Methoden moderner Röntgenphysik II: Streuung und Abbildung

Lecture 8	Vorlesung zum Haupt- oder Masterstudiengang Physik, SoSe 2015	
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Location	Lecture hall AP, Physics, Jungiusstraße	
Date	Tuesday	12:45 - 14:15
	Thursday	8:30 - 10:00

Methoden moderner Röntgenphysik II: Streuung und Abbildung

Part I:

Basics of X-ray Physics

by Gerhard Grübel (GG)

Introduction
Overview, Introduction to X-ray Scattering

X-ray Scattering Primer
Elements of X-ray Scattering

Sources of X-rays, Synchrotron Radiation
Laboratory Sources, Accelerator Bases Sources

Reflection and Refraction from Interfaces
Snell's Law, Fresnel Equations

Kinematical Diffraction (I)
Diffraction from an Atom, a Molecule, from Liquids, Glasses, …

Kinematical Diffraction (II)
Diffraction from a Crystal, Reciprocal Lattice, Structure Factor, …

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 ω_s and damping constant Γ

Include dispersion corrections (f', f"):

[**Note**: $f'' = \left(\frac{k}{4\pi r_0}\right)\sigma_a$]

$$f(\mathbf{Q},\omega) = f^0(\mathbf{Q}) + f'(\omega) + i f''(\omega)$$ [in units of r_0]

Resonant Scattering

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

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

equation of motion of the electron

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

Γ = damping

ω_s resonant frequency

<u>Solution:</u> $x(t) = x_0\, e^{-i\omega t} \longrightarrow$

$$x_0 = -\left(\frac{e\,E_0}{m}\right)\frac{1}{(\omega_s^2 - \omega^2 - i\omega\Gamma)} \qquad \text{(A)}$$

Radiated field strength at distance R and time t

$$E_{rad}(R,t) = \left(\frac{e}{4\,\varepsilon_0 R\,c^2}\right)\ddot{x}\left(t - \frac{R}{c}\right) \qquad \text{(B)}$$

acceleration at “earlier” time $\left(t - \frac{R}{c}\right)$

Resonant Scattering

Inserting $\ddot{x}\left(t-\frac{R}{c}\right) = \omega^2 x_0 e^{-i\omega t} e^{i\left(\frac{\omega}{c}\right)R}$ using (A) into (B):

$$E_{rad}(R,t) = \left(\frac{\omega^2}{(\omega_s^2 - \omega^2 + i\omega\Gamma)}\right)\left(\frac{e^2}{4\,\varepsilon_0 R\, c^2}\right) E_0\, e^{-i\omega t}\left(\frac{e^{ikR}}{R}\right)$$

or

$$\frac{E_{rad}(R,t)}{E_{in}} = -r_0 \frac{\omega^2}{(\omega_s^2 - \omega^2 + i\omega\Gamma)}\left(\frac{e^{ikR}}{R}\right)$$

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

Total cross-section: $\sigma_T = \left(\frac{8\pi}{3}\right) r_o^2$ (free electron)

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

for $\Gamma = 0$ and $\omega << \omega_s$: $\sigma_T = \left(\frac{8\pi}{3}\right) r_o^2 \left(\frac{\omega}{\omega_s}\right)^4$: "Rayleigh Scattering"

Resonant Scattering

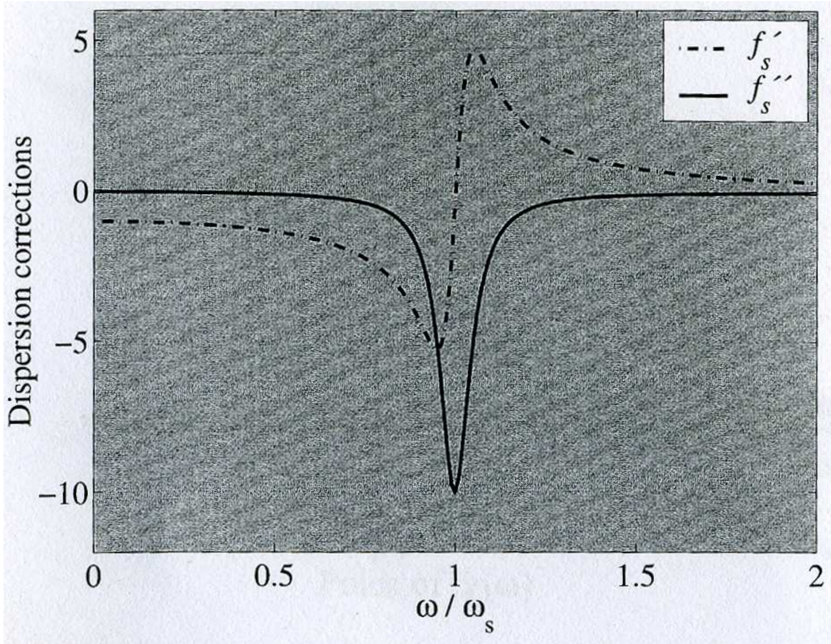
$$f_s = \frac{\omega^2 - \omega_s^2 + i\omega\Gamma + \omega_s^2 - i\omega\Gamma}{(\omega^2 - \omega_{s^2} + i\omega\Gamma)}$$

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

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

dispersion correction $\chi(\omega)$

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



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

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

This function has:

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

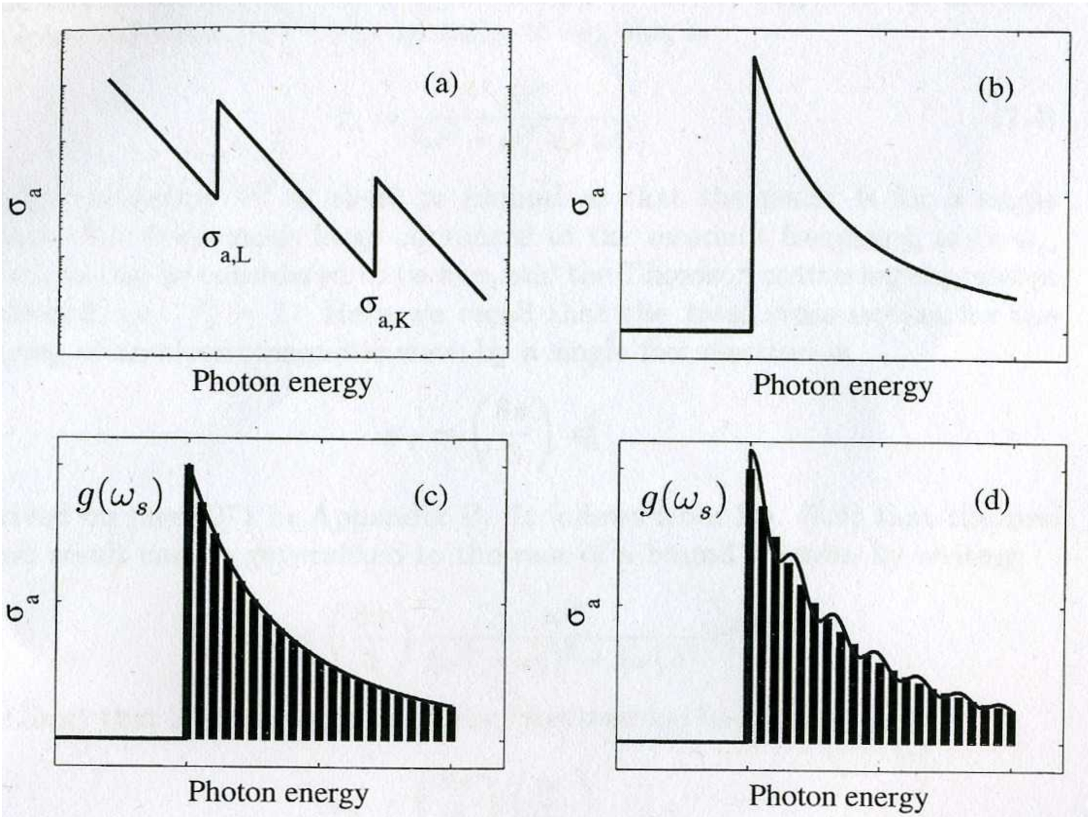
Thus σ_a (E) may be written with help of a delta function:

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

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 ω_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

Geben Sie hier eine Formel ein.

The real part of the dispersion becomes:

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

(F) does not describe e.g. “white lines” or “EXAFS” oscillations (see figure) in the absorption cross-section arising from the particular environement 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