Interaction between matter and radiation: an introduction

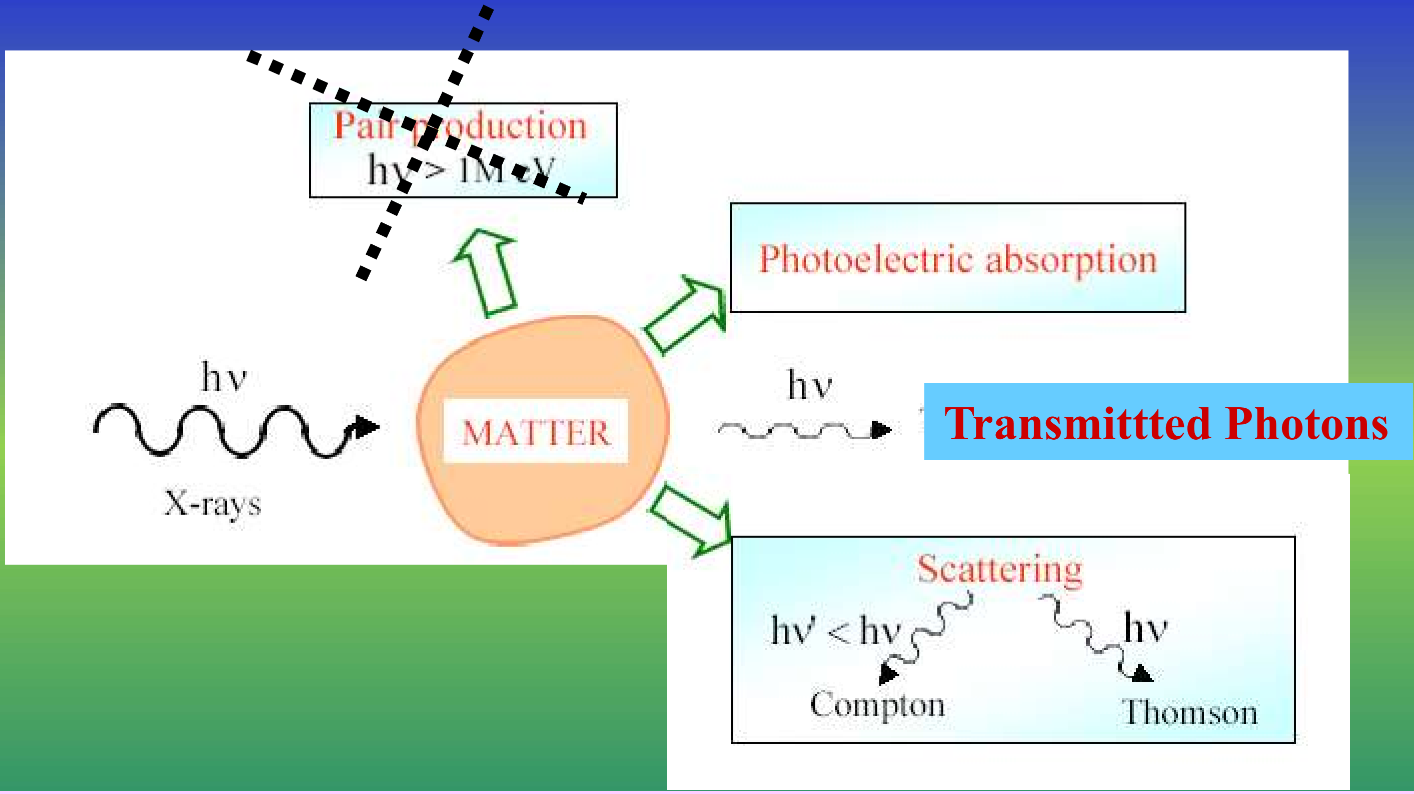
Overview of the basic processes

Absorption (classical and quantum)
Scattering (classical and quantum)

Basic elements to follows lectures

To introduce relativistic effects

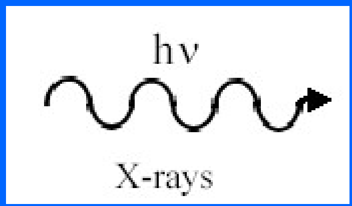
Main interactions



Photon absorption: excitation
with or without emission of electrons

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

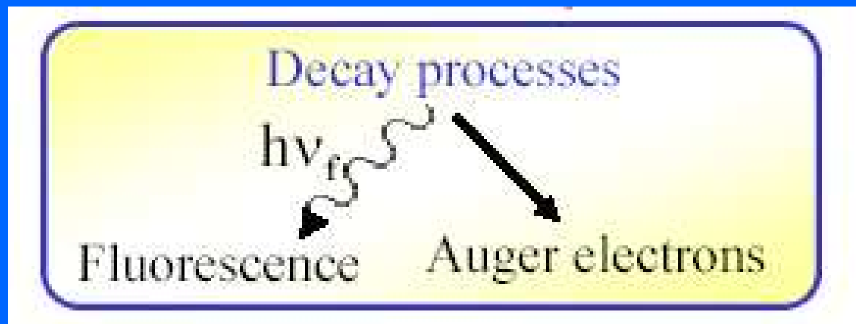
Indirect effects: decay processes



MATTER

Matter is excited by the radiation

It looses energy through decay processes



Experimental techniques

Absorption
Photoemission

Scattering

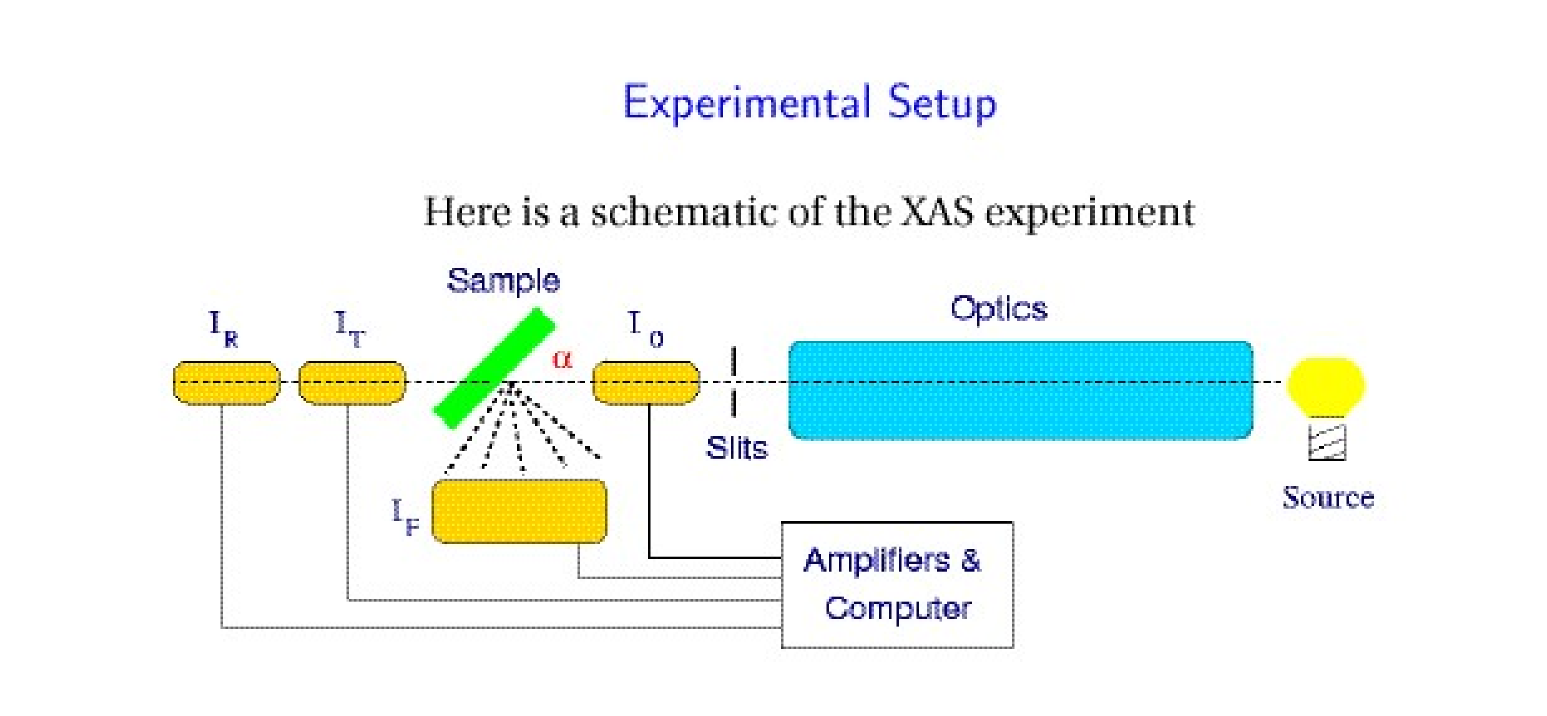
Elastic Scattering: Diffraction, SAXS
Inelastic Scattering: Compton, IXS
Resonant scattering: R(I)XS

Imaging

Fluorescence Yield
Auger spectroscopy

What we measure in experiments?

Experimental techniques: what we measure?

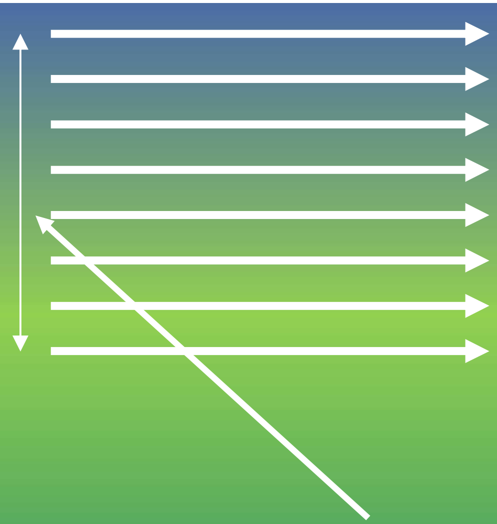


Absorption $I_T(E) = I_0 e^{-\mu(E)x}$

- **μ(E) is called the absorption coefficient**
- **it describes quantitatively how the energy of a beam is transferred to the matter**
- **It is measured in m^{-1}**
- **In a thickness 1/μ the intensity is reduced to 1/e**

The cross section σ

photon beam

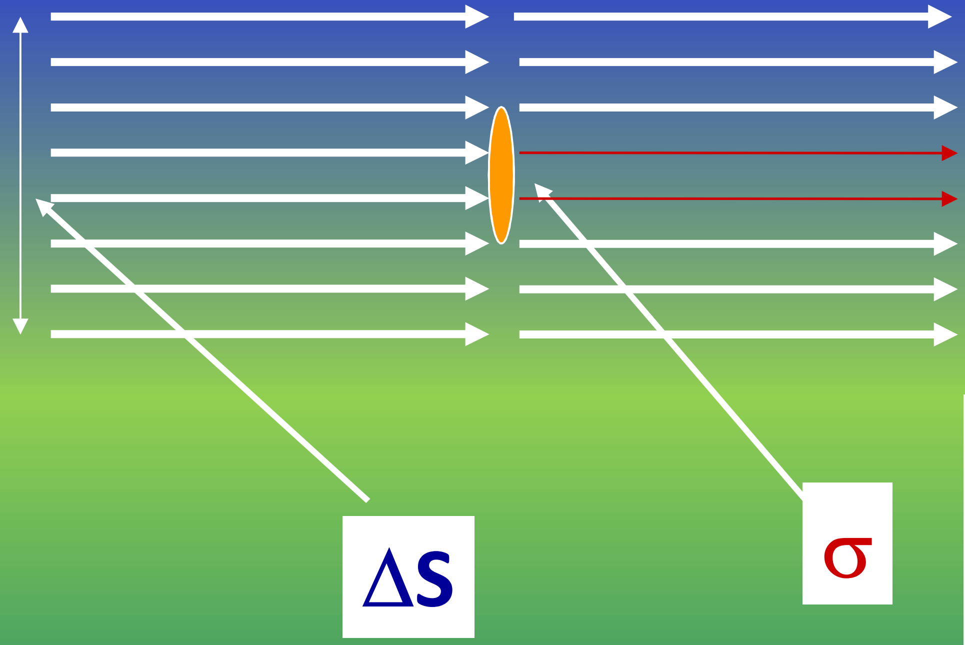


ΔS

$\dot{N}$ **is the number of photons per second per unit cross area of the beam**

$\dot{N} \Delta S \, h\nu$ **is the total power of a photon beam**

The cross section σ



$$\dot{N}_{out}\Delta S = \dot{N}_{in}\left(\Delta S - \sigma\right)$$

$$\frac{\Delta \dot{N}}{\dot{N}_{in}} = \frac{\dot{N}_{out} - \dot{N}_{in}}{\dot{N}_{in}} = -\frac{\sigma}{\Delta S}$$

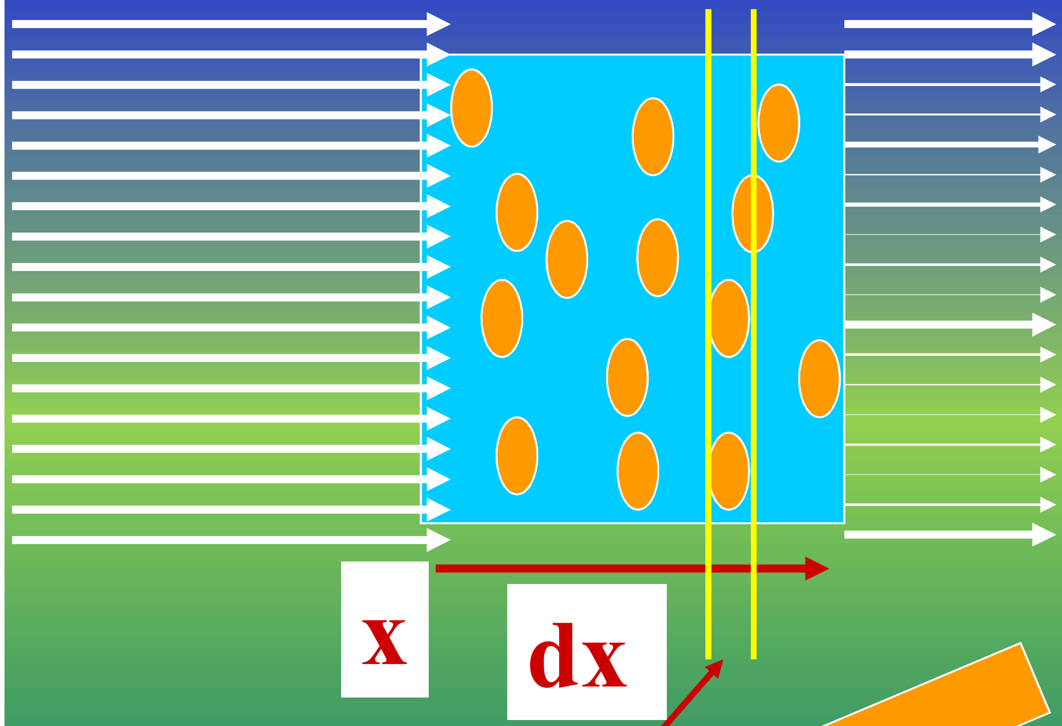
σ has no geometrical meaning:

it is a measure of the interaction

It is called "cross section"

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

The cross section σ and the absorption coefficient μ



ρ is the density of the objects

$$\rho\Delta V = \rho\Delta S\Delta x$$

$$-\frac{\Delta\dot{N}}{\dot{N}_{in}} = \frac{\sigma_{tot}}{\Delta S} = \sigma\rho\Delta x$$

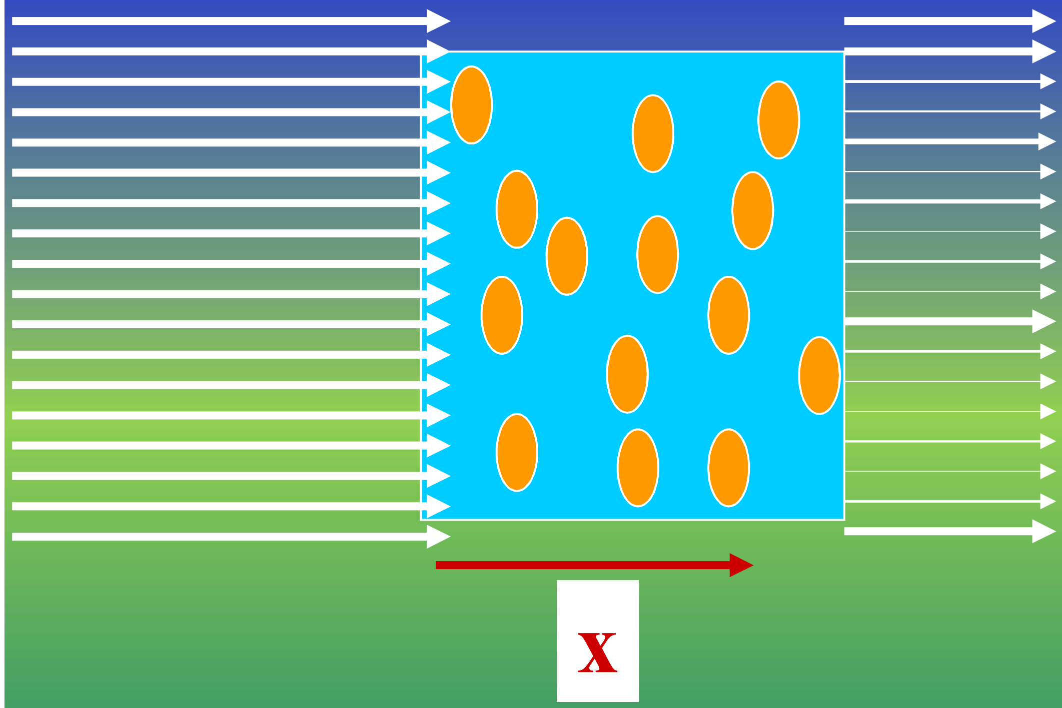
$$\sigma_{tot} = \sigma\rho\Delta S\Delta x$$

$$\frac{d\dot{N}}{\dot{N}} = -\sigma\rho dx$$

$$\dot{N}(x) = \dot{N}_{in} e^{\overbrace{-\sigma\rho x}^{\mu x}}$$

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

Cross section σ – III



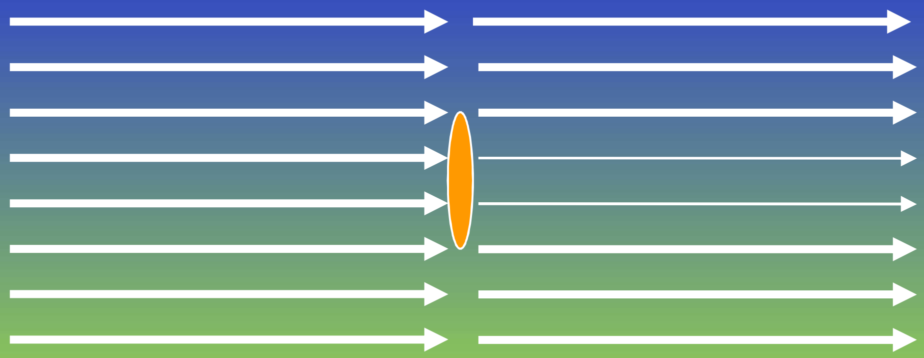
ρ is the density of the objects

σ is the cross section of each object

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

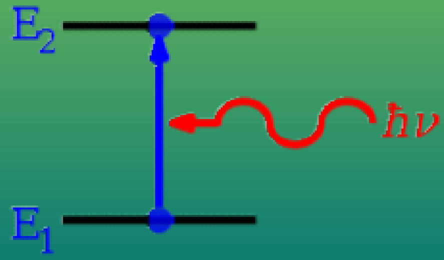
$$\mu = \rho \sigma$$

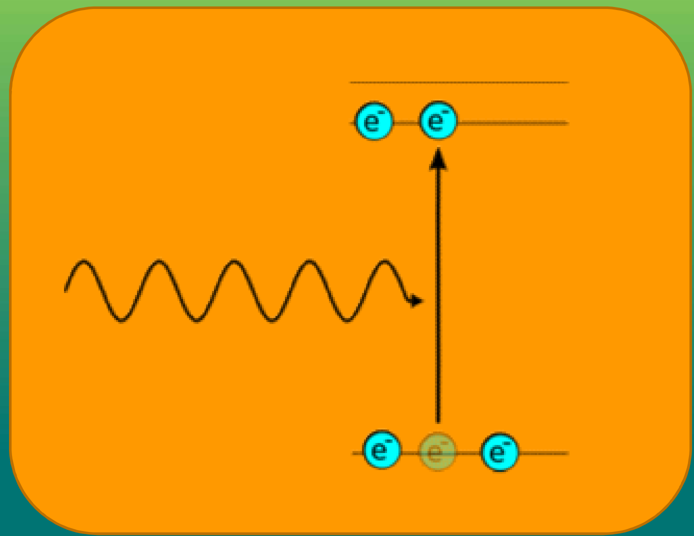
Absorption cross section



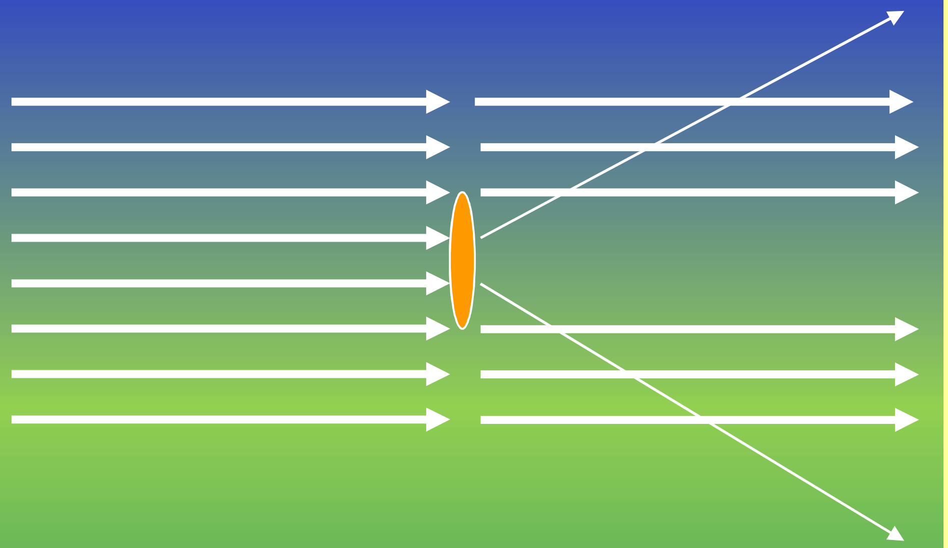
Absorption

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





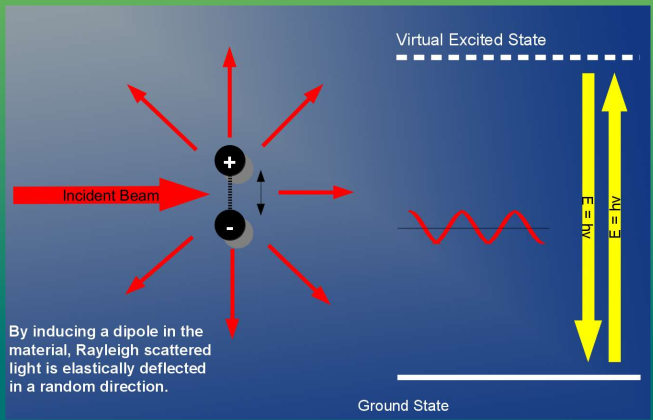
Scattering cross section

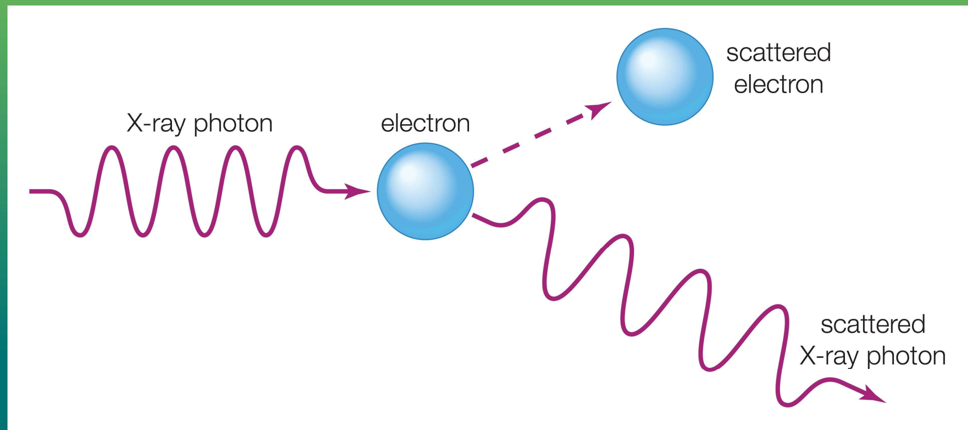


Scattering

Photons are removed because are partially scattered into a different direction

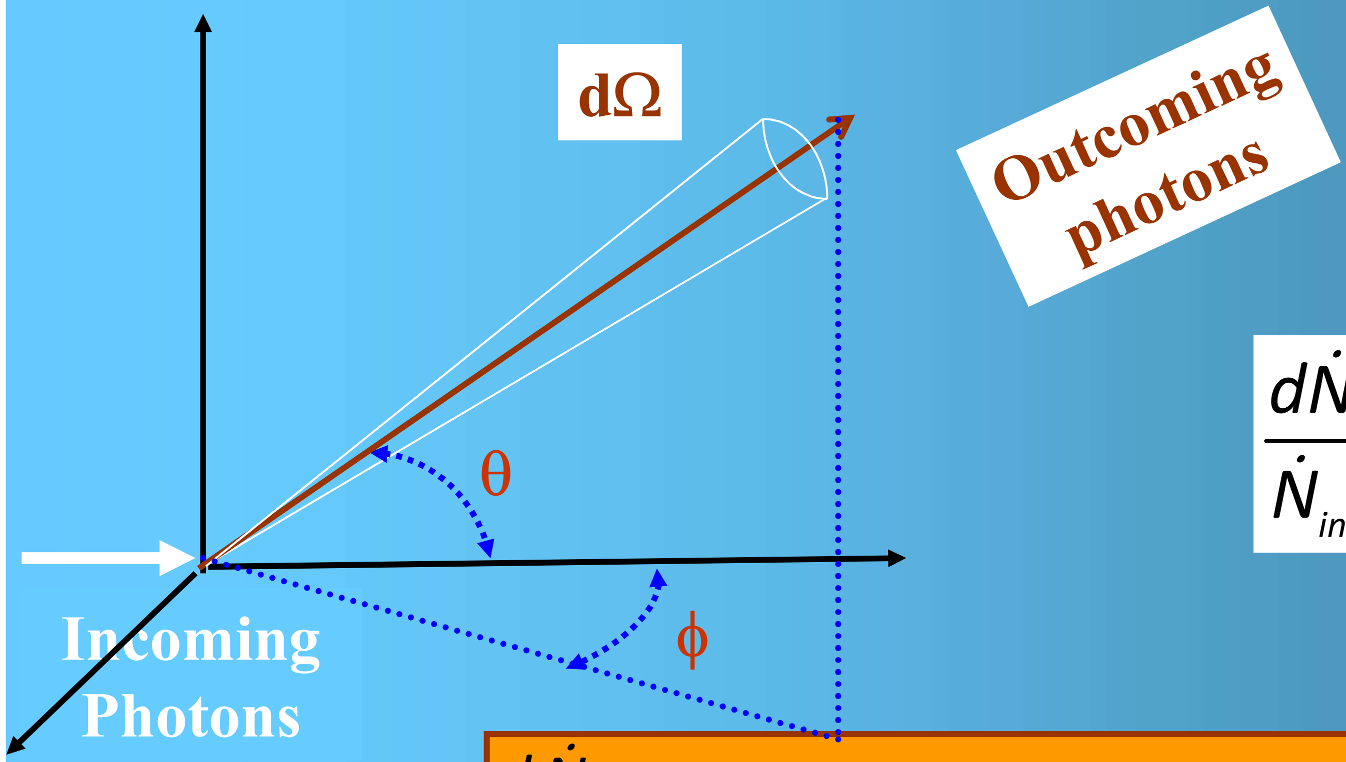
$\sigma_{scatt.}$





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

Differential Cross Section $d\sigma/d\Omega$



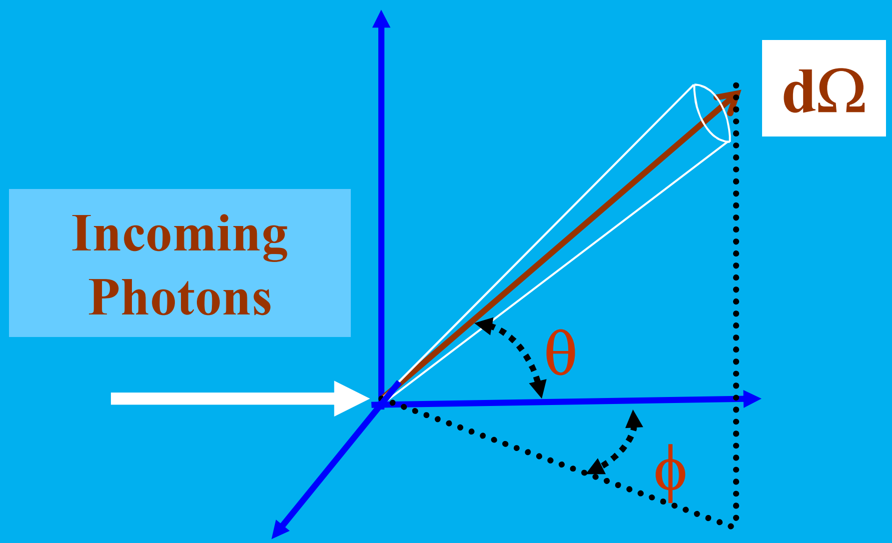
$$\frac{d\dot{N}}{\dot{N}_{in}} = -\sigma_{\text{scatt}}\,\rho\,dx$$

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

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

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

Cross section & Probability



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

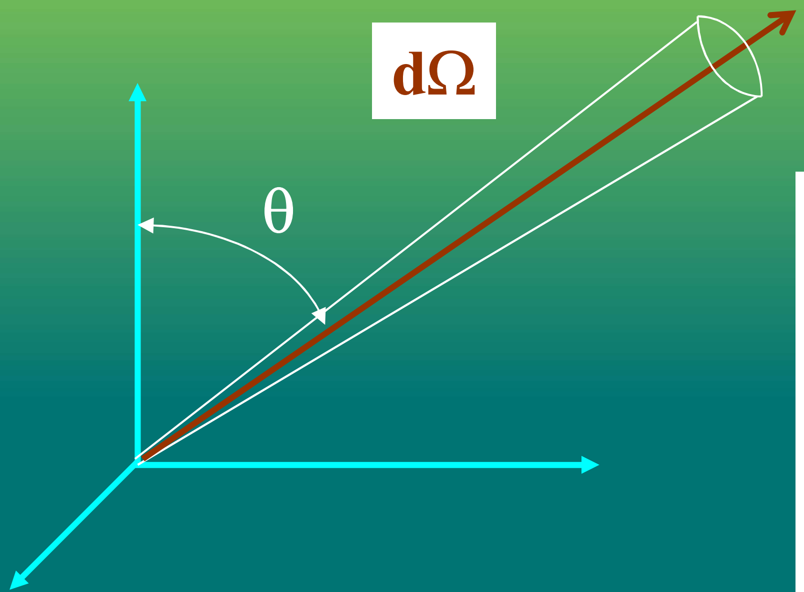
Probability

Cross Sections: Classical definition

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

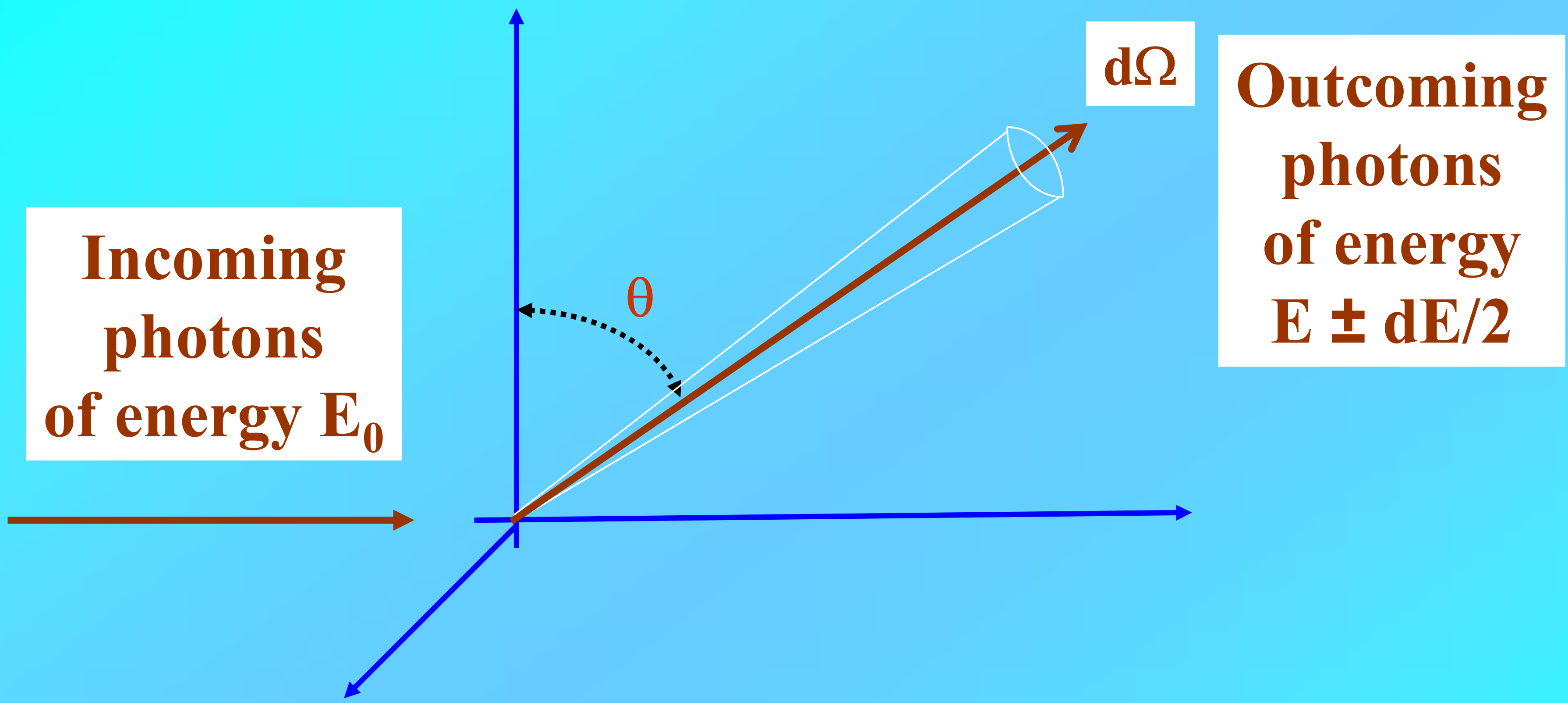
$$\frac{d\dot{N}_{sc.}}{\dot{N}_{in}} = \frac{dI}{I_0}$$

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



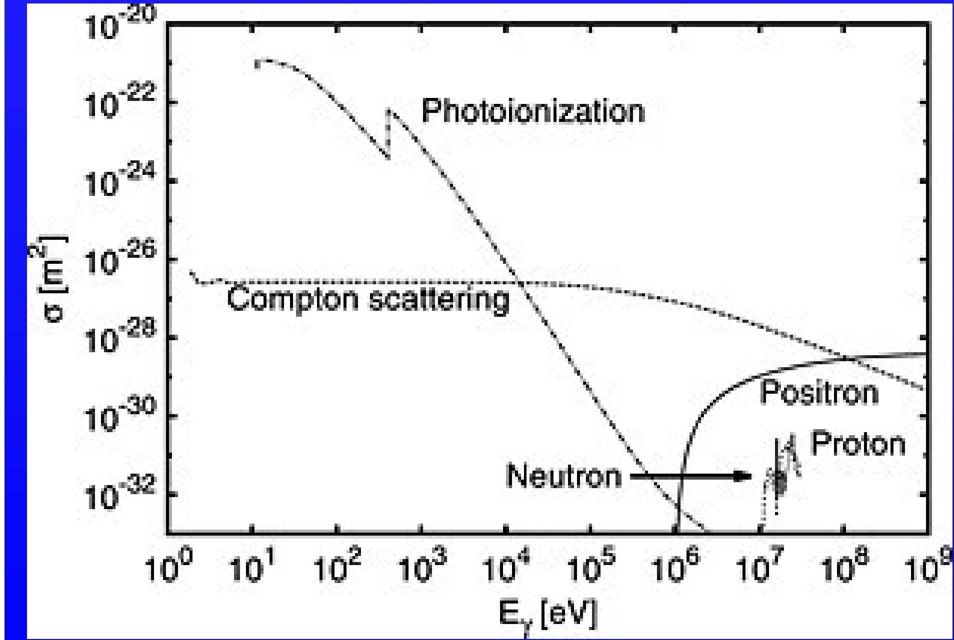
Differential cross section:
it is the differential power scattered in dΩ normalized to the incoming power and to the density of scattering objects

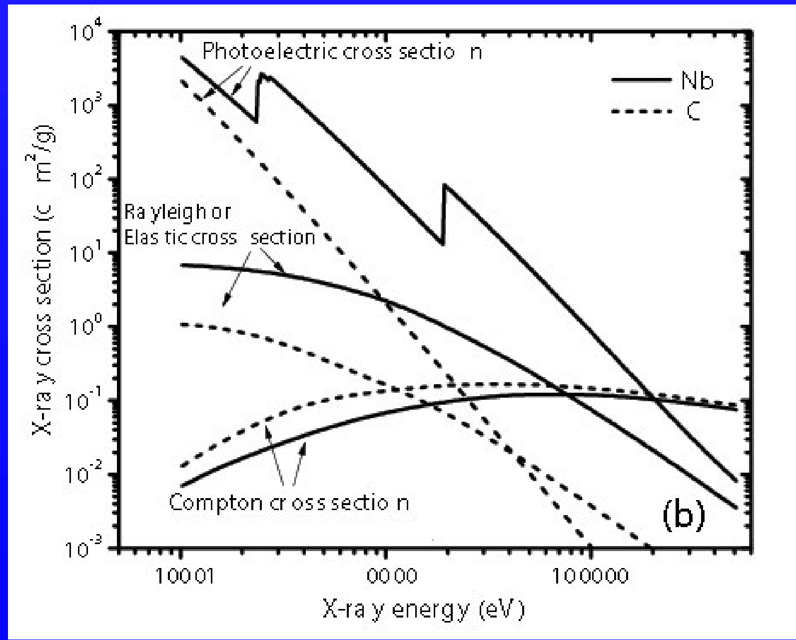
Double Differential Cross Section $d^2\sigma/d\Omega dE$

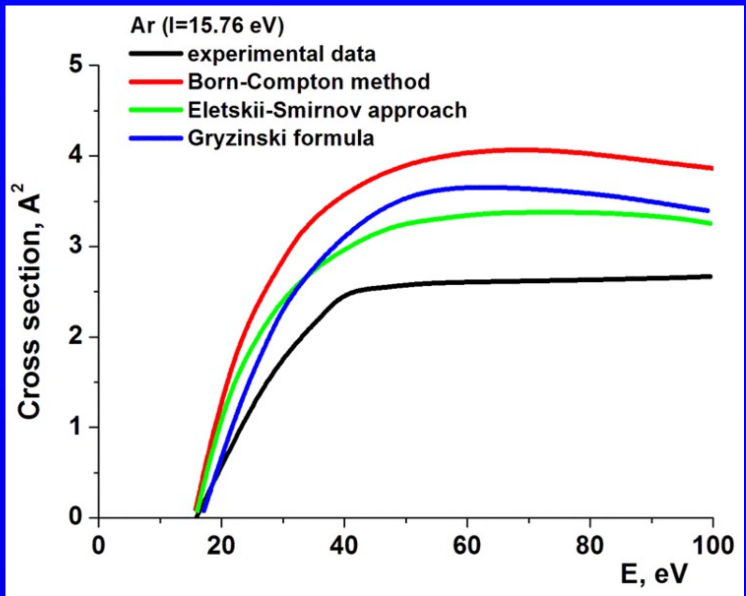


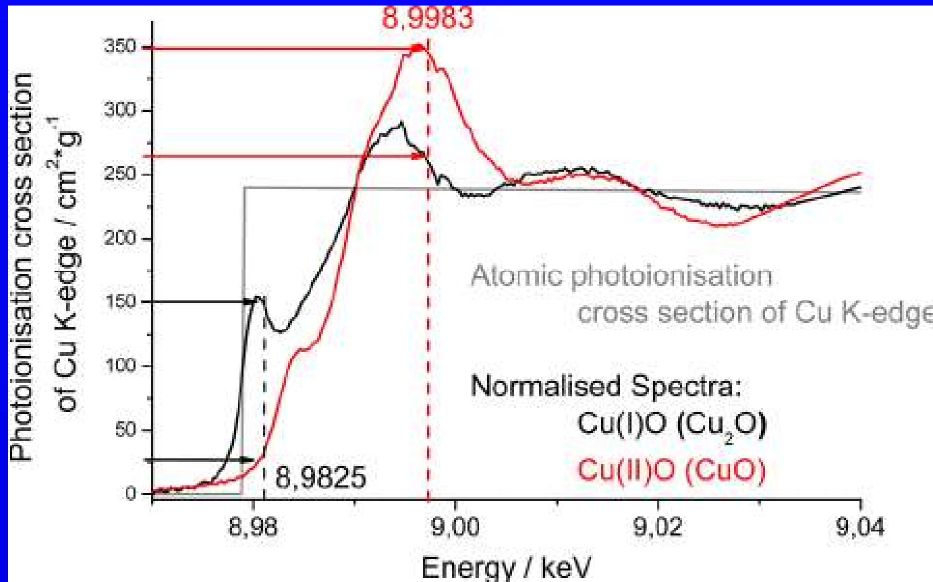
$$\frac{d^2\dot{N}_{events}}{d\Omega dE_k} = \dot{N}_{photons} \times (\rho dx) \times \left(\frac{d^2\sigma}{d\Omega dE_k} \right)$$

Total cross section σ of atoms



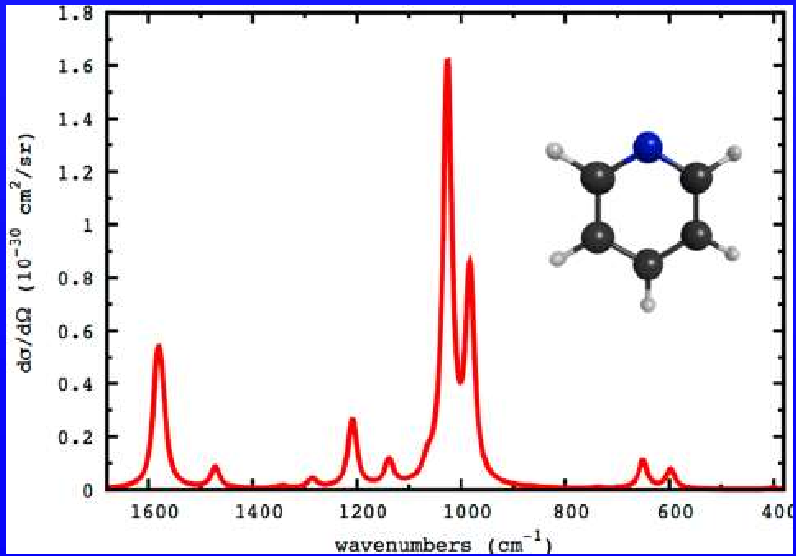




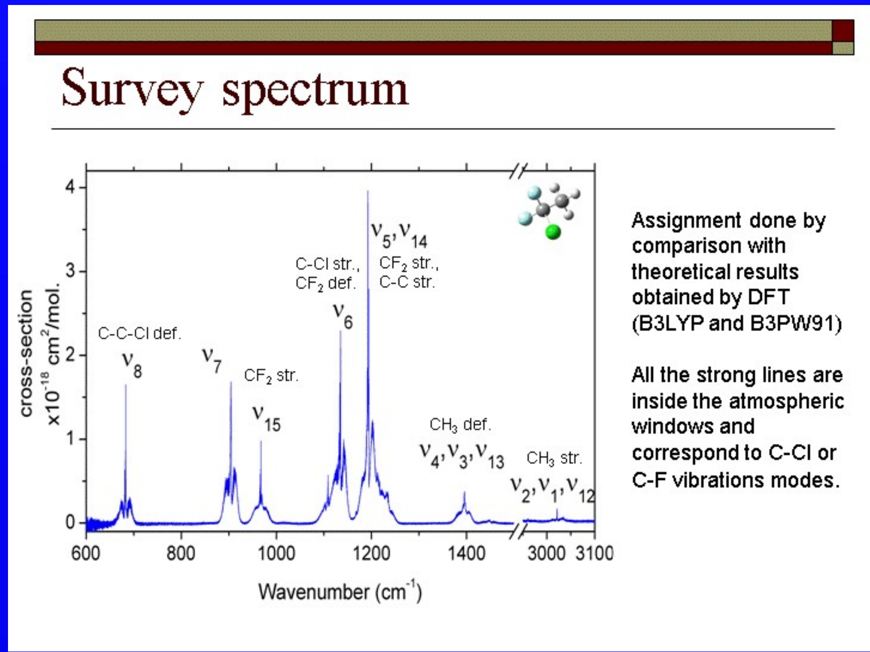


Total cross section σ of atoms

Raman scattering cross section



IR vibrational cross section



Matter ←Interaction→ Radiation I

Classical description

Radiation:

Electromagnetic waves are described by Maxwell equations

Matter:

Macroscopic optical constants: index of refraction, absorption coefficient, reflection coefficient, dielectric function…

Two independent constant are enough in isotropic materials

Deeper:
microscopic origin of optical constants:
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: $\mu(\lambda)$

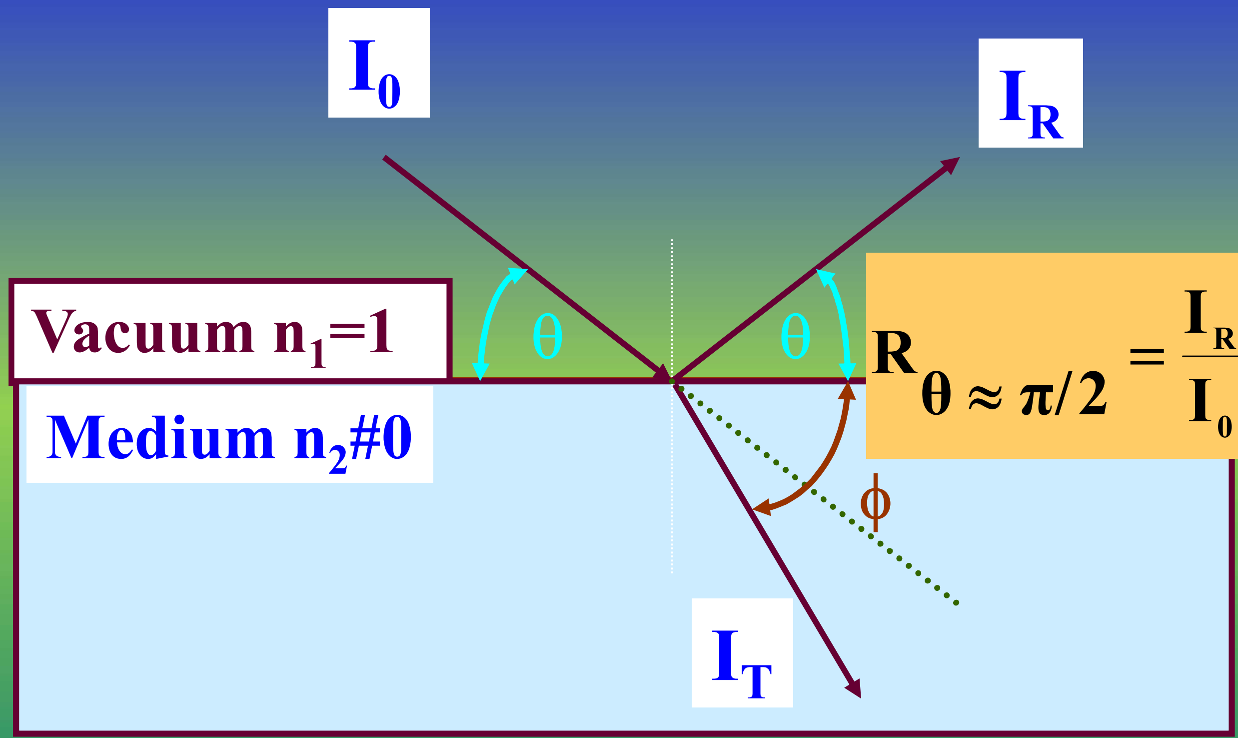
Interaction: Lorentz force

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

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

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

Reflection and refraction



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

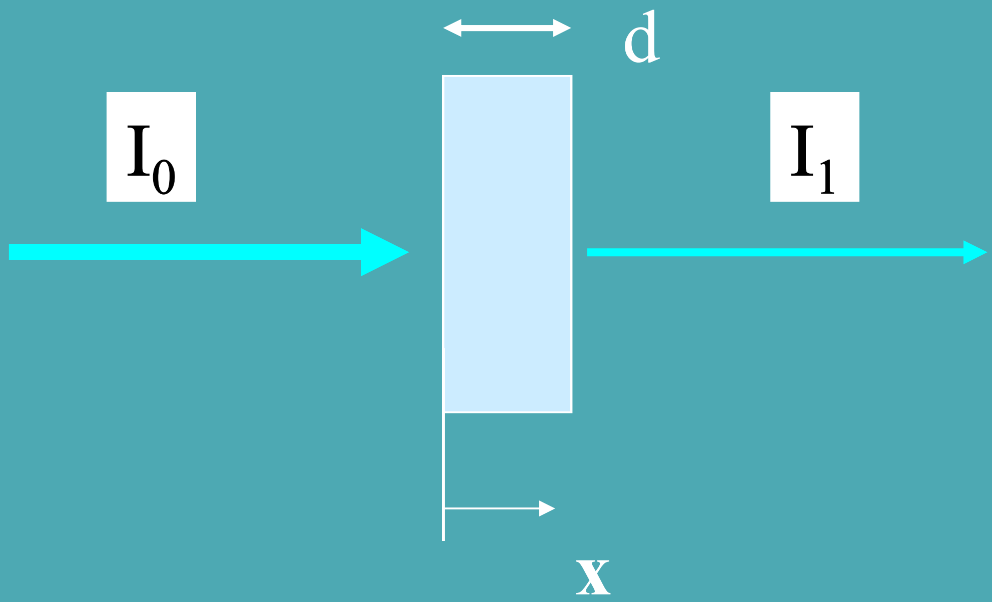
Snell law of refraction

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

n_i is the index of refraction

n is ~ to 1/v → v= c/n

Absorption coefficient



$$I(x) = I_0 e^{-\mu x} \Rightarrow I_1 = I_0 e^{-\mu d}$$

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

Plane Wave in vacuum

$$\nabla^2\vec{E} - \mu_0\varepsilon_0\frac{\partial^2\vec{E}}{\partial t^2} = 0$$

$$\nabla^2\vec{B} - \mu_0\varepsilon_0\frac{\partial^2\vec{B}}{\partial t^2} = 0$$

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

The radiation is a wave and moves with a speed equal to c

Plane waves

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

Real part $\rightarrow \vec{E} = \vec{E}_0 \cos\left(\vec{k}\vec{r} - \omega t\right)$

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

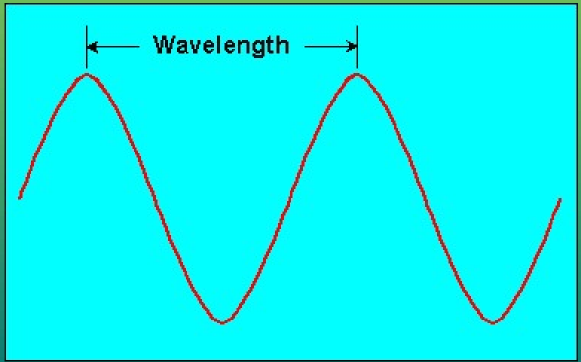
Plane Wave in vacuum

Plane waves

$$\vec{E} = \vec{E}_0 \cos\left(\vec{k}\vec{r} - \omega t\right) \qquad \vec{B} = \vec{B}_0 \cos\left(\vec{k}\vec{r} - \omega t\right)$$

$\vec{k}$ **is the wavevector;**

it gives the direction of the propagation



$$\left|\vec{k}\right| x + 2\pi = \left|\vec{k}\right|\left(x + \lambda_0\right)$$

The modulus of k gives the wavelength of the radiation

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

Plane Wave in vacuum

Plane waves

$$\vec{E} = \vec{E}_0 \cos\left(\vec{k}\vec{r} - \omega t\right) \qquad \vec{B} = \vec{B}_0 \cos\left(\vec{k}\vec{r} - \omega t\right)$$

Dispersion relation

$$\lambda_0 \nu = \frac{\lambda_0}{T} = \lambda_0 \frac{\omega}{2\pi} = c$$

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

$$-k^2 \vec{E} + \frac{\omega^2}{c^2}\vec{E} = 0 \rightarrow k = \frac{\omega}{c} \rightarrow \frac{2\pi}{\lambda_0} = \frac{2\pi\nu}{c} \rightarrow \lambda_0 \nu = c$$

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

Plane Wave in vacuum

$$\lambda_0 \nu = \frac{\lambda_0}{T} = \lambda_0 \frac{\omega}{2\pi} = c$$

$$\left|\vec{\mathbf{k}}\right| = \frac{\mathbf{2\pi}}{\boldsymbol{\lambda}_0}$$

$$\vec{\mathbf{k}} = \frac{\mathbf{2\pi}}{\boldsymbol{\lambda}_0}\hat{\mathbf{k}} = \frac{\boldsymbol{\omega}}{\mathbf{c}}\hat{\mathbf{k}}$$

Plane waves

$$\vec{E} = \vec{E}_0 e^{i\left(\vec{k}\cdot\vec{r} - \omega t\right)} \Rightarrow \vec{E} = \vec{E}_0 e^{i\frac{2\pi}{\lambda_0}\left(x - ct\right)} \Rightarrow$$

$$\vec{E} = \vec{E}_0 \cos\frac{2\pi}{\lambda_0}\left(x - ct\right) \Rightarrow \vec{E} = \vec{E}_0 \cos\left(\frac{2\pi x}{\lambda_0} - \omega t\right)$$

Plane Wave in vacuum

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

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

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

$$\mathbf{w(t)} = \frac{1}{2}\varepsilon_0 \mathbf{E(t)}^2 + \frac{1}{2\mu_0}\mathbf{B(t)}^2$$

$$\frac{1}{2}\varepsilon_0 \mathbf{E}^2 = \frac{1}{2\mu_0}\mathbf{B}^2$$

$$w(t) = \varepsilon_0 E^2 = \frac{B^2}{\mu_0}$$

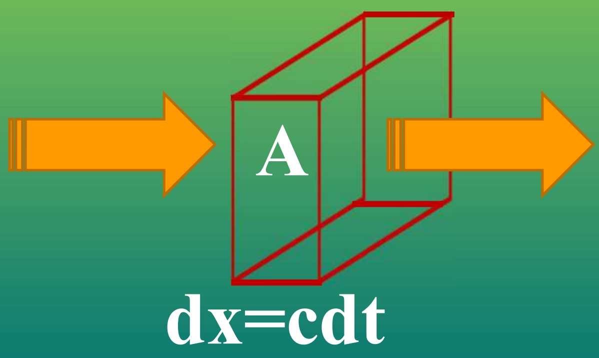
$$\overline{w} = \frac{1}{2}\varepsilon_0 E_0^2$$

Plane Wave in vacuum

$$w(t) = \frac{1}{2}\varepsilon_0 E(t)^2 + \frac{1}{2\mu_0}B(t)^2 = \varepsilon_0 E(t)^2$$

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

Intensity I:
Mean energy flow per unit time and unit area



$$I = \frac{1}{A}\frac{\overline{w}dV}{dt} = \frac{1}{A}\frac{\overline{w}\left(Acdt\right)}{dt} = \overline{w}c = \frac{1}{2}\varepsilon_0 E_0^2 c$$

The intensity I of the beam is: $\mathrm{I} = \overline{\mathrm{w}}\mathrm{c} = \mathrm{c}\frac{1}{2}\varepsilon_0 \mathrm{E}_0^2$

Plane Wave in matter

$$\nabla^2\vec{E} - \mu\varepsilon\frac{\partial^2\vec{E}}{\partial t^2} = 0$$

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

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

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

$\vec{k}$ is the wavevector

$$\varepsilon = \varepsilon_0\varepsilon_r$$

$$\mu = \mu_0\mu_r \cong \mu_0$$

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

Plane Wave in matter

$$\nabla^2\vec{E} - \mu\varepsilon\frac{\partial^2\vec{E}}{\partial t^2} = 0$$

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

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

Dispersion relation:

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

$\lambda 2\pi\nu = 2\pi c/n$

$\lambda = \lambda_0/n$

E.M. Waves in matter

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

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

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

In the matter the light is slower than in the vacuum

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

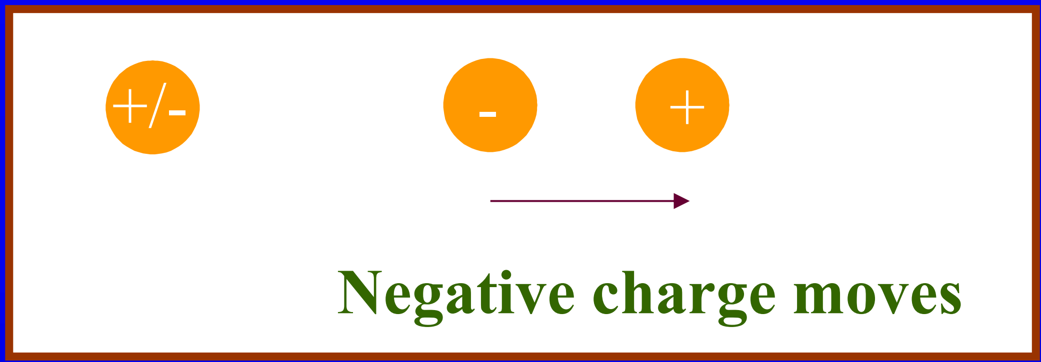
In the matter the wavelength is shorter than in the vacuum

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

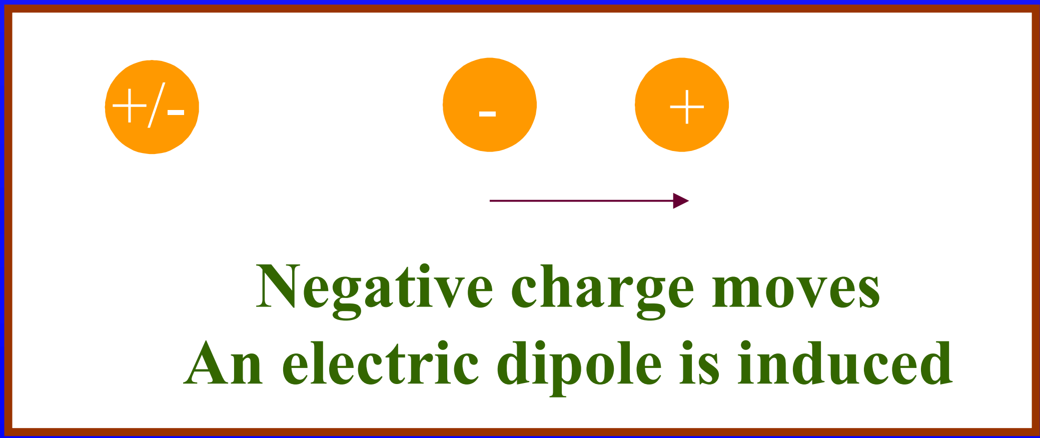
Origin of the dielectric function and of the index of refraction (qualitative)

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

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



Origin of the dielectric function and of the index of refraction (qualitative)

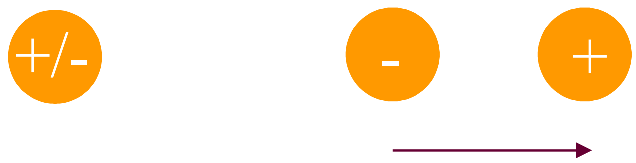


Dipoles generate additional electric fields that add to the external (radiation) one

The dielectric function describe the modifications induced by the microscopic dipoles to the electric field

Origin of the dielectric function and of the index of refraction (qualitative)

$$\vec{\mathbf{E}} = \frac{\varepsilon_0}{\varepsilon}\vec{\mathbf{E}}_{vac.}$$



The induced electric dipole and the electric field are not in phase (because of the electron and nuclei mass)

The dielectric function is a complex quantity with a real and an imaginary part

$$\varepsilon = \varepsilon_1 + i\varepsilon_2 = |\varepsilon| e^{i\phi}$$

Origin of the dielectric function and of the index of refraction (qualitative)

$$\vec{E} = \frac{\varepsilon_0}{\varepsilon} E_{vac.} = \frac{\varepsilon_0}{|\varepsilon| e^{i\phi}} \vec{E}_{vac.} = \frac{\varepsilon_0}{|\varepsilon|} \vec{E}_{vac.} e^{-i\phi}$$

- **Amplitude relation is determined by the modulus (~ real 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

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

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

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

Amplitude reduction

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

Intensity $I \propto E^2$

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

Absorption coefficient μ

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

Kramers-Kronig Relation

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

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

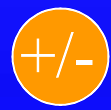
$$\varepsilon_2(\omega) = \frac{2\omega}{\pi}\int_0^{\infty} \frac{\varepsilon_1(\overline{\omega}) - 1}{\overline{\omega}^2 - \omega^2}\, d\overline{\omega}$$

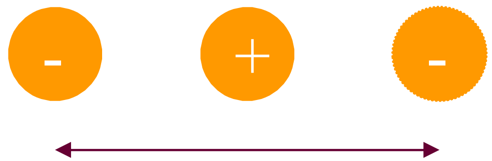
Causality: the dipole moment P(t) at time t is determined only by the values of the electric field at time t'≤ t

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

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

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

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

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

Dielectric function

N = number of atoms per unit volume

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

$$\varepsilon_r = 1 + \chi$$

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

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

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

Electric field and dielectric function
(in simple word)

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

$$\varepsilon_r = 1 + \chi$$

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

$$\vec{E}_0 e^{i(\vec{k}\vec{r} - \omega t)} \rightarrow \vec{E}_{tot.} = \frac{\vec{E}_0 e^{i(\vec{k}\vec{r} - \omega t)}}{\varepsilon_r}$$

Real and imaginary part of the dielectric function

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

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

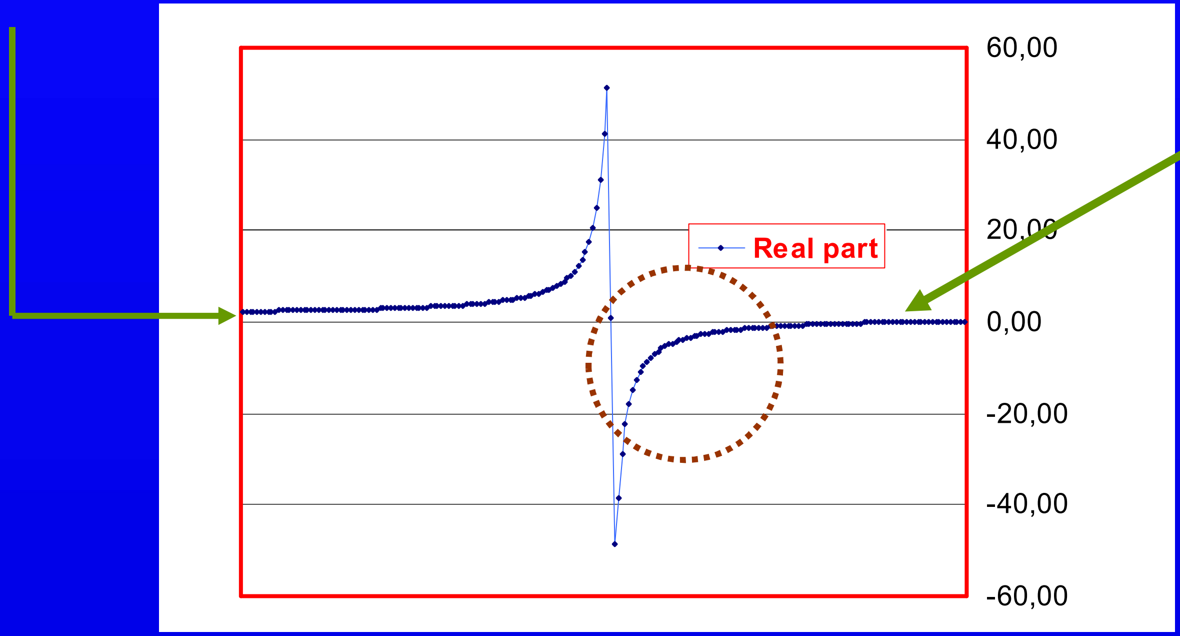
$$\varepsilon_2 = \frac{NZe^2}{\varepsilon_0 m} \frac{\gamma\omega}{\left(\omega_0^2 - \omega^2\right)^2 + \left(\gamma\omega\right)^2}$$

General behavior of the real part of the dielectric function

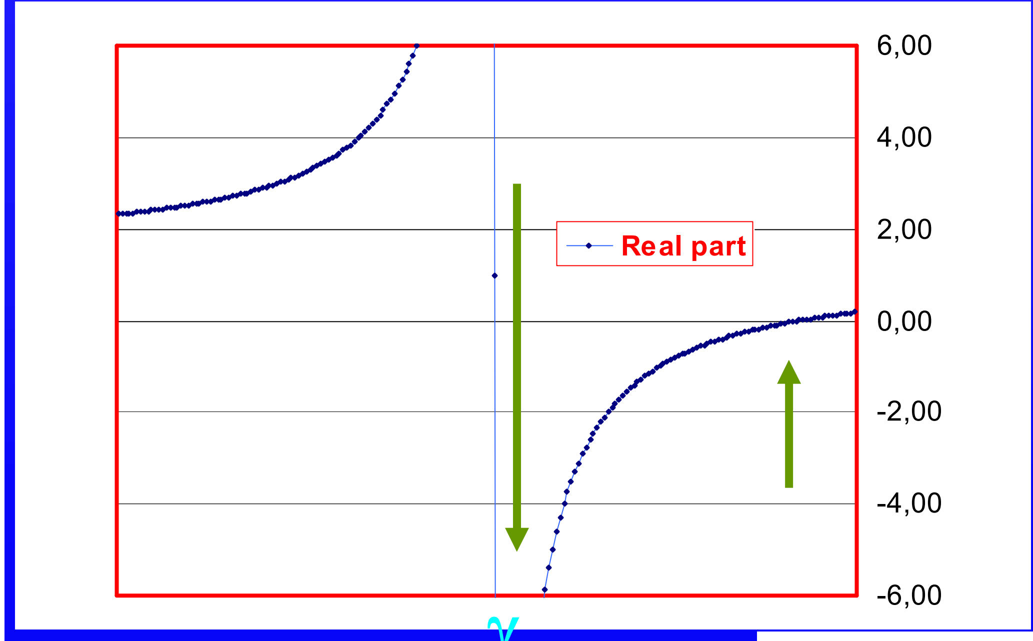
$$\varepsilon_1 = 1 + \frac{NZe^2}{\varepsilon_0 \mathbf{m}} \frac{\omega_0^2 - \omega^2}{\left(\omega_0^2 - \omega^2\right)^2 + (\gamma\omega)^2}$$

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

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



Behavior of the real part above ω_0



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

$\beta = 0$

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

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

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

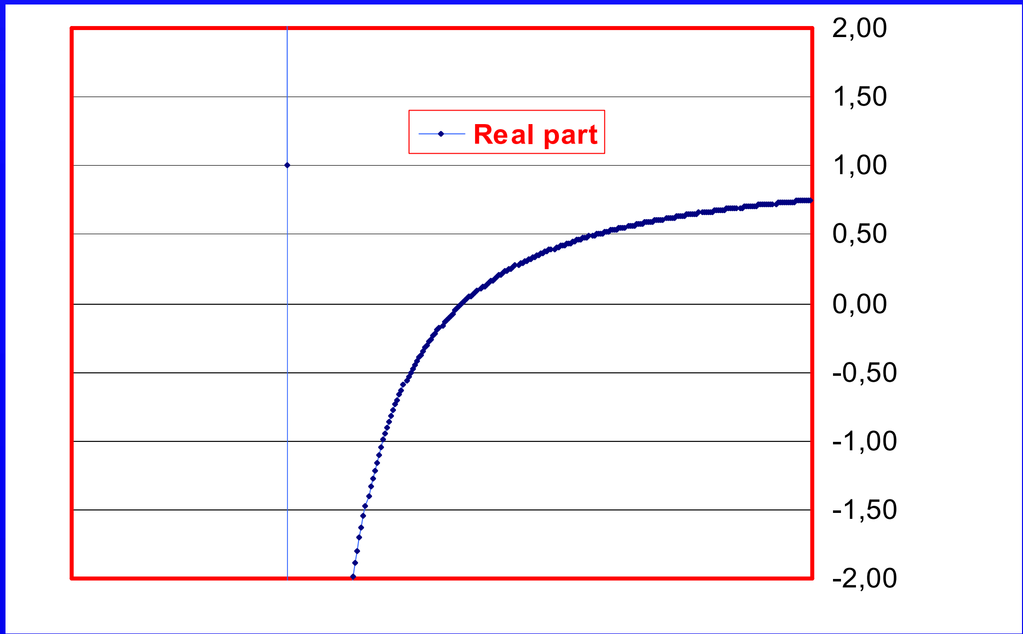
There is no propagation into the matter
no energy exchange

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

is called "extinction length"

Behavior of the real part at high energy

$$\varepsilon_1(\omega >> \omega_0) = 1 - \frac{NZe^2}{\varepsilon_0 m \omega^2}$$



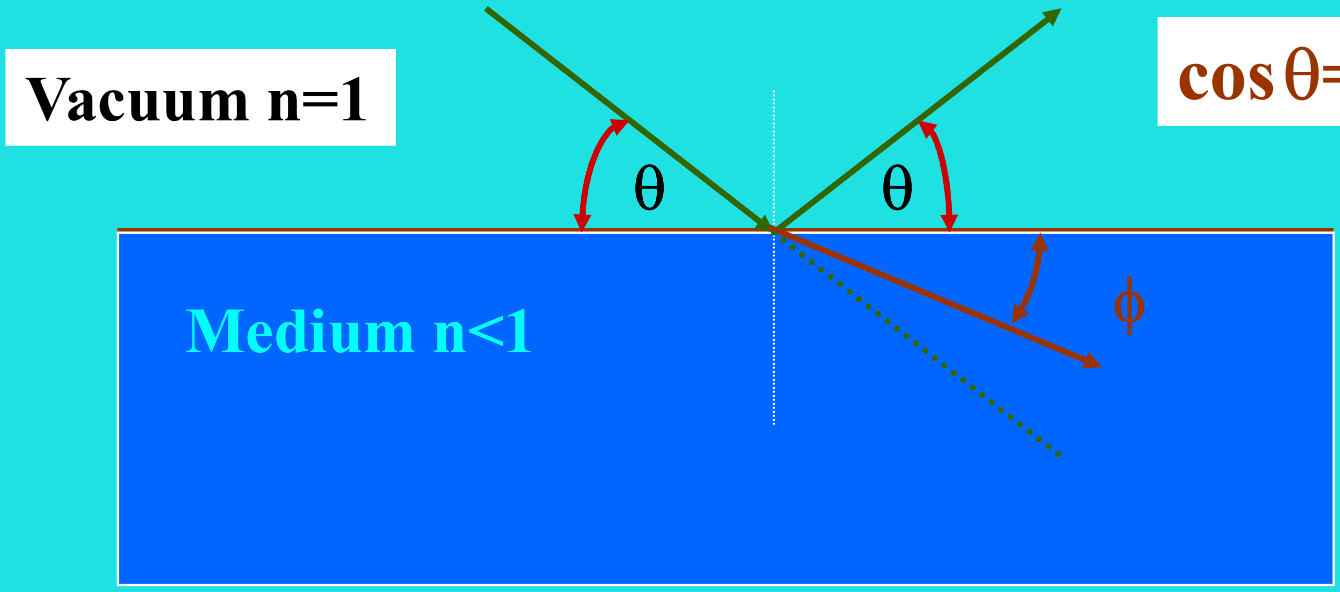
$$\varepsilon_1(\omega >> \omega_0) < 1$$

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



$\cos\theta = n\cos\phi$

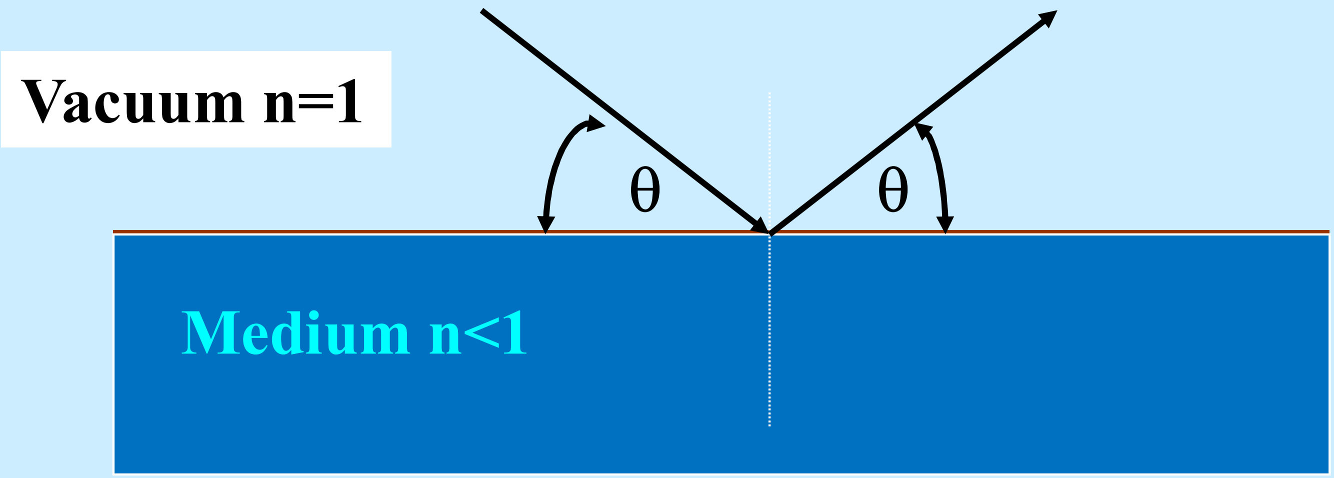
The critical angle θ_c is defined by $\cos\phi=1$

→

$\cos\theta_c = n$

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

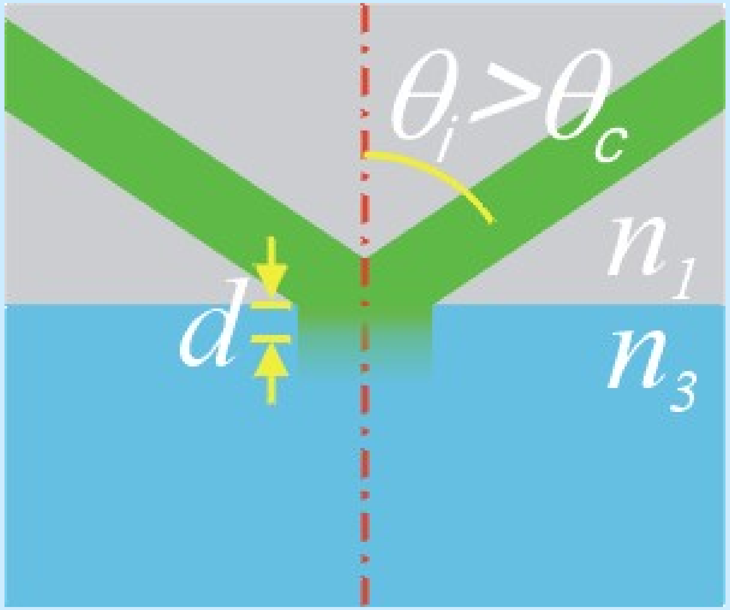
Use of Total Reflection



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

- X-ray Mirrors
- Surface Diffraction
- REFLEXAFS

Total Reflection: evanescent wave



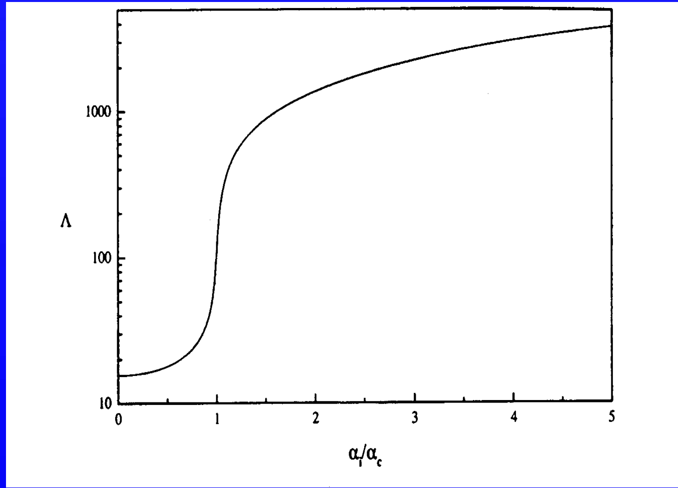
REFLEXAFS: evanescent wave

$$E_T = E_o T e^{ik_{Tx}x} e^{-kn_T z\sqrt{\alpha_c^2-\alpha_i^2}}$$

Λ = penetration length

$$\Lambda = \frac{1}{2kn\sqrt{\alpha_c^2-\alpha_i^2}}$$

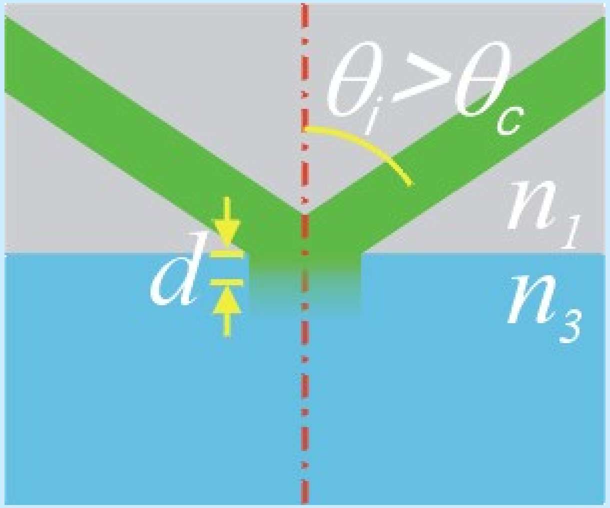
$$\frac{1}{2kn\alpha_c} = 12\ \dot{A}\ (Au)$$



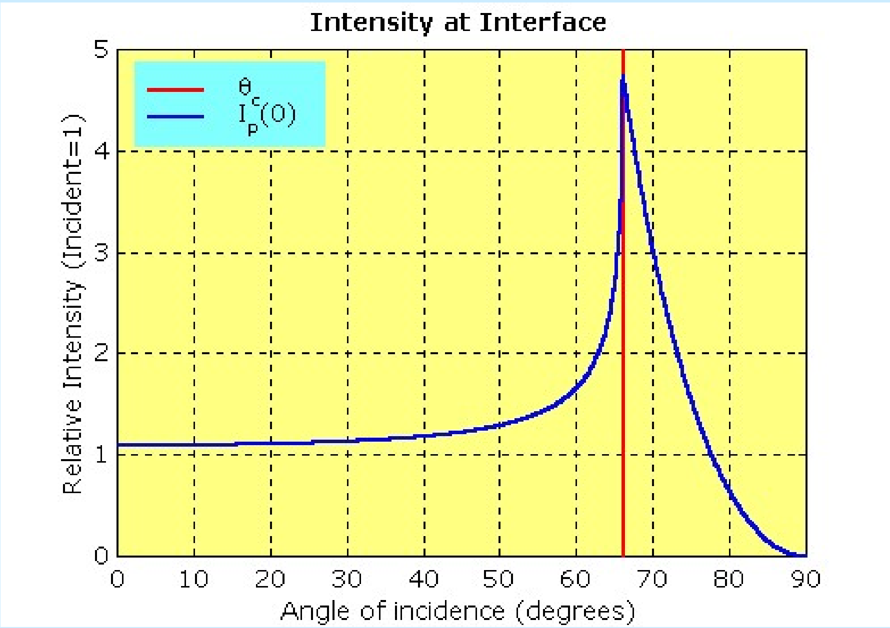
Under total reflection condition the X-ray beam is confined in a layer of few tens of A from the surface

Surface sensitivity

Total Reflection: evanescent wave



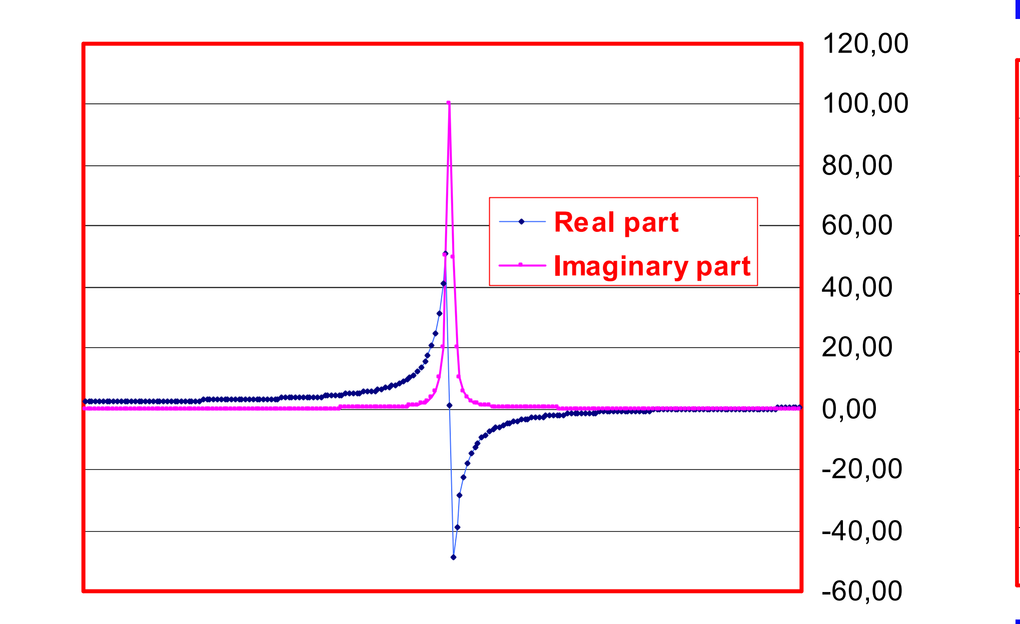
z=0

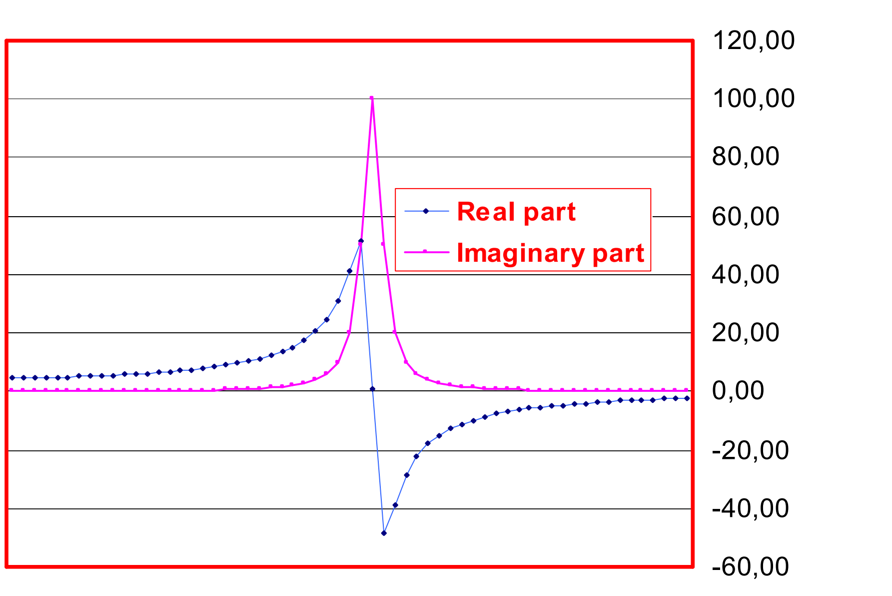


Somewhat counterintuitively, the amplitude of the evanescent wave can actually be greater than the incident one.

Behavior of the imaginary part

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





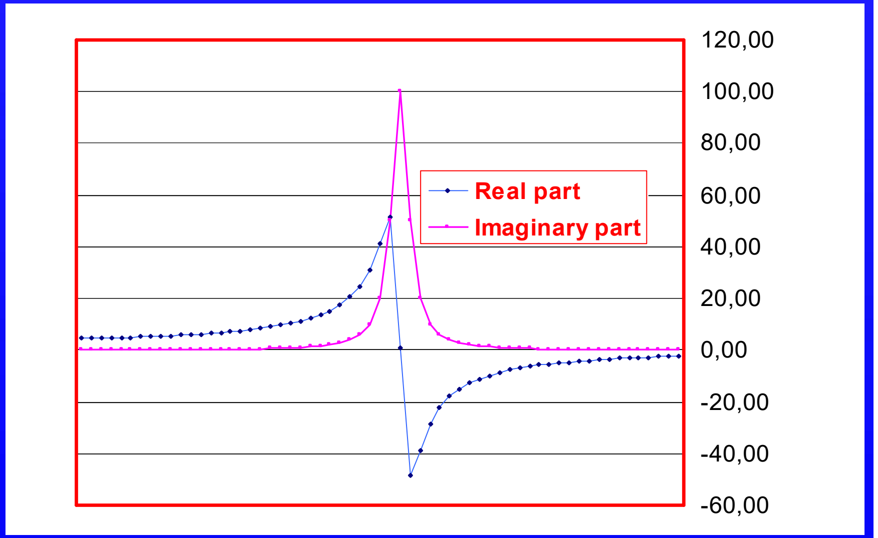
$$\varepsilon_2(\omega >> \omega_0) = \frac{NZe^2}{\varepsilon_0 m} \frac{\gamma}{\omega^3}$$

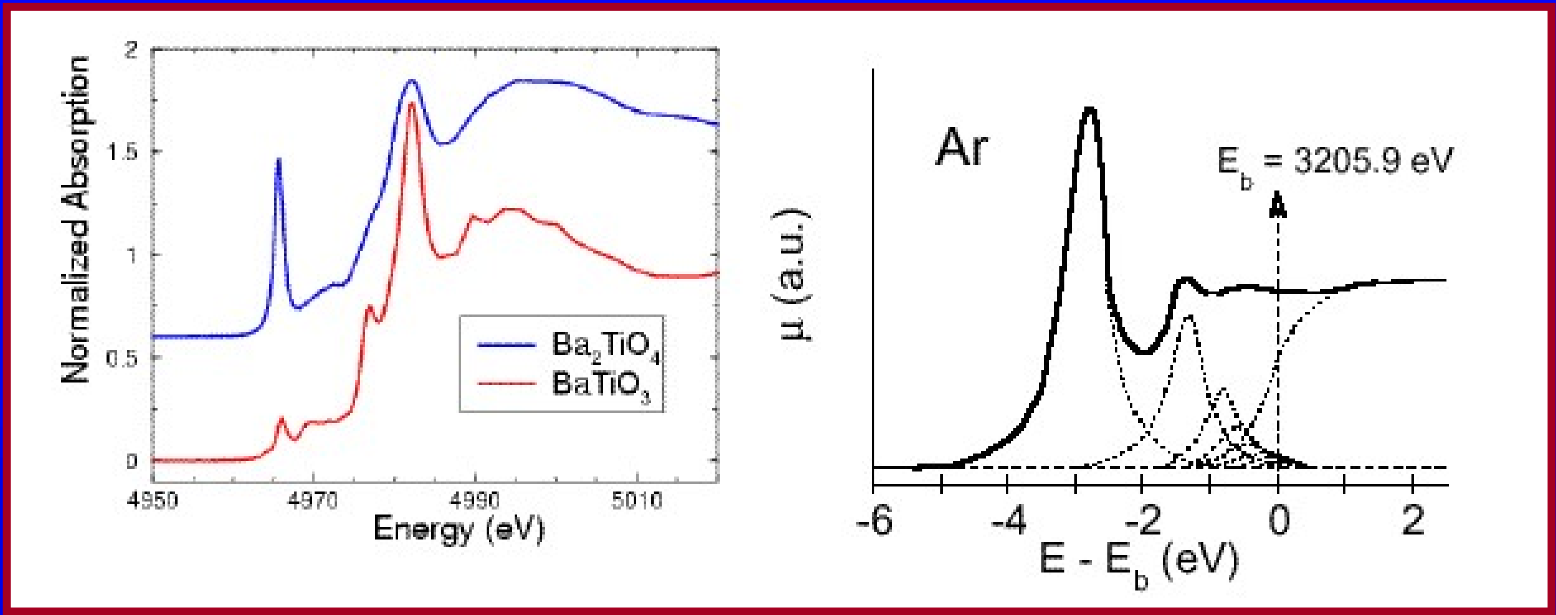
$$\beta = \frac{NZe^2}{2\varepsilon_0 m} \frac{\gamma}{\omega^3}$$

Absorption coefficient

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

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

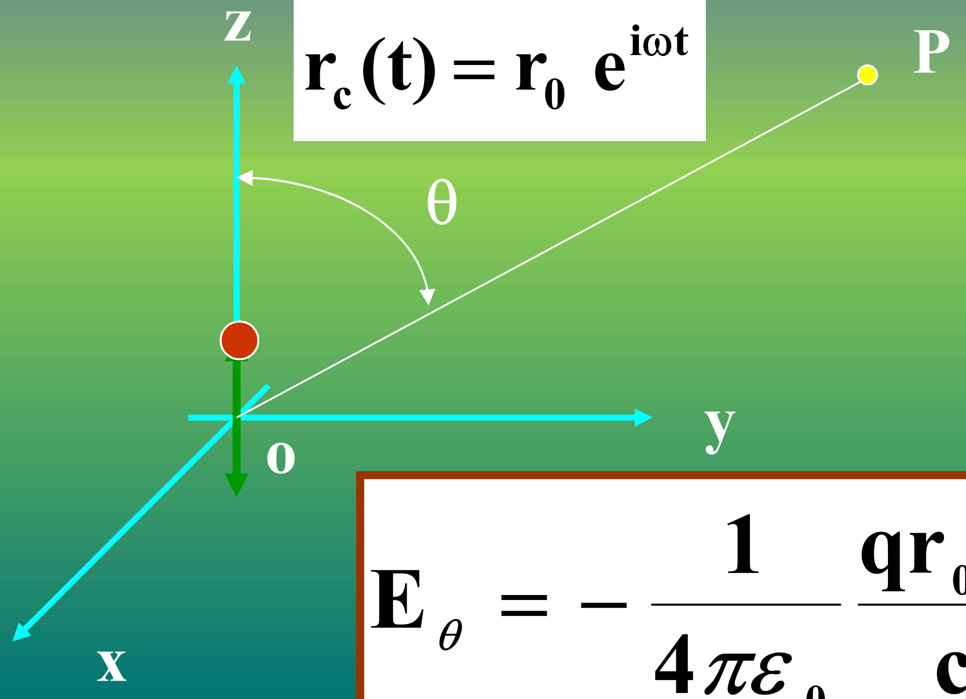




Scattering

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

$$r_c(t) = r_0\ e^{i\omega t}$$



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

The electric field is in the plane (OzP)

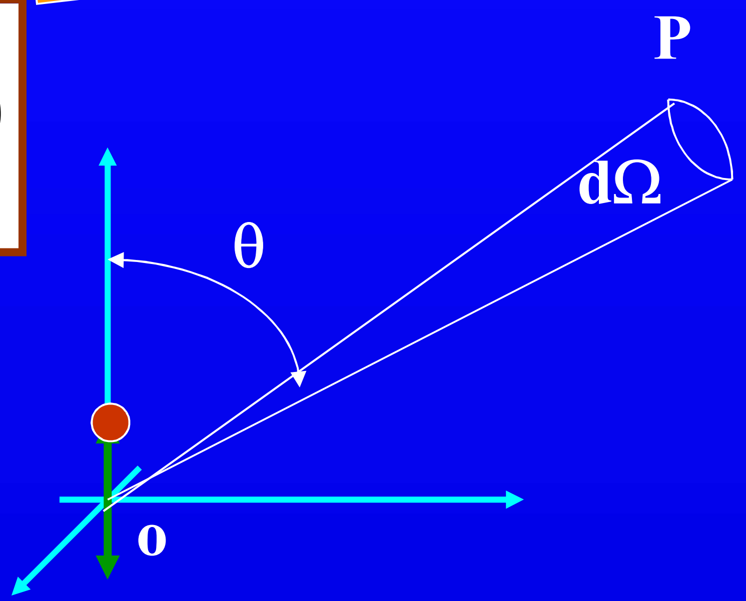
Scattering by a free electron ($\omega >> \omega_0$)

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

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

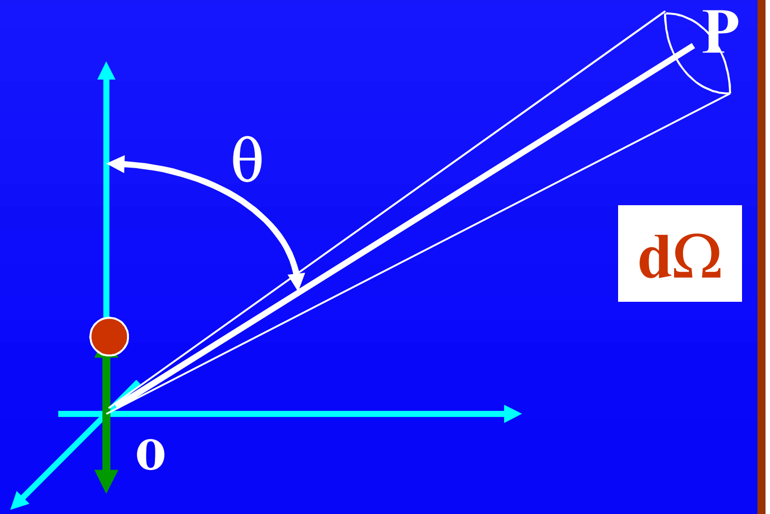
$$\vec{r}_e(t) = -\frac{e}{m\omega^2}\vec{E}_0 e^{i\omega t}$$

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



Differential cross section

Differential cross section (normalized differential scattered power)



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

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

$$\frac{1}{2}\frac{cE_0^2}{(4\pi)^2\varepsilon_0}\left(\frac{e^2}{mc^2}\right)^2 \sin^2\theta\, d\Omega$$

$$\frac{d\sigma}{d\Omega} = \frac{1}{I_0}\frac{dW}{d\Omega} = \frac{1}{{}^1\!/_2\,\varepsilon_0 c E_0^2}\frac{dW}{d\Omega} = \left(\frac{1}{4\pi\varepsilon_0}\frac{e^2}{mc^2}\right)^2 \sin^2\theta$$

Electron classical radius

Electron classical radius

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

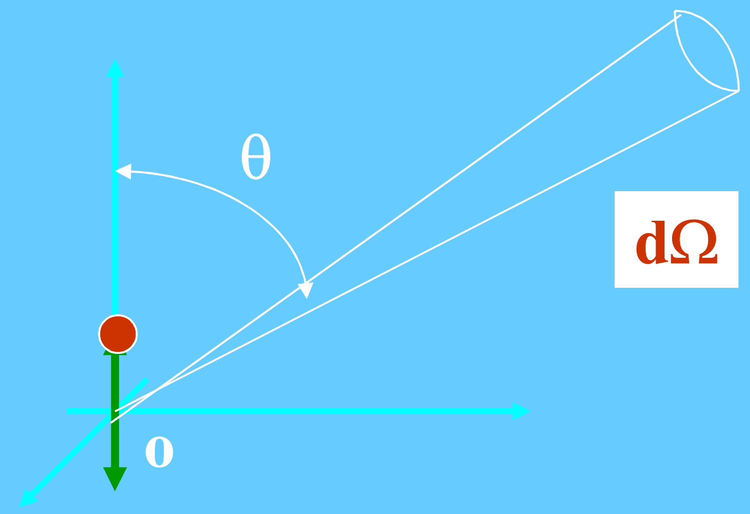
r_e is called the electron classical radius=2.818 10^{-15} m

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

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

Total scattering cross section: polarized radiation

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



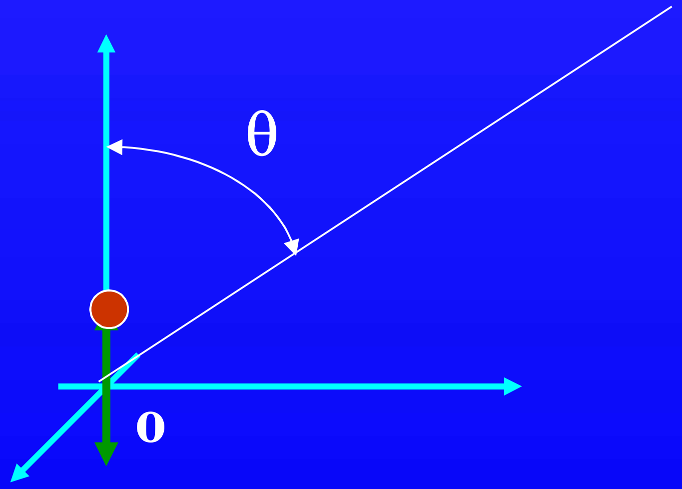
Linear Polarization

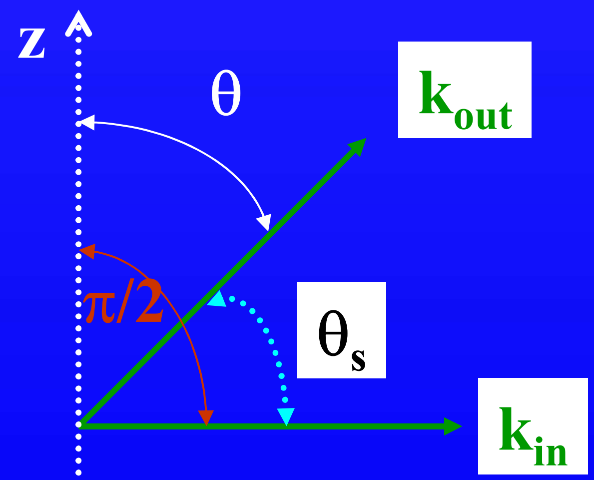
$$\sigma = \int r_e^2 \sin^2\theta d\Omega = r_e^2 \int_0^{\pi} \sin^2\theta\, 2\pi \sin\theta d\theta =$$

$$= r_e^2\, 2\pi \int_0^{\pi} \sin^3\theta d\theta = \frac{8\pi}{3} r_e^2 = 6.7x10^{-29}\ m^2\ /\ electron$$

Thomson cross section

Scattering Plane

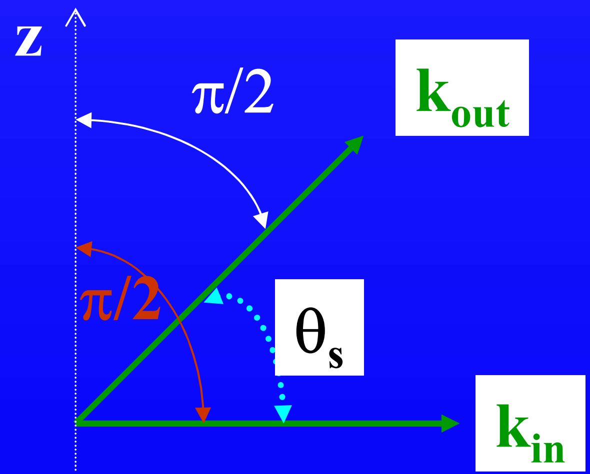




The plane formed by the direction of the incoming and outcoming radiation is called is scattering angle It is the plane formed by k_{in} and k_{out}

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

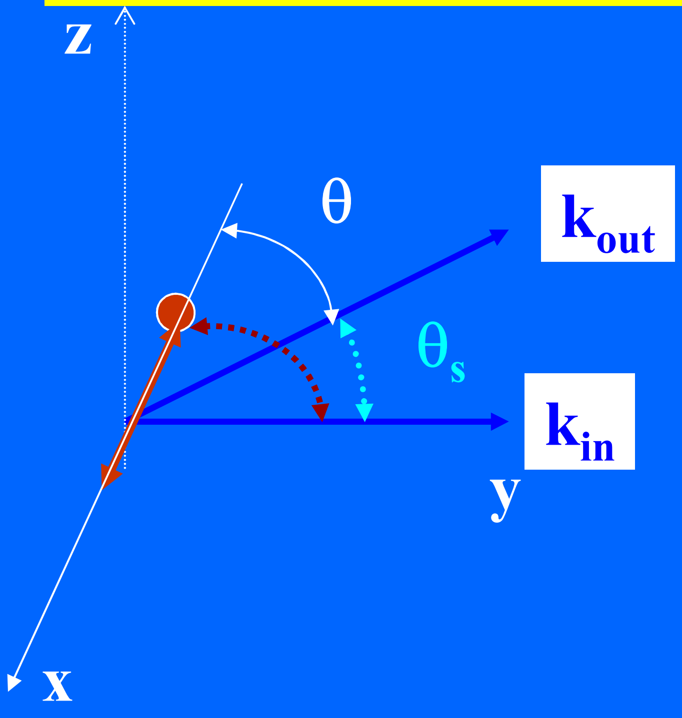


Incoming radiation polarized perpendicular to the scattering plane π_s
→θ=π/2 → sinθ=1
Scattering radiation perpendicular to the scattering plane

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

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

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

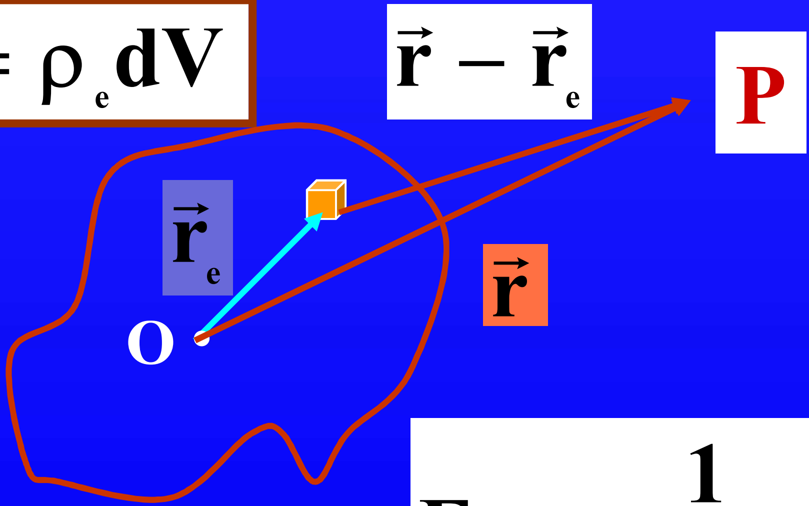
$$\theta + \theta_s = \frac{\pi}{2}$$

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

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

Charge distributions: Scattering Factor

$$dN_e = \rho_e dV$$



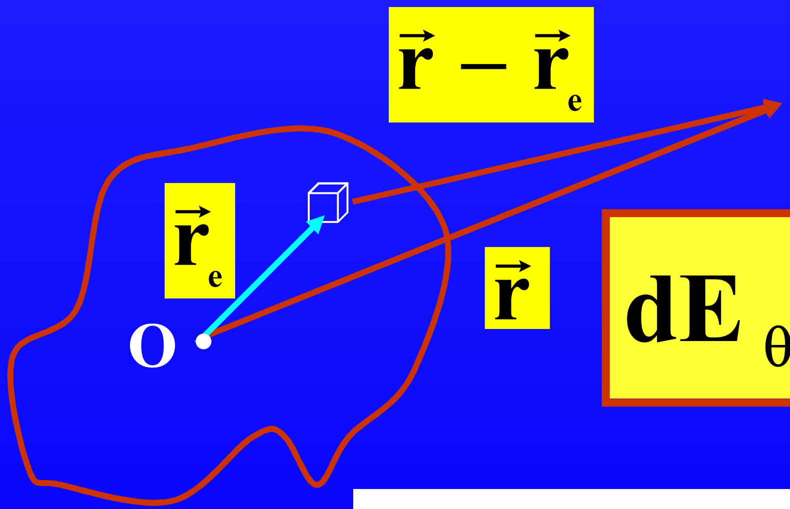
$$E_{in} = E_0 e^{i\left(\vec{k}_{in}\vec{r} - \omega t\right)}$$

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

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

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

Scattering Factor IV



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

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

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

f is called the scattering factor

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

Scattering Factor V

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

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

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 …

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

→ **Phase Problem**

Overview

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

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

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

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

Anomalous correction

Electrons are not free but are bound

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

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

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

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

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

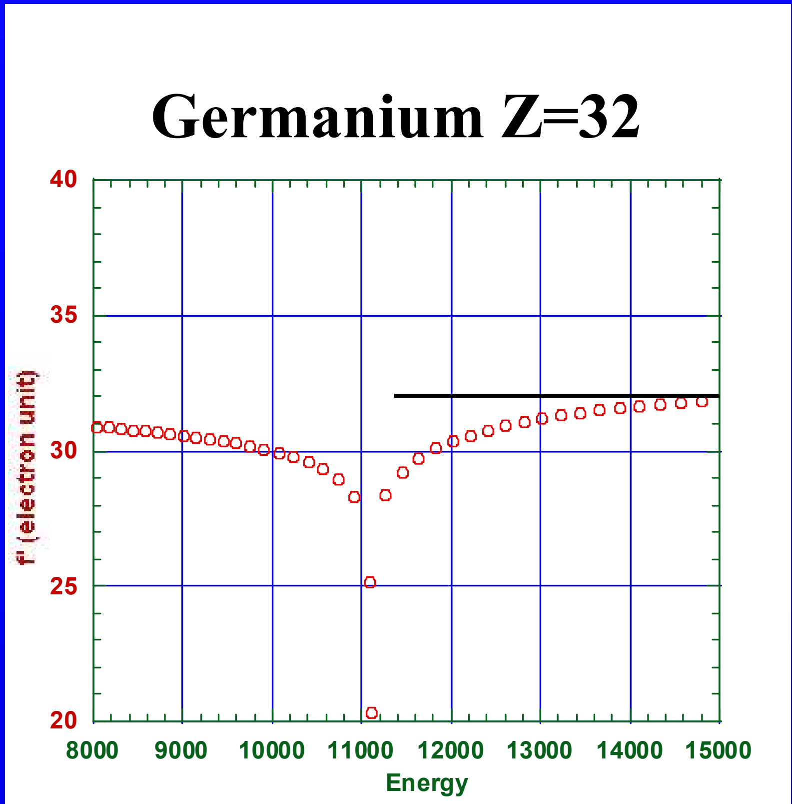
$\omega >> \omega_0$

$$f_i = f_i^{free}$$

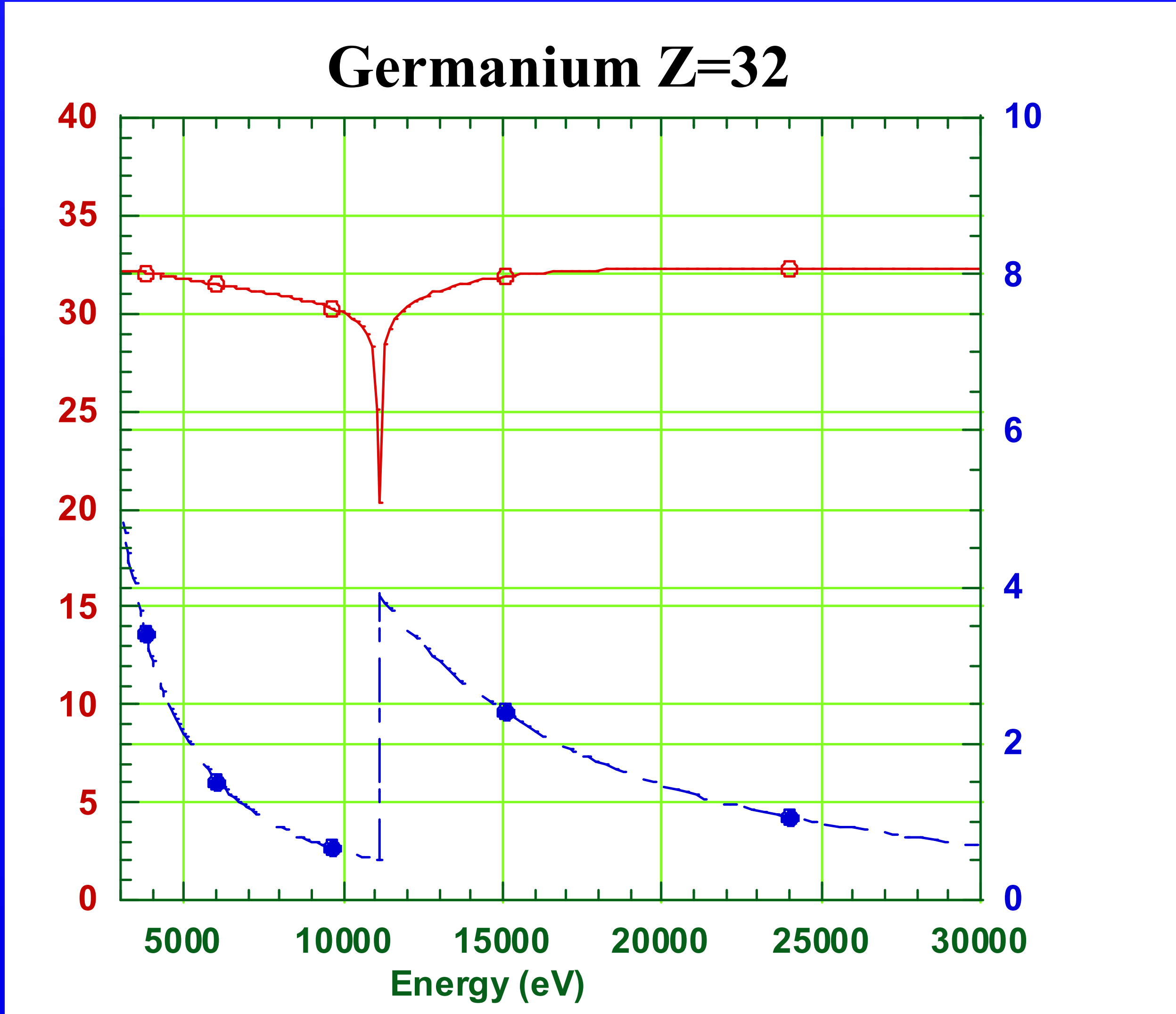
At high frequency the electron behaves like free electrons

Anomalous correction for atoms

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



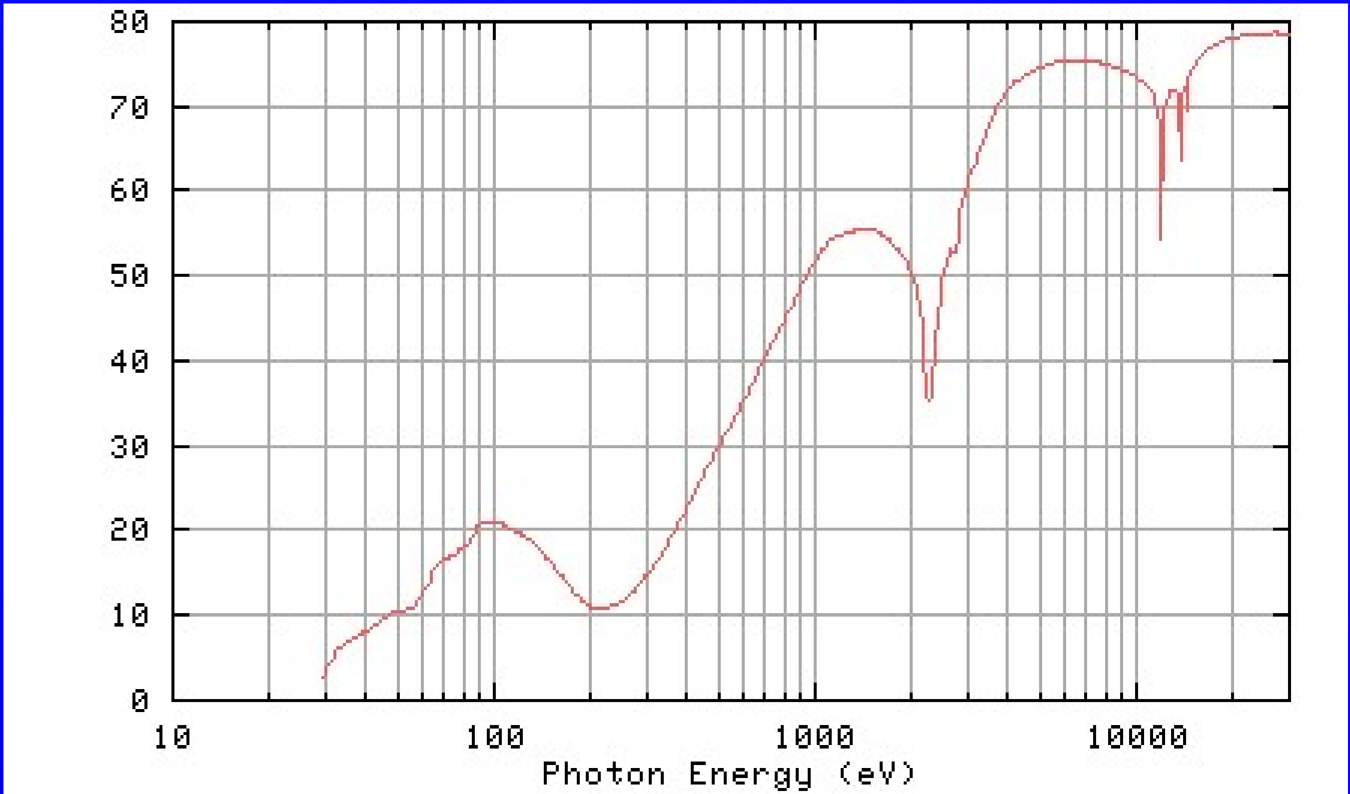
Anomalous correction for atoms: f’ and f” of Ge



Anomalous correction for Au

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

Gold Z=



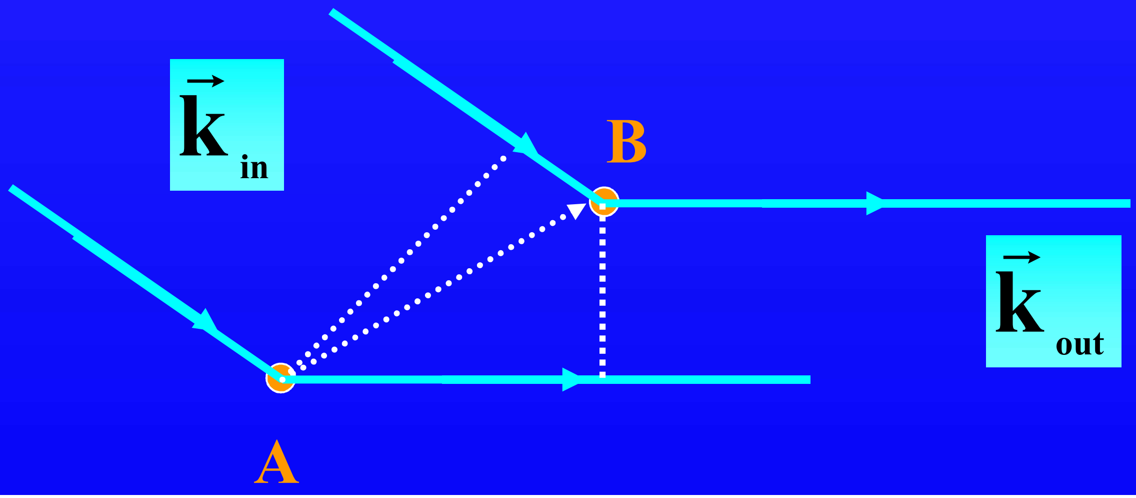
KK & Optical theorem

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

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

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

Anomalous scattering to solve the phase problem



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

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

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

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

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 → $I(q) \neq I(-q)$

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

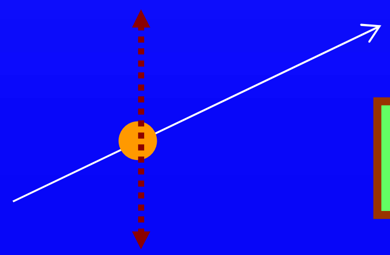
$$\left|\left(f_A + f_B e^{-i\vec{q}(\vec{r}_A - \vec{r}_B)}\right)\right|^2 = \left(f_A + f_B e^{-i\vec{q}(\vec{r}_A - \vec{r}_B)}\right)\left(f_A^* + f_B^* e^{+i\vec{q}(\vec{r}_A - \vec{r}_B)}\right)$$

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

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

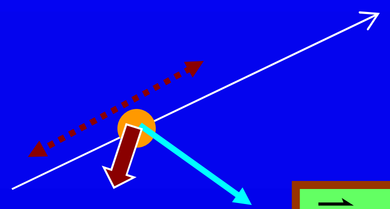
Magnetic Interactions

An electromagnetic wave transport both an electric and a magnetic field



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

Thomson scattering

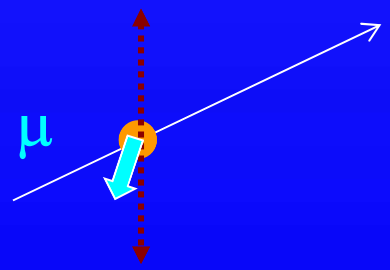


$$E = -\vec{\mu}\vec{H}$$

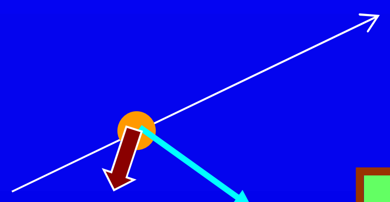
$$\vec{F} = \mathrm{grad}\left(\vec{\mu}\vec{H}\right)$$

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

Magnetic Interactions



Magnetic dipole oscillations

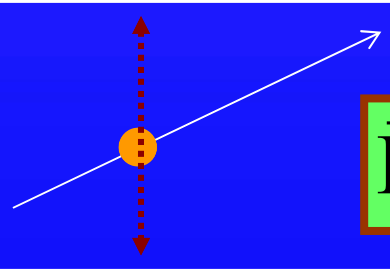


Torque

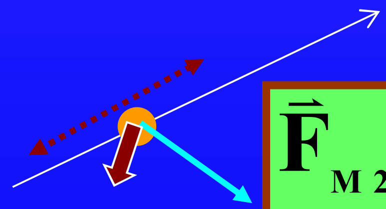
$$\vec{M} = \left(\vec{\mu} \times \vec{H}\right)$$

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

Strength of Magnetic Interactions



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



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

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

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

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)

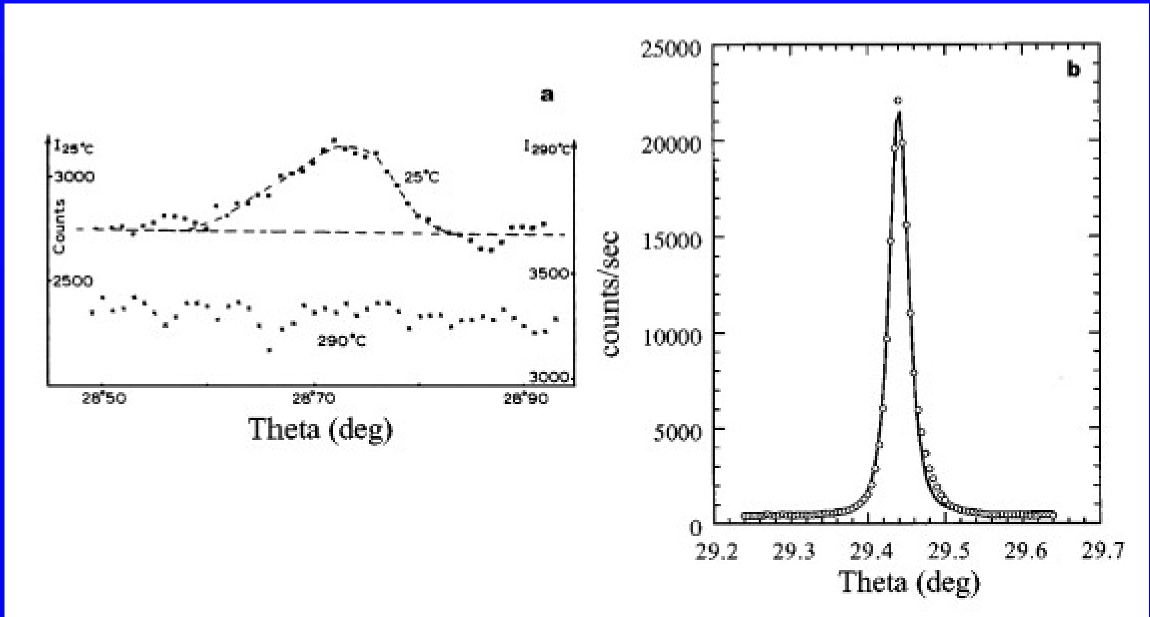


Figure 10: Panel a: Superlattice magnetic reflection (3/2, 3/2, 3/2) of NiO measured in magnetic phase (25°), and in the paramagnetic phase. The disappearance of the peak shows its magnetic origin. Panel b: The magnetic reflection (3/2, 3/2, 3/2) of NiO measured today at a third generation synchrotron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

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

Semiclassical approach: the radiation

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

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

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

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

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

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

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

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

Semiclassical approach: the radiation

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

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

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

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

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

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

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

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

Absorption

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

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

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

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

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

Absorption Coefficient

$$I = I_0 e^{-\mu x} \Rightarrow \mu = -\frac{1}{I}\frac{dI}{dx}$$

$$I = \frac{1}{2\pi c}\omega^2 A_0^2$$

$$dI = \sum w_{fi}\hbar\omega N dx$$

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

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

Absorption Coefficient:dipole approximation

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

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

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

Optical transitions: $\lambda \approx 5000$ 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.

Absorption Coefficient: electric dipole

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

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

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

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

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

Scattering

The full elastic and inelastic scattering cross section

In particular:

- **the anomalous scattering**
- **the resonant scattering**
- **additional scattering arising from the magnetic interaction between the electromagnetic field and the electrons**

Full quantum approach is needed, in which:

- **the matter is treated as a quantum system**
- **the electromagnetic field as a ensamble of photons**

The electromagnetic field and its quantum states

$$\mathbf{A} = \sum_{\vec{k},\lambda} \hat{e}_{\vec{k},\lambda} \sqrt{\frac{2\pi\hbar c^2}{L^3 \omega_k}} \left(\hat{a}_{\vec{k},\lambda} e^{i\vec{k}\vec{r}} + \hat{a}^{+}_{\vec{k},\lambda} e^{-i\vec{k}\vec{r}} \right)$$

$$\left| n_{\vec{k},\lambda}, \ldots, n_{\vec{k}',\lambda,} \right\rangle$$

$$\left\langle m_{\vec{k},\lambda}, \ldots, m_{\vec{k}',\lambda,} \right| \hat{O} \left| n_{\vec{k},\lambda}, \ldots, n_{\vec{k}',\lambda,} \right\rangle$$

$$\left\langle n_{\vec{k},\lambda} + 1, \ldots, n_{\vec{k}',\lambda,} \right| \hat{a}^{+}_{k,\lambda} \left| n_{\vec{k},\lambda}, \ldots, n_{\vec{k}',\lambda,} \right\rangle \neq 0$$

$$\left\langle n_{\vec{k},\lambda} - 1, \ldots, n_{\vec{k}',\lambda,} \right| \hat{a}_{k,\lambda} \left| n_{\vec{k},\lambda}, \ldots, n_{\vec{k}',\lambda,} \right\rangle \neq 0$$

Interactions in quantum approach

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + V$$

$$\hat{H} = \frac{1}{2m}\left(\hat{p} - \frac{e}{c}A\right)^2 + V = \hat{H}_0 - \frac{e}{mc}A \bullet \hat{p} + \frac{e^2}{2mc^2}A^2$$

$$\hat{H}_1 = -\frac{e}{mc}A \bullet \hat{p} = -\frac{e}{mc}\sum_{\vec{k},\lambda}\hat{e}_{\vec{k},\lambda}\sqrt{\frac{2\pi\hbar c^2}{L^3\omega_k}}\left(\hat{a}_{\vec{k},\lambda}e^{i\vec{k}\vec{r}} + \hat{a}^{+}_{\vec{k},\lambda}e^{-i\vec{k}\vec{r}}\right) \bullet \hat{p}$$

$$\hat{H}_2 = \frac{e^2}{2mc^2}A^2 = \frac{e^2}{2mc^2}\sum_{\vec{k},\lambda;\vec{k}'\lambda'}\sqrt{\frac{2\pi\hbar c^2}{L^3\omega_k}}\sqrt{\frac{2\pi\hbar c^2}{L^3\omega_{k'}}}\hat{e}_{\vec{k},\lambda} \bullet \hat{e}_{\vec{k}',\lambda'}$$

$$\left(\hat{a}_{\vec{k},\lambda}\hat{a}_{\vec{k}',\lambda'}e^{i(\vec{k}+\vec{k}')\vec{r}} + \hat{a}^{+}_{\vec{k},\lambda}\hat{a}^{+}_{\vec{k}',\lambda'}e^{-i(\vec{k}+\vec{k}')\vec{r}} + \hat{a}_{\vec{k},\lambda}\hat{a}^{+}_{\vec{k}',\lambda'}e^{i(\vec{k}-\vec{k}')\vec{r}} + \hat{a}^{+}_{\vec{k},\lambda}\hat{a}_{\vec{k}',\lambda'}e^{i(-\vec{k}+\vec{k}')\vec{r}}\right)$$

Fermi Golden Rule

The perturbation induces transitions between initial and Final states with a propability w_{if}

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

$$M_{if} = \langle f|\hat{H}_{int.}|i\rangle + \sum_n \frac{\langle f|\hat{H}_{int.}|n\rangle\langle n|\hat{H}_{int.}|i\rangle}{E_i - E_n + i\varepsilon}$$

$$|m\rangle = |\psi\rangle_{el.}|n_1 n_2 \ldots, n_{\vec{k}} \ldots\rangle_{photons}$$

Scattering - I

Scattering involves two photons:
one is removed from the initial state k_i
The second is created in the final state k_f

$$|\mathbf{i}\rangle = |\psi_i\rangle_{el.} |\ldots, n_{\vec{k}\,in} \ldots, 0_{\vec{k}\,out}, \ldots\rangle_{fotoni}$$

$$|\mathbf{f}\rangle = |\psi_f\rangle_{el.} |\ldots, n_{\vec{k}\,in} - 1, \ldots, 1_{\vec{k}\,out}, \ldots\rangle_{fotoni}$$

Such transitions are due to:

1. **terms in A^2 in the first order (Thompson and Compton scattering)**
2. **terms in A•p in the second order (Anomalous and resonant scattering)**

Elastic and inelastic scattering

I order perturbation theory for the term ~ A²

$$\left|i\right\rangle = \left|\psi_i\right\rangle_{el.}\left|\ldots,n_{\vec{k}\,in},\ldots,0_{\vec{k}\,out},\ldots\right\rangle_{photons}$$

$$\left|f\right\rangle = \left|\psi_f\right\rangle_{el.}\left|\ldots,n_{\vec{k}\,in}-1,\ldots,1_{\vec{k}\,out},\ldots\right\rangle_{photons}$$

$$M_{if} = \left\langle \psi_f;\ldots n_{\vec{k}_{in}} - 1\ldots 1_{\vec{k}_{out}} \middle| \hat{H}_2 \middle| \psi_i;\ldots n_{\vec{k}_{in}}\ldots 0_{\vec{k}_{out}}\ldots \right\rangle =$$

$$= \left(\frac{e^2}{2mc^2}\right)\sqrt{\left(\frac{2\pi\hbar c^2}{V\omega_{k_{in}}}\right)}\sqrt{\left(\frac{2\pi\hbar c^2}{V\omega_{k_{out}}}\right)}$$

$$\Big\{ \sum_{\vec{k}_i,\lambda}\sum_{\vec{k}_o,\lambda'} \Big\langle f \Big| \left(\hat{e}_{\vec{k}_i,\lambda}\bullet\hat{e}_{\vec{k}_o,\lambda'}\right)e^{i\left(\vec{k}_i+\vec{k}_o\right)\vec{r}}\hat{a}_{\vec{k}_i,\lambda}\hat{a}_{\vec{k}_o,\lambda'} + \left(\hat{e}_{\vec{k}_i,\lambda}\bullet\hat{e}_{\vec{k}_o,\lambda\lambda}\right)e^{i\left(\vec{k}_i-\vec{k}_o\right)\vec{r}}\hat{a}_{\vec{k}_i,\lambda}\hat{a}^{+}_{\vec{k}_o,\lambda'} +$$

$$+\left(\hat{e}_{\vec{k}_i,\lambda}\bullet\hat{e}_{\vec{k}_o,\lambda'}\right)e^{i\left(-\vec{k}_i+\vec{k}_o\right)\vec{r}}\hat{a}^{+}_{\vec{k}_i,\lambda}\hat{a}_{\vec{k}_o,\lambda'} + \left(\hat{e}_{\vec{k}_i,\lambda}\bullet\hat{e}_{\vec{k}_o,\lambda''}\right)e^{i\left(-\vec{k}_i-\vec{k}_o\right)\vec{r}}\hat{a}^{+}_{\vec{k}_i,\lambda}\hat{a}^{+}_{\vec{k}_o,\lambda'}\Big| i \Big\rangle \Big\}$$

Scattering - III

$$M_{if} = \left(\frac{e^2}{2mc^2}\right)\sqrt{\left(\frac{2\pi\hbar c^2}{V\omega_{k_{in}}}\right)}\sqrt{\left(\frac{2\pi\hbar c^2}{V\omega_{k_{out}}}\right)}$$

$$\left\{ \sum_{\vec{k}_i,\lambda} \sum_{\vec{k}_o,\lambda} \left\langle f \left| \left(\hat{e}_{\vec{k}_i,\lambda} \bullet \hat{e}_{\vec{k}_o,\lambda\lambda}\right) e^{i(\vec{k}_i - \vec{k}_o)\vec{r}} \hat{a}_{\vec{k}_i,\lambda} \hat{a}^+_{\vec{k}_o,\lambda\lambda} + \left(\hat{e}_{\vec{k}_i,\lambda} \bullet \hat{e}_{\vec{k}_o,\lambda\lambda}\right) e^{i(-\vec{k}_i + \vec{k}_o)\vec{r}} \hat{a}^+_{\vec{k}_i,\lambda} \hat{a}_{\vec{k}_o,\lambda\lambda} \right| i \right\rangle \right\}$$

$$M_{if} = \left(\frac{e^2}{2mc^2}\right)\sqrt{\left(\frac{2\pi\hbar c^2}{V\omega_{k_{in}}}\right)}\sqrt{\left(\frac{2\pi\hbar c^2}{V\omega_{k_{out}}}\right)}$$

$r_0 = e^2/mc^2 = 2.8179\ 10^{-13}$ cm

$$\left\{ \left\langle f \left| \left(\hat{e}_{\vec{k}_i,\lambda} \bullet \hat{e}_{\vec{k}_{out},\lambda\lambda}\right) e^{i(\vec{k}_{in} - \vec{k}_{out})\vec{r}} \hat{a}_{\vec{k}_{in},\lambda} \hat{a}^+_{\vec{k}_{out},\lambda\lambda} + \left(\hat{e}_{\vec{k}_{out},\lambda\lambda} \bullet \hat{e}_{\vec{k}_{in},\lambda}\right) e^{i(-\vec{k}_{out} + \vec{k}_{in})\vec{r}} \hat{a}^+_{\vec{k}_{out},\lambda\lambda} \hat{a}_{\vec{k}_{in},\lambda} \right| i \right\rangle \right\} =$$

$$= \left(\frac{e^2}{2mc^2}\right)\sqrt{\left(\frac{2\pi\hbar c^2}{V\omega_{k_{in}}}\right)}\sqrt{\left(\frac{2\pi\hbar c^2}{V\omega_{k_{out}}}\right)} \left(\hat{e}_{\vec{k}_i,\lambda} \bullet \hat{e}_{\vec{k}_{out},\lambda\lambda}\right) \sqrt{n_{\vec{k}_{in}}} \left\langle \psi_f \left| 2e^{-i\vec{q}\vec{r}} \right| \psi_i \right\rangle =$$

$$= r_0 \left(\frac{2\pi\hbar c^2}{V}\right)\sqrt{\frac{1}{\omega_{k_{in}}\omega_{k_{out}}}} \left(\hat{e}_{\vec{k}_i,\lambda} \bullet \hat{e}_{\vec{k}_{out},\lambda\lambda}\right)\sqrt{n_{\vec{k}_{in}}} \left\langle \psi_f \left| e^{-i\vec{q}\vec{r}} \right| \psi_i \right\rangle$$

Scattering - IV

Cross section →

$$\frac{d^2\sigma}{d\Omega\, dE_k} = \frac{\sum_f \Gamma_{if}}{n_{\vec{k}_{in}} c / V}$$

Density of states

$$g(E_k) = \frac{dN}{dE_k} = \frac{V}{(2\pi)^3} \frac{\omega_{k_{out}}^2}{\hbar c^3} d\Omega$$

$$w_{if} = \frac{2\pi}{\hbar} |M_{if}|^2 g(E_f) = r_0^2 \left(\frac{c}{V}\right) n_{\vec{k}_{in}} \frac{\omega_{k_{out}}}{\omega_{k_{in}}} \left(\hat{e}_{\vec{k}_i,\lambda} \bullet \hat{e}_{\vec{k}_{out},\lambda\lambda}\right)^2 \left|\langle \psi_i | e^{-i\vec{q}\vec{r}} | \psi_f \rangle\right|^2$$

$$\frac{d^2\sigma}{dE d\Omega} = \Sigma_f\ r_0^2 \left(\hat{e}_{\vec{k}_i,\lambda} \bullet \hat{e}_{\vec{k}_f,\lambda'}\right)^2 \frac{\omega_{k_{out}}}{\omega_{k_{in}}} \left|\langle \psi_i | e^{-i\vec{q}\vec{r}} | \psi_f \rangle\right|^2$$

Scattering Cross Section
(non relativistic)

$$\frac{d^2\sigma}{d\Omega dE_k} = \Sigma_f\ r_0^2 \left(\hat{e}_{\vec{k}_i,\lambda} \bullet \hat{e}_{\vec{k}_{out},\lambda\lambda}\right)^2 \frac{\omega_{k_{out}}}{\omega_{k_{in}}} \sum_f \left| \left\langle \psi_i \left| e^{-i\vec{q}\vec{r}} \right| \psi_f \right\rangle \right|^2$$

Elastic scattering

$$\frac{d^2\sigma}{d\Omega dE_k} = \Sigma_f \, r_0^2 \left(\hat{e}_{\vec{k}_i,\lambda} \bullet \hat{e}_{\vec{k}_{out},\lambda'}\right)^2 \frac{\omega_{k_{out}}}{\omega_{k_{in}}} \sum_f \left|\left\langle \psi_i \left| e^{-i\vec{q}\vec{r}} \right| \psi_f \right\rangle\right|^2$$

Elastic scattering → $\omega_{k'} = \omega_k$

Final electronic state equal to their initial one

$$\frac{d\sigma}{d\Omega} = r_0^2 \left(\hat{e}_{\vec{k}_i,\lambda} \bullet \hat{e}_{\vec{k}_{out},\lambda'}\right)^2 \left|\left\langle \psi_i \left| e^{-i\vec{q}\vec{r}} \right| \psi_i \right\rangle\right|^2$$

Inelastic Scattering at very high energy

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

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

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

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

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

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

Contribution due to A•p

$$\hat{H}_1 = -\frac{e}{mc}\mathbf{A}\bullet\hat{\mathbf{p}} = -\frac{e}{mc}\sum_{\vec{k},\lambda}\hat{e}_{\vec{k},\lambda}\sqrt{\frac{2\pi\hbar c^2}{V\omega_k}}\left(\hat{a}_{\vec{k},\lambda}e^{i\vec{k}\vec{r}} + \hat{a}^{+}_{\vec{k},\lambda}e^{-i\vec{k}\vec{r}}\right)\bullet\hat{\mathbf{p}}$$

$$M_{if} = \langle f|\hat{H}_{int.}|i\rangle + \sum_n \frac{\langle f|\hat{H}_{int.}|n\rangle\langle n|\hat{H}_{int.}|i\rangle}{E_i - E_n + i\varepsilon}$$

$$|i\rangle = |\psi_i\rangle_{el.}|\ldots, n_{\vec{k}\,in}\ldots, 0_{\vec{k}\,out},\ldots\rangle_{fotoni}$$

$$|f\rangle = |\psi_f\rangle_{el.}|\ldots, n_{\vec{k}\,in}\text{-}1,\ldots,1_{\vec{k}\,out},\ldots\rangle_{fotoni}$$

$$\Rightarrow M_{if} = \sum_n \frac{\langle f|\hat{H}_{int.}|n\rangle\langle n|\hat{H}_{int.}|i\rangle}{E_i - E_n + i\varepsilon}$$

$$|n\rangle = |\psi_a\rangle_{el.}|\ldots, n_{\vec{k}\,in}\text{-}1\ldots,0_{\vec{k}\,out},\ldots\rangle \Rightarrow E_i - E_n = \left(E_i^{el} - E_a^{el}\right) - \hbar\omega$$

$$|n'\rangle = |\psi_a\rangle_{el.}|\ldots, n_{\vec{k}\,in},\ldots,1_{\vec{k}\,out},\ldots\rangle \Rightarrow E_i - E_n = \left(E_i^{el} - E_a^{el}\right) + \hbar\omega$$

Elastic cross section

$$\frac{d\sigma}{d\Omega} = r_0^2 \frac{1}{m^2}$$

$$\left| \sum_n \frac{\langle \psi_i | e^{i\vec{k}_{in}\vec{r}} \hat{e}_{\vec{k}_{in}\lambda} \bullet \hat{p} | \psi_n \rangle \langle \psi_n | e^{-i\vec{k}_{out}\vec{r}} \hat{e}_{\vec{k}_{out}\lambda'} \bullet \hat{p} | \psi_i \rangle}{\varepsilon_i - \varepsilon_n + \hbar\omega} + \sum_n \frac{\langle \psi_i | e^{-i\vec{k}_{out}\vec{r}} \hat{e}_{\vec{k}_{out}\lambda'} \bullet \hat{p} | \psi_n \rangle \langle \psi_n | e^{i\vec{k}_{in}\vec{r}} \hat{e}_{\vec{k}_{in}\lambda} \bullet \hat{p} | \psi_i \rangle}{\varepsilon_i - \varepsilon_n - \hbar\omega} \right|^2$$

At the resonance→

$$\frac{d\sigma}{d\Omega} \cong r_0^2 \frac{1}{m^2}$$

$$\left| \sum_n \frac{\langle \psi_i | e^{i\vec{k}_{in}\vec{r}} \hat{e}_{\vec{k}_{in}\lambda} \bullet \hat{p} | \psi_n \rangle \langle \psi_n | e^{-i\vec{k}_{out}\vec{r}} \hat{e}_{\vec{k}_{out}\lambda'} \bullet \hat{p} | \psi_i \rangle}{\varepsilon_i - \varepsilon_n + \hbar\omega + i\Gamma/2} \right|^2$$

Total cross section at high energy

At high energy the contribution becomes:

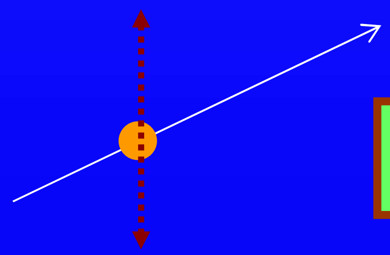
$$M_{if} = -i r_0 \left(\frac{2\pi\hbar c^2}{V}\right)\left(\frac{\hbar\omega_k}{mc^2}\right)\left\langle \psi_i \left| e^{i\vec{q}\vec{r}} \frac{i\vec{q}\times\hat{p}}{\hbar k^2} \right| \psi_i \right\rangle \left(\widehat{e}_{k_{out}\lambda'} \times \widehat{e}_{k_{in}\lambda}\right)$$

$$\frac{d\sigma}{d\Omega} = \frac{\frac{2\pi}{\hbar}\left|M_{if}^{A^2} + M_{if}^{Ap}\right|^2 g(E_f)}{n_{k_{in}} c \big/ V} =$$

$$r_0^2 \left| \left(\hat{e}_{k_{in}\lambda} \bullet \hat{e}_{k_{out}\lambda'}\right) \left\langle \psi_i \left| e^{-i\vec{q}\vec{r}} \right| \psi_i \right\rangle - i \left(\frac{\hbar\omega_k}{mc^2}\right) \left\langle \psi_i \left| e^{i\vec{q}\vec{r}} \frac{i\vec{q}\times\hat{p}}{\hbar k^2} \right| \psi_i \right\rangle \left(\widehat{e}_{k_{out}\lambda'} \times \widehat{e}_{k_{in}\lambda}\right) \right|^2$$

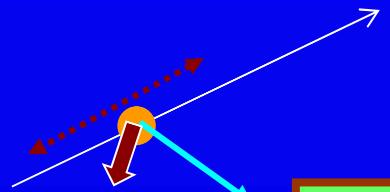
Magnetic Interactions

An electromagnetic wave transport both an electric and a magnetic field



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

Thomson scattering

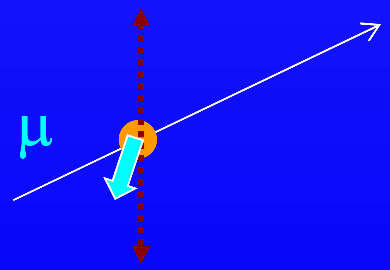


$$E = -\vec{\mu}\vec{H}$$

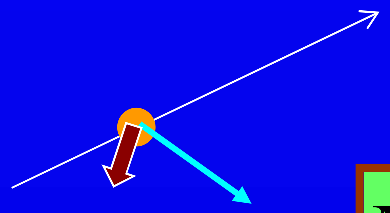
$$\vec{F} = \mathrm{grad}\left(\vec{\mu}\vec{H}\right)$$

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

Magnetic Interactions



Magnetic dipole oscillations

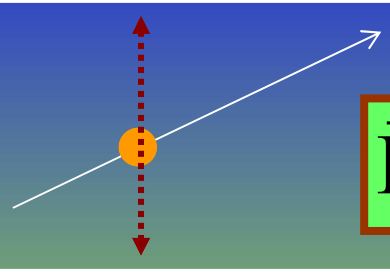


Torque

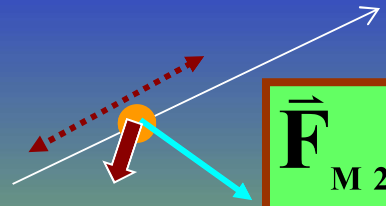
$$\vec{M} = \left(\vec{\mu} \times \vec{H}\right)$$

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

Strength of Magnetic Interactions



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



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

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

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

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 is an antiferromagnetic cubic crystal (T_{Neel}=250 ^{0}C)
- Ni^{++} have only two electrons
- Electron spin are ferro-magnetically aligned in (111) plane
- They are anti-ferromagnetically aligned between (111) planes

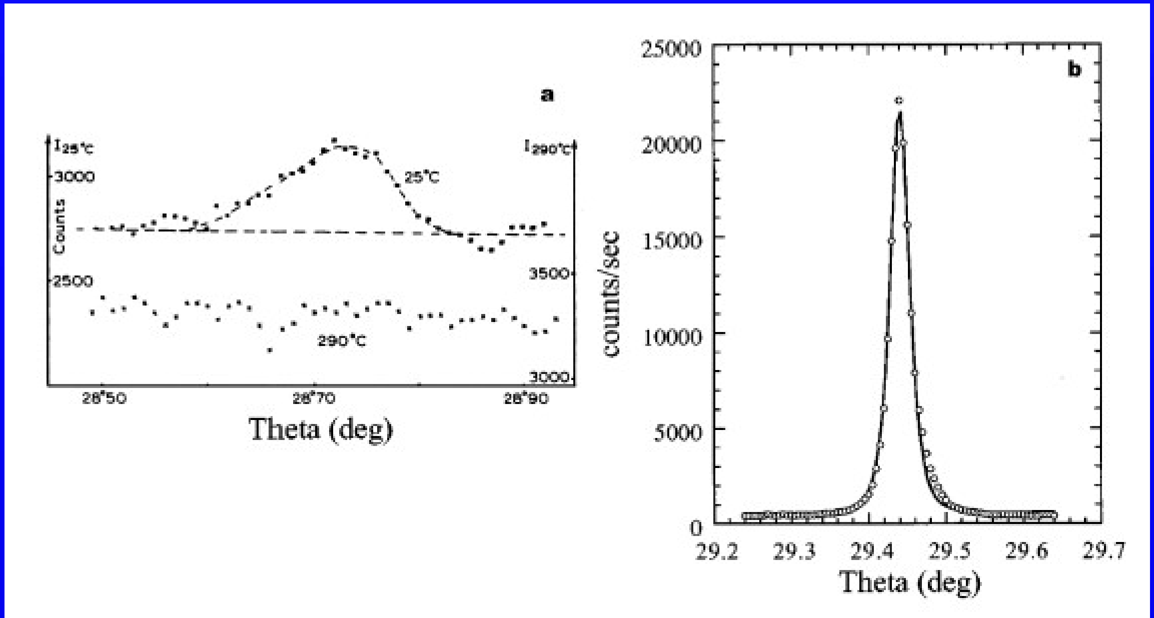


Figure 10: Panel a: Superlattice magnetic reflection (3/2, 3/2, 3/2) of NiO measured in magnetic phase (25°), and in the paramagnetic phase. The disappearance of the peak shows its magnetic origin. Panel b: The magnetic reflection (3/2, 3/2, 3/2) of NiO measured today at a third generation synchrotron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

Hamiltonian in the relativistic approximation

$$\hat{H}_{tot} = \hat{H}_{el.} + \hat{H}_{rad.} = \sum_i \left(\frac{\left(\hat{p}_i - {}^{e}\!/_{c}\,\vec{A}\right)^2}{2m} + V(\vec{r}_i) \right) +$$

$$\sum_i \left(-\frac{e\hbar}{mc}\vec{s}_i \bullet \mathrm{rot}\vec{A} + \frac{e\hbar}{2m^2c^2}\vec{s}_i \bullet \frac{\partial \vec{A}}{\partial t} \times \left(\hat{p}_i - \frac{e}{c}\vec{A}(\vec{r}_i) \right) \right) +$$

$$\sum_{\vec{k},\lambda} \hbar\omega_{\vec{k}\lambda} \left(a^{+}_{\vec{k}\lambda} a_{\vec{k}\lambda} + \frac{1}{2} \right)$$

Interaction terms in the relativistic approximation

$$\hat{H}_1 = \frac{e^2}{2mc^2}\sum_i A^2(\vec{r}_i)$$

$$\hat{H}_2 = \frac{e}{mc}\sum_i \vec{A}(\vec{r}_i)\bullet\hat{p}_i$$

$$\hat{H}_3 = -\frac{e\hbar}{mc}\sum_i \vec{s}_i \bullet \mathrm{rot}\vec{A}$$

→ Produces scattering (II order in P.T.)

a

$$\hat{H}_4 = \frac{e\hbar}{2m^2c^3}\sum_i \vec{s}_i \bullet \frac{\partial\vec{A}}{\partial t}\times\left(\hat{p}_i - \frac{e}{c}\vec{A}(\vec{r}_i)\right)$$

b

I order scattering in P.T.

$$\frac{a}{b} \cong \left(\frac{\hbar\omega}{mc^2}\right)^2$$

Relativistic approximation

$$\hat{H}_1 = \frac{e^2}{2mc^2}\sum_i A^2(\vec{r}_i)$$

$$\hat{H}_2 = \frac{e}{mc}\sum_i \vec{A}(\vec{r}_i)\bullet\hat{p}_i$$

$$\hat{H}_3 = -\frac{e\hbar}{mc}\sum_i \vec{s}_i \bullet \mathrm{rot}\vec{A}$$

$$\hat{H}_4 \cong \frac{e\hbar}{2m^2c^3}\left(-\frac{e}{c}\right)\sum_i \vec{s}_i \bullet \frac{\partial\vec{A}}{\partial t}\times\vec{A}(\vec{r}_i)$$

$$\Gamma_{if} = \frac{2\pi}{\hbar}\left|\langle f|\hat{H}_1+\hat{H}_4|i\rangle + \sum_n \frac{\langle f|\hat{H}_2+\hat{H}_3|n\rangle\langle n|\hat{H}_2+\hat{H}_3|i\rangle}{E_i - E_n + i\varepsilon}\right|^2 \delta(E_i - E_f)$$

Contributo di H_4 allo scattering

$$M_{if} = \langle f | \hat{H}_1 + \hat{H}_4 | i \rangle + \sum_n \frac{\langle f | \hat{H}_2 + \hat{H}_3 | n \rangle \langle n | \hat{H}_2 + \hat{H}_3 | i \rangle}{E_i - E_n + i\varepsilon}$$

$$M_{if}^{A^2} = r_0 \left(\frac{2\pi\hbar c^2}{V\omega_{k_t}} \right) \sum_i \langle \psi_f | e^{-i\vec{q}\vec{r}_i} | \psi_i \rangle \left(\hat{e}_{\vec{k}_i,\lambda} \bullet \hat{e}_{\vec{k}_{out},\lambda'} \right)$$

$$\langle f | \hat{H}_4 | i \rangle = -i \left(\frac{\hbar\omega_k}{mc^2} \right) r_0 \left(\frac{2\pi\hbar c^2}{V\omega_k} \right) \sum_i \langle \psi_i | e^{-i\vec{q}\vec{r}_i} \vec{s}_i | \psi_i \rangle \bullet \left(\hat{e}^*_{k_{out}\lambda'} \times \hat{e}_{k_{in}\lambda} \right)$$

Out of phase

Reduction factor

Fourier transform of the spin density

Polarization dependance

Scattering from I order perturbation

$$M_{if}^{I} = \frac{2\pi\hbar c^2}{V\omega} r_0$$

$$\left(\sum_i \langle \psi_i | e^{-i\vec{q}\,\vec{r}_i} | \psi_i \rangle \left(\hat{e}^*_{k_{out}\lambda'} \bullet \hat{e}_{k_{in}\lambda} \right) - i \left(\frac{\hbar\omega_k}{mc^2} \right) \sum_i \langle \psi_i | e^{-i\vec{q}\,\vec{r}_i} \vec{s}_i | \psi_i \rangle \bullet \left(\hat{e}^*_{k_{out}\lambda'} \times \hat{e}_{k_{in}\lambda} \right) \right)$$

Contribution of H_2 and H_3

$$M^{II}_{if} = \left| \langle f | \hat{H}_1 + \hat{H}_4 | i \rangle + \sum_n \frac{\langle f | \hat{H}_2 + \hat{H}_3 | n \rangle \langle n | \hat{H}_2 + \hat{H}_3 | i \rangle}{E_i - E_n + i\varepsilon} \right|^2$$

$$\hat{H}_2 = \frac{e}{mc} \sum_i \vec{A}(\vec{r}_i) \bullet \hat{p}_i \rightarrow \hat{H}_2 = \frac{e}{mc} \sum_i \hat{e}_{k\lambda} \bullet \hat{p}_i \ldots$$

$$\hat{H}_3 = -\frac{e\hbar}{mc} \sum_i \vec{s}_i \bullet \mathrm{rot}\vec{A} \rightarrow \hat{H}_3 = -\frac{e\hbar}{mc} \sum_i \vec{s}_i \bullet \left(\vec{k} \times \hat{e}_{\vec{k}\lambda}\right) \ldots$$

$$\hat{e}_{\vec{k}\lambda} \bullet \hat{p}_i \rightarrow -\hbar \vec{s}_i \bullet \left(\vec{k} \times \hat{e}_{\vec{k}\lambda}\right)$$

Resonant term at high energy

After some hours of a tedious calculation we get:

$$M_{if} = -i\left(\frac{\hbar\omega_k}{mc^2}\right) r_0 \left(\frac{2\pi\hbar c^2}{V\omega_k}\right) \times \sum_i \left\langle \psi_i \middle| e^{i\vec{q}\vec{r}} \vec{s}_i \middle| \psi_i \right\rangle \times$$

$$\left\{ \left(\hat{k}_{out} \times \hat{e}^*_{k_{out}\lambda'}\right) \hat{k}_{out} \bullet \hat{e}_{k_{in}\lambda} - \left(\hat{k}_{in} \times \hat{e}_{k_{in}\lambda}\right) \hat{k}_{in} \bullet \hat{e}^*_{k_{out}\lambda'} - \left(\hat{k}_{out} \times \hat{e}^*_{k_{out}\lambda'}\right) \times \left(\hat{k}_{in} \times \hat{e}_{k_{in}\lambda}\right) \right\}$$

Out of phase

Reduction factor

Fourier transform of the spin density

Polarization dependance

Total contribution at high energy from the I order term in A

(II order perturbation theory)

$$\mathbf{M}_{if} = -i\left(\frac{\hbar\omega_k}{mc^2}\right) r_0 \left(\frac{2\pi\hbar c^2}{V\omega_k}\right)$$

$$\sum_i \left\langle \psi_i \left| e^{i\vec{q}\vec{r}} \frac{i\vec{q}\times\hat{p}}{\hbar k^2} \right| \psi_i \right\rangle \left(\hat{e}_{k_{out}\lambda'} \times \hat{e}_{k_{in}\lambda}\right) + \sum_i \left\langle \psi_i \left| e^{i\vec{q}\vec{r}} \vec{s}_i \right| \psi_i \right\rangle \times$$

$$\times \left\{ \left(\hat{k}_{out} \times \hat{e}^*_{k_{out}\lambda'}\right) \hat{k}_{out} \bullet \hat{e}_{k_{in}\lambda} - \left(\hat{k}_{in} \times \hat{e}_{k_{in}\lambda}\right) \hat{k}_{in} \bullet \hat{e}^*_{k_{out}\lambda'} - \left(\hat{k}_{out} \times \hat{e}^*_{k_{out}\lambda'}\right) \times \left(\hat{k}_{in} \times \hat{e}_{k_{in}\lambda}\right) \right\}$$

Total cross section at high energy

$$\frac{d\sigma}{d\Omega} = \frac{\frac{2\pi}{\hbar}\left|M_{if}^{totale}\right|^2 g(E_f)}{n_k c / V}$$

$$\Bigg| \sum_i \langle \psi_i | e^{i\vec{q}\vec{r}} | \psi_i \rangle \left(\hat{e}_{k_{out}\lambda'} \cdot \hat{e}_{k_{in}\lambda}\right) - i\left(\frac{\hbar\omega_k}{mc^2}\right)\Big\{ \sum_i \langle \psi_i | e^{i\vec{q}\vec{r}} \frac{i\vec{q}\times\hat{p}}{\hbar k^2} | \psi_i \rangle \left(\hat{e}_{k_{out}\lambda'} \times \hat{e}_{k_{in}\lambda}\right) +$$

$$\sum_i \langle \psi_i | e^{i\vec{q}\vec{r}} \vec{s}_i | \psi_i \rangle \times$$

$$\times \Big\{ \left(\hat{e}_{k_{out}\lambda'} \times \hat{e}_{k_{in}\lambda}\right) + \left(\hat{k}_{out} \times \hat{e}^*_{k_{out}\lambda'}\right) \hat{k}_{out} \bullet \hat{e}_{k_{in}\lambda} - \left(\hat{k}_{in} \times \hat{e}_{k_{in}\lambda}\right) \hat{k}_{in} \bullet \hat{e}^*_{k_{out}\lambda'} - \left(\hat{k}_{out} \times \hat{e}^*_{k_{out}\lambda'}\right) \vec{k}_{in} \times \hat{e}_{k_{in}\lambda} \Big\} \Bigg|^2$$

Orbital momentum

$$\sum_i \langle \psi_i | e^{i\vec{q}\vec{r}} \frac{i\vec{q}\times\hat{p}}{\hbar k^2} | \psi_i \rangle = \frac{i}{\hbar q}\left(4\sin^2\theta_B\right)\langle \psi_i | e^{i\vec{q}\vec{r}} \widehat{q}\times\hat{p} | \psi_i \rangle =$$

$$\frac{i}{\hbar q}\left(4\sin^2\theta_B\right)\widehat{q}\times\langle \psi_i | e^{i\vec{q}\vec{r}} \hat{p} | \psi_i \rangle = -\frac{im}{e\hbar q}\left(4\sin^2\theta_B\right)\widehat{q}\times\langle \psi_i | e^{i\vec{q}\vec{r}} \hat{j} | \psi_i \rangle =$$

$$-\frac{im}{e\hbar q}\left(4\sin^2\theta_B\right)\widehat{q}\times\vec{j}(\vec{q})$$

$$\vec{j} = c\left[\nabla\times\vec{M}_L\right] \;\Rightarrow\; \vec{j}(\vec{q}) = -ic\left[\vec{q}\times\vec{M}_L(\vec{q})\right]$$

$$\sum_i \langle \psi_i | e^{i\vec{q}\vec{r}} \frac{i\vec{q}\times\hat{p}}{\hbar k^2} | \psi_i \rangle = \frac{mc}{e\hbar q}\left(4\sin^2\theta_B\right)\widehat{q}\times\left(\vec{q}\times M_L(\vec{q})\right) =$$

$$\frac{mc}{e\hbar}\left(4\sin^2\theta_B\right)\hat{q}\times\left(\hat{q}\times M_L(\vec{q})\right)$$

Total cross section at high energy

$$\frac{d\sigma}{d\Omega} = r_0^2 \left| \begin{array}{l} \sum_i \langle \psi_i | e^{i\vec{q}\vec{r}} | \psi_i \rangle \left(\widehat{e}_{k_{out}\lambda'} \widehat{e}_{k_{in}\lambda} \right) \\ -i \left(\frac{\hbar\omega_k}{mc^2} \right) \sum_i \left\{ \langle \psi_i | e^{i\vec{q}\vec{r}} \frac{i\vec{q}\times\hat{p}}{\hbar k^2} | \psi_i \rangle P_L + \langle \psi_i | e^{i\vec{q}\vec{r}} \vec{s}_i | \psi_i \rangle P_S \right\} \end{array} \right|^2$$

$$P_L = \left(\widehat{e}_{k_{out}\lambda'} \times \widehat{e}_{k_{in}\lambda} \right)$$

$$P_S = \left(\widehat{e}_{k_{out}\lambda'} \times \widehat{e}_{k_{in}\lambda} \right) + \left(\hat{k}_{out} \times \hat{e}^*_{k_{out}\lambda'} \right) \hat{k}_{out} \bullet \hat{e}_{k_{in}\lambda} + \\ - \left(\hat{k}_{in} \times \hat{e}_{k_{in}\lambda} \right) \hat{k}_{in} \bullet \hat{e}^*_{k_{out}\lambda'} - \left(\hat{k}_{out} \times \hat{e}^*_{k_{out}\lambda'} \right) \times \left(\hat{k}_{in} \times \hat{e}_{k_{in}\lambda} \right)$$

Total cross section at high energy

$$\frac{d\sigma}{d\Omega} = r_0^2 \left| \begin{array}{l} \sum_i \langle \psi_i | e^{i\vec{q}\vec{r}} | \psi_i \rangle \left(\hat{e}_{k_{out}\lambda'} \cdot \hat{e}_{k_{in}\lambda} \right) \\ -i \left(\frac{\hbar\omega_k}{mc^2} \right) \sum_i \left\{ \langle \psi_i | e^{i\vec{q}\vec{r}} \frac{i\vec{q}\times\hat{p}}{\hbar k^2} | \psi_i \rangle P_L + \langle \psi_i | e^{i\vec{q}\vec{r}} \vec{s}_i | \psi_i \rangle P_S \right\} \end{array} \right|^2$$

$$\sum_i \langle \psi_i | e^{i\vec{q}\vec{r}} \frac{i\vec{q}\times\hat{p}}{\hbar k^2} | \psi_i \rangle \; P_L = \frac{mc}{e\hbar q^2} \vec{q} \times \left(\vec{M}_L(\vec{q}) \times \vec{q} \right) P_L'$$

$$P_L' = \left(\hat{e}_{k_{out}\lambda'} \times \hat{e}_{k_{in}\lambda} \right) 4 \sin^2 \theta_B$$

$$\sum_i \langle \psi_i | e^{i\vec{q}\vec{r}} \vec{s}_i | \psi_i \rangle = \frac{mc}{e\hbar} \vec{M}_S(\vec{q})$$

Total cross section at high energy

$$\frac{d\sigma}{d\Omega} = r_0^2 \left| \sum_i \langle \psi_i | e^{i\vec{q}\vec{r}} | \psi_i \rangle \left(\hat{e}_{k_{out}\lambda'} \hat{e}_{k_{in}\lambda} \right) - i \left(\frac{\hbar\omega_k}{mc^2} \right) \left(\frac{mc}{e\hbar q^2} (\vec{q} \times \vec{M}_L(\vec{q}) \times \vec{q}) P'_L + \frac{mc}{e\hbar} \vec{M}_s(\vec{q}) P_S \right) \right|^2$$

$$\vec{P}'_L = \left(\hat{e}_{k_{out}\lambda'} \times \hat{e}_{k_{in}\lambda} \right) 4 \sin^2\theta_B$$

$$\vec{P}_S = \left(\hat{e}_{k_{out}\lambda'} \times \hat{e}_{k_{in}\lambda} \right) + \left(\hat{k}_{out} \times \hat{e}^*_{k_{out}\lambda'} \right) \hat{k}_{out} \bullet \hat{e}_{k_{in}\lambda} - \left(\hat{k}_{in} \times \hat{e}_{k_{in}\lambda} \right) \hat{k}_{in} \bullet \hat{e}^*_{k_{out}\lambda'} - \left(\hat{k}_{out} \times \hat{e}^*_{k_{out}\lambda'} \right) \times \left(\hat{k}_{in} \times \hat{e}_{k_{in}\lambda} \right)$$