

# Methoden moderner Röntgenphysik II: Streuung und Abbildung

## Lecture 8

Vorlesung zum Haupt/Masterstudiengang Physik

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Location: Hörs AP, Physik, Jungiusstrasse

Tuesdays 12.45 – 14.15

Thursdays 8:30 – 10.00

# ■ Methoden moderner Röntgenphysik II: Streuung und Abbildung

## Small Angle Scattering, and Soft Matter

Introduction, form factor, structure factor, applications, ..

## Anomalous Diffraction

Introduction into anomalous scattering,..

## Introduction into Coherence

Concept, First order coherence, ..

## Coherent Scattering

Spatial coherence, second order coherence,..

## Applications of coherent Scattering

Imaging and Correlation spectroscopy,..

# Resonant Scattering (phasing, magnetism,...)

Scattering length of an atom:  $-r_0 f^0(\mathbf{Q})$

$f^0(\mathbf{Q})$  atomic form factor (fourier transform of charge distribution)

$r_0$  thomson scattering length of single electron

in order to include absorption effects ( $f''$ ) atoms a more elaborate model than the free electron gas is needed.

→ Electrons are bound to atoms

→ Forced oscillator model with resonant frequency  $\omega_s$  and damping constant  $\Gamma$

include dispersion corrections ( $f'$ ,  $f''$ ):

[note:  $f'' = (k/4\pi r_0) \sigma_a$ ]

$$f(\mathbf{Q}, \omega) = f^0(\mathbf{Q}) + f'(\omega) + i f''(\omega)$$

[in units of  $r_0$ ]

# Resonant Scattering

classical model of  
an electron bound  
in an atom in E field

$$\mathbf{E}(\mathbf{r},t) = \hat{\mathbf{x}} E_0 \exp\{-i\omega t\} \longrightarrow$$

equation of motion  
of the electron

$$\ddot{x} + \Gamma \dot{x} + \omega_s^2 x = - \left( \frac{e E_0}{m} \right) \exp\{-i\omega t\}$$

$\Gamma$  = damping  
 $\omega_s$  resonant  
frequency

Solution:  $x(t) = x_0 \exp\{-i\omega t\} \longrightarrow x_0 = - \left( \frac{e E_0}{m} \right) \frac{1}{(\omega_s^2 - \omega^2 - i\omega\Gamma)}$  (A)

radiated field strength at  
distance R and time t

$$E_{\text{rad}}(R,t) = \left( \frac{e}{4\pi \epsilon_0 R c^2} \right) \ddot{x}(t - R/c) \quad \text{(B)}$$

↑  
acceleration at “earlier” time (t-R/c)

# Resonant scattering

inserting  $\ddot{x}(t - R/c) = \omega^2 x_0 \exp\{-i\omega t\} \exp\{i(\omega/c)R\}$  using (A) into (B):

$$E_{\text{rad}}(R,t) = \frac{\omega^2}{(\omega_s^2 - \omega^2 - i\omega\Gamma)} \left( \frac{e^2}{4\pi \epsilon_0 m c^2} \right) E_0 \exp\{-i\omega t\} \left( \frac{\exp\{ikR\}}{R} \right)$$

or

$$\frac{E_{\text{rad}}(R,t)}{E_{\text{in}}} = \underbrace{-r_0 \frac{\omega^2}{(\omega_s^2 - \omega^2 + i\omega\Gamma)}}_{\text{atomic scattering length } f_s} \left( \frac{\exp\{ikR\}}{R} \right)$$

atomic scattering length  $f_s$  (in units of  $-r_0$ ) for bound electron (C)  
 note:  $f_s \rightarrow 1$  ( $\omega \gg \omega_s$ )

total cross-section:  $\sigma_T = (8\pi/3) r_0^2$  (free electron)

$$\sigma_T = \left( \frac{8\pi}{3} \right) \frac{\omega^4}{(\omega^2 - \omega_s^2)^2 + (\omega\Gamma)^2} r_0^2$$

for  $\Gamma = 0$  and  $\omega \ll \omega_s$ :  $\sigma_T = (8\pi/3) r_0^2 (\omega / \omega_s)^4$ : “Rayleigh Scattering”

# Resonant scattering

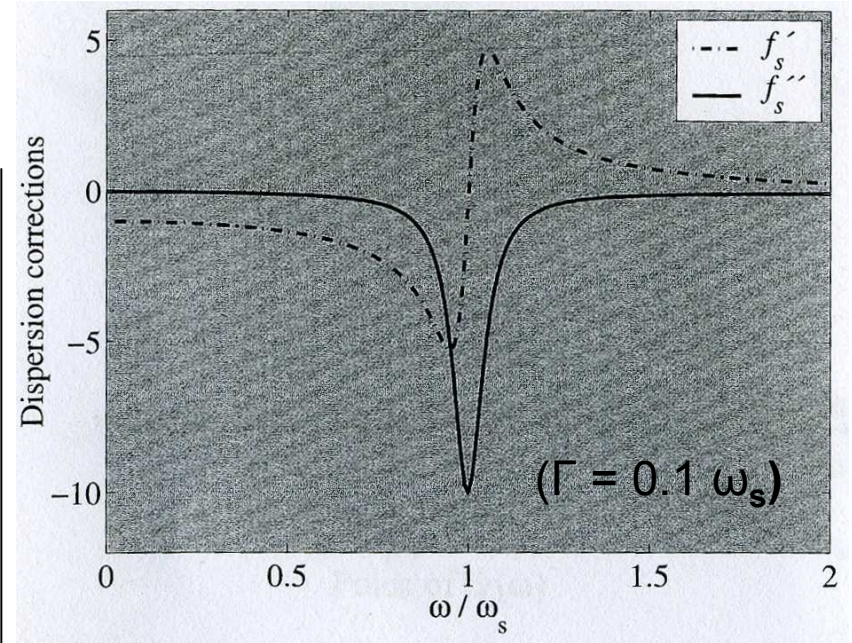
$$f_s = \frac{\omega^2 - \omega_s^2 + i\omega\Gamma + \omega_s^2 - i\omega\Gamma}{(\omega^2 - \omega_s^2 + i\omega\Gamma)}$$

$$= 1 + \frac{\omega_s^2 - i\omega\Gamma}{(\omega^2 - \omega_s^2 + i\omega\Gamma)}$$

$$\approx 1 + \frac{\omega_s^2}{(\omega^2 - \omega_s^2 + i\omega\Gamma)}$$

dispersion correction  $\chi(\omega)$

$$\chi(\omega) = f'_s + i f''_s = \frac{\omega_s^2}{(\omega^2 - \omega_s^2 + i\omega\Gamma)}$$



with:

$$f'_s = \frac{\omega_s^2 (\omega^2 - \omega_s^2)}{(\omega^2 - \omega_s^2)^2 + (\omega\Gamma)^2}$$

$$f''_s = \frac{\omega_s^2 \omega \Gamma}{(\omega^2 - \omega_s^2)^2 + (\omega\Gamma)^2}$$

# Resonant scattering

Note: since  $f'' = -(k/4\pi) \sigma_a(E)$  (see J. A-N. & D. McM. p. 70) it follows that the absorption cross-section for a single oscillator model is:

$$\sigma_{a,s}(\omega) = 4 \pi r_0 c \frac{\omega_s^2 \Gamma}{(\omega - \omega_s)^2 + (\omega \Gamma)^2}$$

this function has:

- sharp peak at  $\omega = \omega_s$
- $\Delta\omega_{\text{FWHM}} \approx \Gamma$

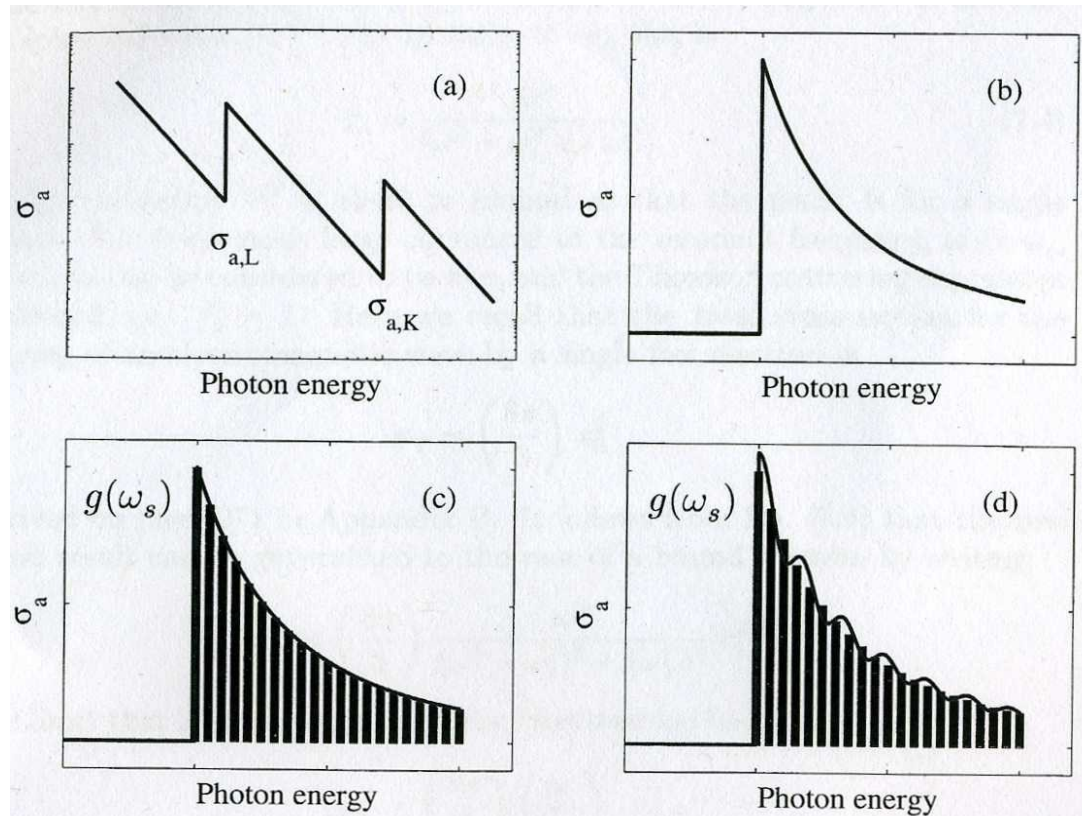
thus  $\sigma_a(E)$  may be written with help of a delta function:

$$\sigma_{a,s}(\omega) = 4 \pi r_0 c \frac{\pi}{2} \delta(\omega - \omega_s) \quad (\text{D})$$

# Resonant scattering

The experimentally observed absorption cross-section is NOT a single line spectrum as suggested by (D).

There is a continuum of free states above an absorption edge that the electron can be excited into. This implies a series of different  $\omega_s$ :





# Resonant scattering

Absorption cross section for multiple harmonic oscillators:

$$\sigma_a(\omega) = 2 \pi^2 r_0 c \sum_s g(\omega_s) \delta(\omega - \omega_s)$$

where  $g(\omega_s)$  is the relative weight of each transition

The real part of the dispersion becomes:

$$f'(\omega) = \sum_s g(\omega_s) f'_s(\omega, \omega_s) \quad (\text{F})$$

(F) does not describe e.g. “white lines” or “EXAFS” oscillations (see figure) in the absorption cross section arising from the particular environment of the resonantly scattering atom.

# Resonant scattering

measure absorption cross-section and use (E) to obtain  $f''$ :

$$f''(\omega) = - \left( \frac{\omega}{4 \pi r_0 c} \right) \sigma_a(\omega)$$

use [Kramers-Kronig relations](#) to obtain  $f'$ :

$$f'(\omega) = \frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{f''(\omega')}{(\omega' - \omega)} d\omega' = \frac{2}{\pi} P \int_0^{+\infty} \frac{\omega' f''(\omega')}{(\omega'^2 - \omega^2)} d\omega'$$

$$f''(\omega) = - \frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{f'(\omega')}{(\omega' - \omega)} d\omega' = - \frac{2\omega}{\pi} P \int_0^{+\infty} \frac{f'(\omega')}{(\omega'^2 - \omega^2)} d\omega'$$

$P$  stands for “principal value” (see also comments J. A-N & D. McM p. 242)

- # Resonant scattering

Friedel's law and Bijvoet pairs

The phase problem in crystallography

The MAD method

(Resonant) Magnetic Scattering