0}\frac{e^2E_0}{mc^2}\left(\hat{e}_{in}\bullet\hat{e}_{out}\right)\frac{e^{i\left(\vec{k}_{out}\vec{r}-\omega t\right)}}{\left|\vec{r}\right|}e^{i\left(\vec{k}_{out}-\vec{k}_{in}\right)\vec{r}_e}\rho_e dV$$

$$\frac{d\sigma}{d\Omega} = r_e^2\left(\hat{e}_{in}\bullet\hat{e}_{out}\right)^2\left|f\left(\vec{q}\right)\right|^2$$

Inelastic Scattering at high energy

$$\vec{j}_{nm} \cong -\frac{e^2}{mc}\vec{A}\left\langle \Psi_n \| \Psi_m \right\rangle =$$

$$-\frac{e^2}{mc}\vec{A}_k e^{i\vec{k}\vec{r}-\omega_0 t}\left\langle \psi_n \| \psi_m \right\rangle e^{i(\omega_n-\omega_m)t}$$

$$\omega = \omega_0 \pm (\omega_n - \omega_m)$$

$$\vec{j} = e\vec{v} = ei\omega\vec{r} = -\frac{e^2}{mc}\vec{A}\left(\frac{\omega}{\omega_0}\right) \Longleftrightarrow \left(\frac{d\sigma}{d\Omega}\right)_{in.} = r_e^2(\hat{e}_{in}\bullet\hat{e}_{out})^2\left(\frac{\omega}{\omega_0}\right)^2$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{in.} = r_e^2(\hat{e}_{in}\bullet\hat{e}_{out})^2\left(\frac{\omega}{\omega_0}\right)^2 \sum_{m\#n}\left|\left\langle \psi_n \left| e^{i\vec{q}\vec{r}} \right| \psi_m \right\rangle\right|^2$$

Inelastic Scattering at very high energy

$$\left(\frac{d\sigma}{d\Omega}\right)_{in.} = r_e^2\,(\hat{e}_{in}\bullet\hat{e}_{out})^2\left(\frac{\omega}{\omega_0}\right)^2\sum_{m\#n}\left|\langle\psi_m|e^{i\vec{q}\vec{r}}|\psi_n\rangle\right|^2$$

$$\sum_{m\#n}\left|\langle\psi_m|e^{i\vec{q}\vec{r}}|\psi_n\rangle\right|^2 = \sum_{m\#n}\langle\psi_n|e^{i\vec{q}\vec{r}}|\psi_m\rangle\langle\psi_m|e^{-i\vec{q}\vec{r}}|\psi_n\rangle =$$

$$\langle\psi_n|e^{i\vec{q}\vec{r}}\left(\sum_{m\#n}|\psi_m\rangle\langle\psi_m|\right)e^{-i\vec{q}\vec{r}}|\psi_n\rangle = 1-\left|\langle\psi_n|e^{i\vec{q}\vec{r}}|\psi_n\rangle\right|^2 =$$

$$1-\left|f(\vec{q})\right|^2$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{in.} = r_e^2\,(\hat{e}_{in}\bullet\hat{e}_{out})^2\left(1-\left|f(\vec{q})\right|^2\right)$$

Inelastic Scattering at very high energy

$$\left(\frac{d\sigma}{d\Omega}\right)_{in.} \cong r_e^2 \left(\hat{e}_{in} \bullet \hat{e}_{out}\right)^2 \left(1 - \left|f(\vec{q})\right|^2\right)$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{el.} + \left(\frac{d\sigma}{d\Omega}\right)_{in.} \cong r_e^2 \left(\hat{e}_{in} \bullet \hat{e}_{out}\right)^2$$

The sum of the elastic and inelastic cross sections is equal to the Classical cross section of a free electron

Anomalous and Resonant Scattering

$$\Psi_n' = \psi_n e^{-i\frac{E_n}{\hbar}t} + \text{correction}$$

$$\vec{j}_{nm} = \frac{e}{2m}\left\langle \Psi_n' \middle| \hat{p} \middle| \Psi_m' \right\rangle - \frac{e^2}{mc}\vec{A}\left\langle \Psi_n' \middle\| \Psi_m' \right\rangle$$

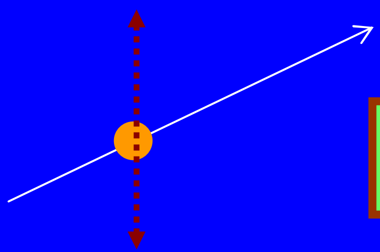
$$\Psi_n' = \psi_n e^{-i\frac{E_n}{\hbar}t} + \frac{eA_k}{mc} \sum_{l \# n}\left(\frac{\left\langle \psi_l \middle| e^{i\vec{k}\vec{r}}\hat{p} \middle| \psi_n \right\rangle}{\hbar\omega_{ln} - \hbar\omega} e^{i(\omega_{ln}-\omega)t} - \frac{\left\langle \psi_n \middle| e^{i\vec{k}\vec{r}}\hat{p} \middle| \psi_l \right\rangle}{\hbar\omega_{ln} + \hbar\omega} e^{i(\omega_{ln}+\omega)t} \right)\psi_l e^{-i\frac{E_l}{\hbar}t}$$

Corrections are frequency dependent ➔ anomalous scattering

One term is resonant

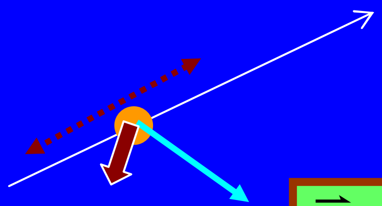
Magnetic Interactions

An electromagnetic wave transport both an electric and a magnetic field



$$\vec{F} = -e\vec{E}$$

Thomson scattering

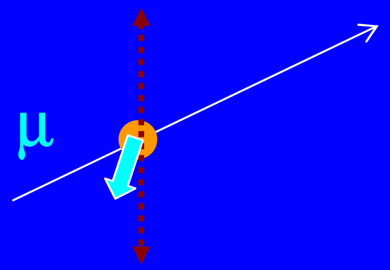


$$E = -\vec{\mu}\vec{H}$$

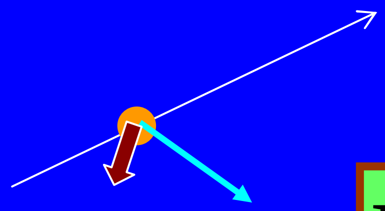
$$\vec{F} = \mathrm{grad}\left(\vec{\mu}\vec{H}\right)$$

Is due to the variation of the energy for the non uniformity of the magnetic field of the radiation

Magnetic Interactions



Magnetic dipole oscillations

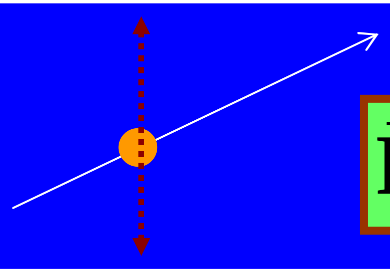


Torque

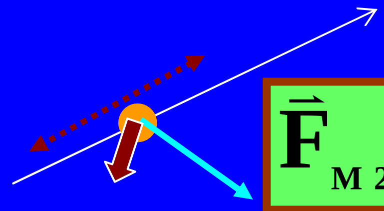
$$\vec{M} = \left(\vec{\mu} \times \vec{H}\right)$$

Due to the variation of the torque associated with the time dependance of the magnetic field of the radiation

Strength of Magnetic Interactions



$$\vec{F}_T = -e\vec{E}$$



$$\vec{F}_{M2} = \mathrm{grad}\left(\vec{\mu}\vec{H}\right)$$

$$\frac{\left|\vec{F}_{M2}\right|}{\left|\vec{F}_T\right|} = \frac{\left|\mathrm{grad}\left(\vec{\mu}\bullet\vec{H}\right)\right|}{\left|eE\right|} = \frac{\left|\mathrm{grad}\left(\vec{\mu}\bullet\vec{H}_0 e^{i\vec{k}\vec{r}}\right)\right|}{eE_0} =$$

$$k\frac{\mu\bullet H_0}{eE_0} = \frac{2\pi}{\lambda}\left(\frac{e\hbar}{2m}\right)\frac{1}{e}\frac{H_0}{E_0} \cong \frac{\pi\hbar}{mc\lambda} = \frac{\lambda_{Compton}}{\lambda} \approx 10^{-2}$$

Only magnetic Electrons are active

$$\frac{I_{mag.}}{I_{T.}} \approx 10^{-4}\left(\frac{Z_{mag.}}{Z}\right)^2 \approx 10^{-6} \div 10^{-7}$$

de Bergevin e Brunel on NiO(1972)

- NiO e' un cristallo cubico antiferromagnetico (T_{Neel}=250 ^{0}C)
- Gli ioni Ni^{++} hanno due soli spin accoppiati
- Gli spin sono allineati magneticamente nel piano (111)
- Ed antiferromagneticamente tra i piani (111)

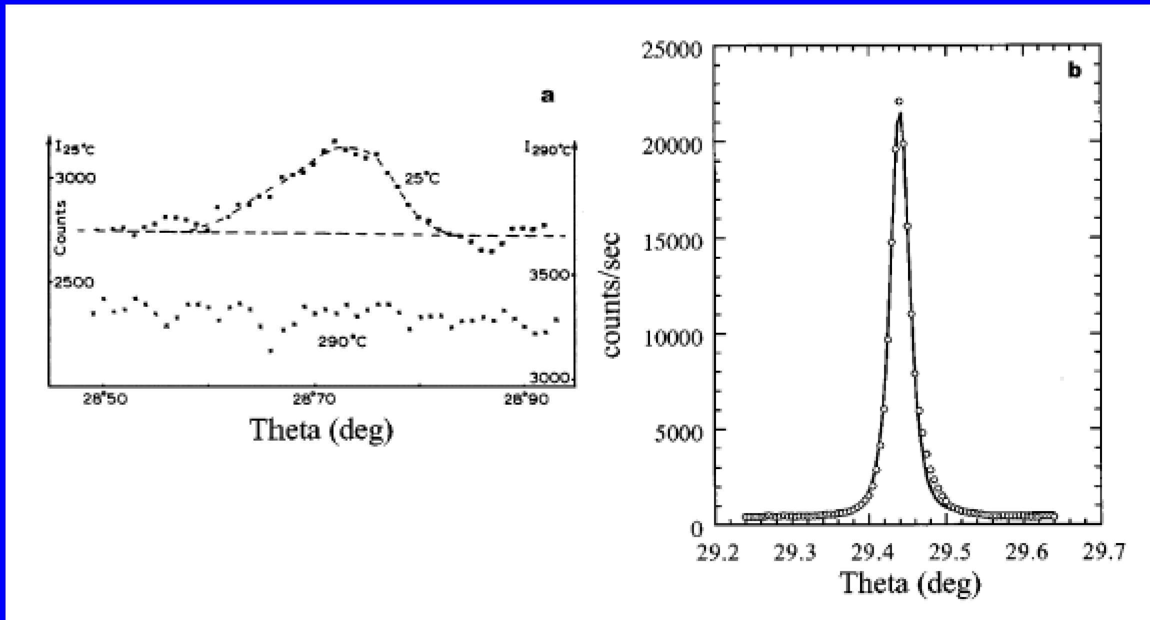


Figure 10: Panel a: Superlattice magnetic reflection (3/2, 3/2, 3/2) of NiO measured in magnetic phase (25°), and in the paramagnetic phase. The disappearance of the peak shows its magnetic origin. Panel b: The magnetic reflection (3/2, 3/2, 3/2) of NiO measured today at a third generation synchrotron radiation facility.

Quantum origin of the magnetic interactions

Relativistic correction
To the kinetic energy

Darwin term
Do not depend on A because

$\vec{\ } \bullet \vec{\ }^{\cdot} =$

$$\hat{H}'_{el.} = \sum_i \frac{\left(\hat{p}_i - {}^{e}\!/_{c}\vec{A}\right)^2}{2m} + V(\vec{r}_i) - \frac{p_i^4}{8m^3c^2} + \frac{e}{8m^2c^2}\nabla\vec{E}$$

$$-\frac{e\hbar}{mc}\vec{s}_i \bullet \vec{B} - \frac{e\hbar}{2m^2c^2}\vec{s}_i \bullet \vec{E} \times \left(\hat{p}_i - \frac{e}{c}\vec{A}(\vec{r}_i)\right)$$

Spin – magnetic field
interaction

Spin-orbit
interaction