

Methoden moderner Röntgenphysik II: Streuung und Abbildung

Vorlesung zum Haupt- oder Masterstudiengang Physik, SoSe 2019

G. Grübel, F. Lehmkuhler, L. Müller, O. Seeck

Location Lecture hall INF, Physics, Jungiusstraße 11

Time Tuesday 12:30 - 14:30
Thursday 8:30 - 10:00



Outline

Part II/1:

Studies on Magnetic Nanostructures

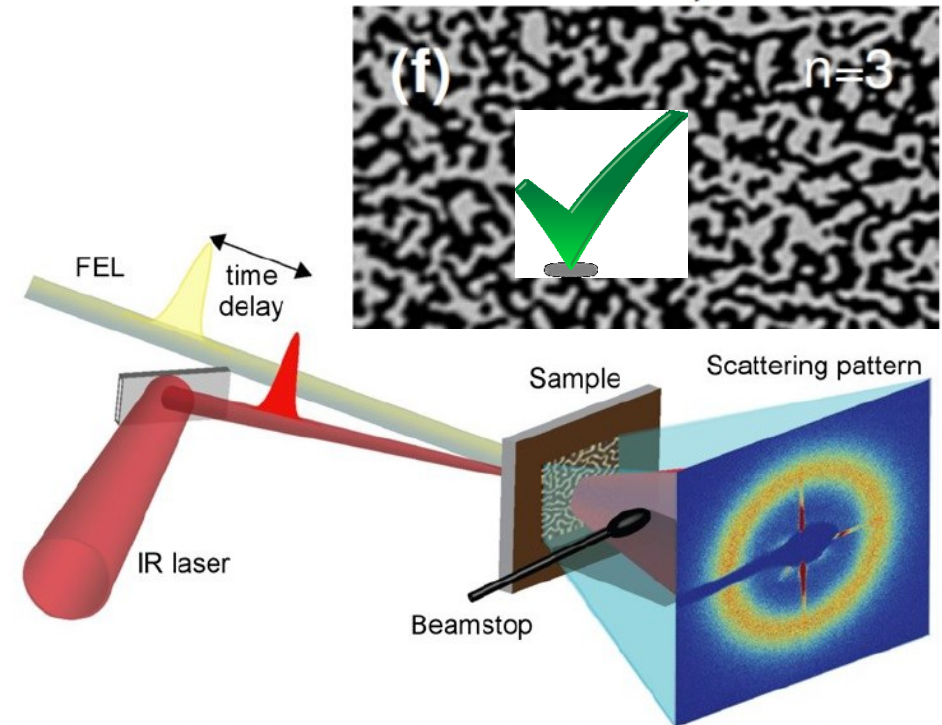
by André Philippi-Kobs (AP)

[28.5.] Ferromagnetism in a Nutshell

- Introduction to Magnetic Materials
- Magnetic Phenomena
- Magnetic Free Energy
- Perpendicular Magnetic Anisotropy
- Magnetic Domains and Domain Walls

[4.6.] Interaction of Polarized Photons with Ferromagnetic Materials

- Charge and Spin X-ray Scattering by a Single Electron
- Absorption and Resonant Scattering of Ferromagnets (Semi-Classical and Quantum-Mechanical Concepts)



B. Pfau et al., Nature Communications, Vol. 3, 11; DOI:doi:10.1038/ncomms2108 (2012)
L. Müller et al., Rev. Sci. Instrum., 84, 013906 (2013)

Interaction of **polarized** photons with matter

2.) Interaction of **polarized** photons with matter

- Recap: Interaction of X-rays with Matter
- Recap: Charge and **Spin** X-ray Scattering by a single electron
- Recap: Classical concept of Resonant Absorption & Scattering (forced oscillator)
- Resonant Absorption and Scattering (**QM concept**, Fermi's Golden rule)
- Interactions of photons with ferromagnetic materials → XMCD effect

Interaction of polarized photons with matter

- > Recap: Interaction of X-rays with matter (consider also light's polarization ϵ)

$$n(\omega, \epsilon) = 1 - \delta(\omega, \epsilon) + i \beta(\omega, \epsilon) \quad \text{Refractive index (classical refraction theory)}$$

$$f(\mathbf{q}, \omega, \epsilon) = f^0(\mathbf{q}) + f'(\omega, \epsilon) - i f''(\omega, \epsilon) \quad \text{Atomic scattering factor (scattering theory)}$$

Atomic form factor
 ~ Z for forward scattering (or soft X-rays)

Anomalous scattering factors
 (electrons are bound in a solid
 → “resonances” at atomic transitions)

- Equivalence between scattering and refraction picture

$$1 - n(\omega, \epsilon) = \frac{r_0 \lambda^2}{2\pi} \rho f(\omega, \epsilon)$$

Atomic density

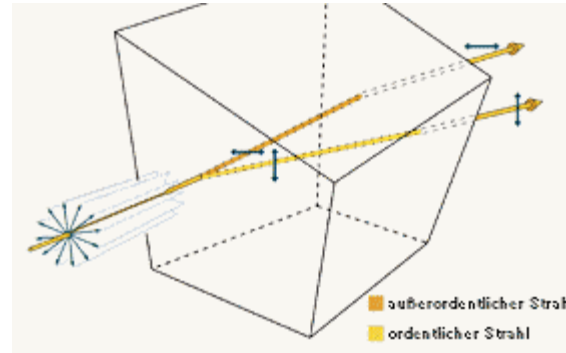
$$\delta(\omega, \epsilon) = \frac{r_0 \lambda^2}{2\pi} \rho (Z + f'(\omega, \epsilon))$$

$$\beta(\omega, \epsilon) = \frac{r_0 \lambda^2}{2\pi} \rho f''(\omega, \epsilon)$$

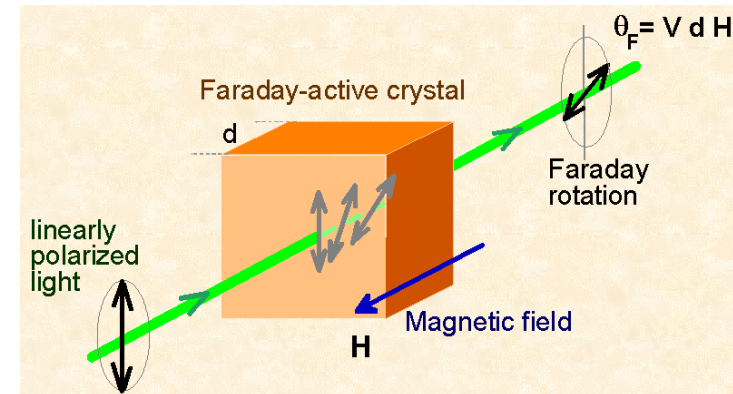
Interaction of polarized photons with matter

> Polarization ϵ dependent effects in transmission geometry

- The dependence of δ on ϵ is called birefringence (Doppelbrechung)



- The change of polarization ϵ is called optical rotation (Faraday effect in case of magnetic materials)



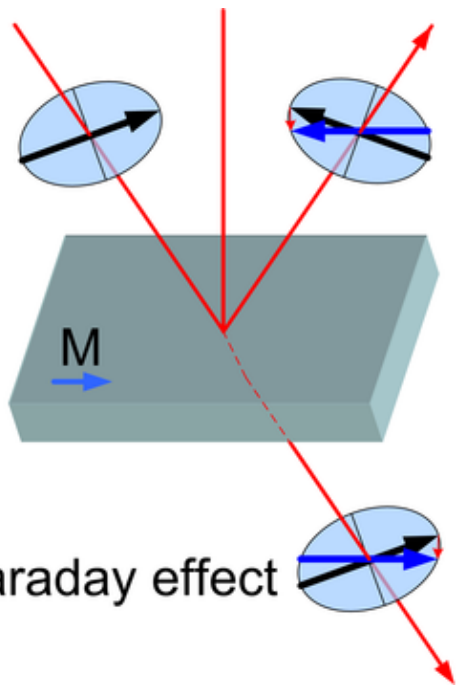
- The dependence of β on ϵ is called dichroism (Zweifarbigkeit)
 - X-ray Natural (charge) linear dichroism (XNLD)
 - X-ray Natural (charge) circular dichroism (XNCD)
 - X-ray magnetic linear dichroism (XMLD)
 - **X-ray magnetic circular dichroism (XMCD)**

Interaction of polarized photons with matter

> History of the interaction between light and ferromagnets

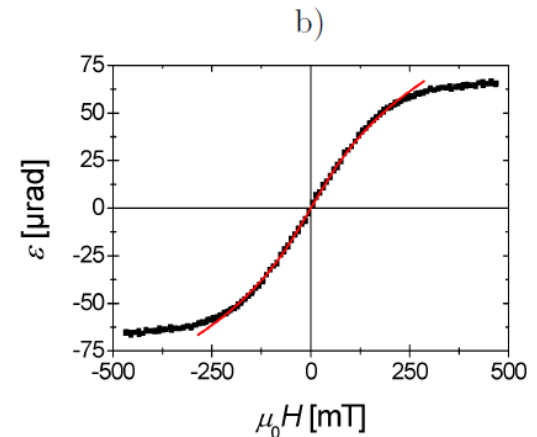
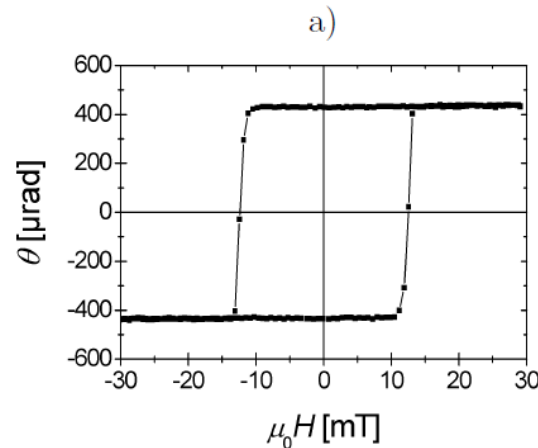
Faraday (1845) and magneto-optical Kerr effect (MOKE) (1876):

Polarization of visible light changes when transmitted/ reflected by a ferromagnetic material



Kerr effect

→ Magnetic hysteresis



Interaction of polarized photons with matter

> History of the interaction between light and ferromagnets

XMCD effect:

Erskine and Stern (1975):

First theoretical formulation of XMCD for the excitation from a core to valence state for the M2,3 edge of Ni

G. Schütz et al. (1987):

First experimental demonstration of the XMCD effect at the K-edge of Fe at DORIS at DESY

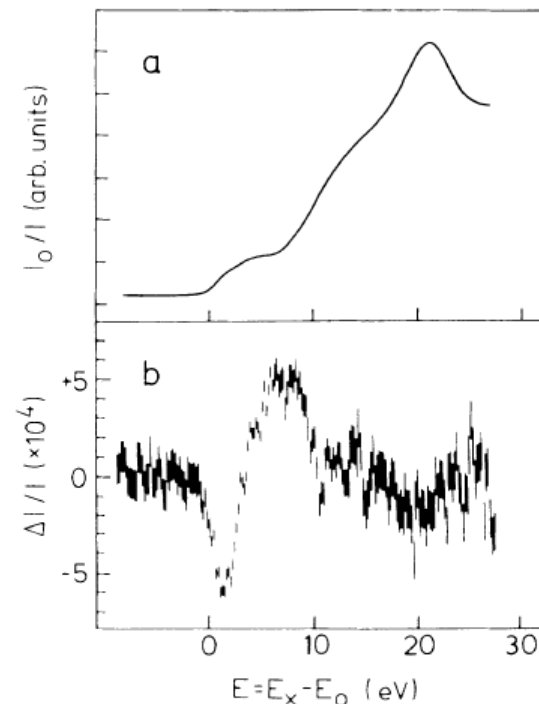


FIG. 1. (a) Absorption I_0/I of x rays as function of the energy E above the K edge of iron and (b) the difference of the transmission $\Delta I/I$ of x rays circularly polarized in and opposite to the direction of the spin of the magnetized d electrons.

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PHYSICAL REVIEW LETTERS

16 FEBRUARY 1987

Absorption of Circularly Polarized X Rays in Iron

G. Schütz, W. Wagner, W. Wilhelm, and P. Kienle^(a)

Physik Department, Technische Universität München, D-8046 Garching, West Germany

R. Zeller

Institut für Festkörperforschung der Kernforschungsanlage Jülich, D-5175 Jülich, West Germany

and

R. Frahm and G. Materlik

Hamburger Synchrotronstrahlungslabor am Deutsches Elektronen-Synchrotron DESY, D-2000 Hamburg 52, West Germany

(Received 22 September 1986)

May 2019 814 citations! (~20 in the last year)



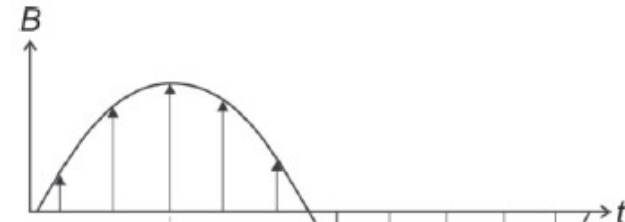
Interaction of polarized photons with matter

- > Scattering of X-rays by a single electron (also consider spin of electron → magnetic XRD)

Incoming plane wave

$$E(\mathbf{r}, t) = \epsilon E_0 e^{-i(\omega t - \mathbf{k} \cdot \mathbf{r})}$$

$$B(\mathbf{r}, t) = \frac{1}{c} (\mathbf{k}_0 \times \epsilon) E_0 e^{-i(\omega t - \mathbf{k} \cdot \mathbf{r})}$$



Electric dipole moment (charge movement) oscillates along **E**

$$p(t) = -\frac{e^2}{m_e \omega^2} E_0 e^{-i\omega t}$$

Spin of electron precesses around magnetic field according to

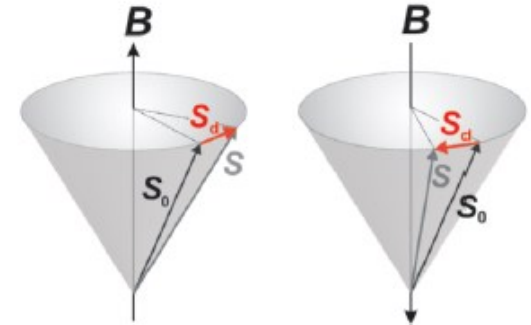
$$\frac{d\vec{S}_d(t)}{dt} = -\frac{e}{m_e} \vec{S}(t) \times \vec{B}(t) \quad \text{Landé-factor}$$

With definition of magnetic moment $m = -2\mu_B s_d$

Magnet dipole moment (spin movement) oscillates in the direction perpendicular to **B** and **S** (initial spin direction)

$$m(t) = i \frac{e^2 \hbar \mu_0}{\omega m_e^2} \mathbf{s} \times \mathbf{B}_0 e^{-i\omega t}$$

Note: different oscillation directions of p and m



Interaction of polarized photons with matter

- > Scattering by a single electron (also consider Spin of electron)

Electric fields radiated by

- electric dipole (Jackson text book):

$$E'(t) = \frac{\omega^2}{4\pi\epsilon_0 c^2} \frac{e^{ik'r}}{r} \cdot [\mathbf{k}'_0 \times \mathbf{p}(t)] \times \mathbf{k}'_0$$

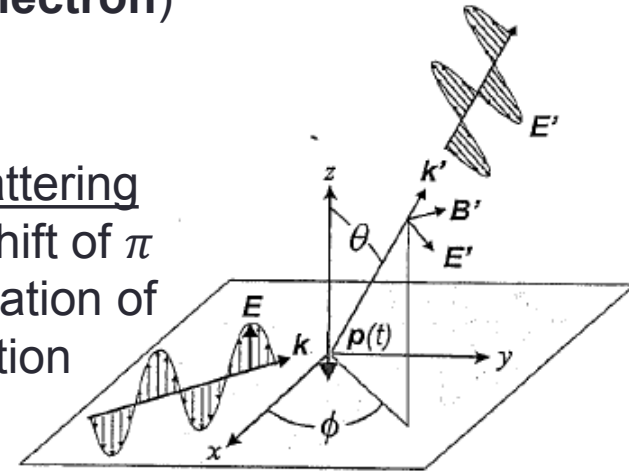
$$E'(t) = -\frac{1}{4\pi\epsilon_0} \cdot \frac{e^2}{m_e c^2} \cdot \frac{e^{ik'r}}{r} [\mathbf{k}'_0 \times \mathbf{E}(t)] \times \mathbf{k}'_0$$

- magnetic dipole (Jackson text book):

$$E'(t) = -\frac{\omega^2}{4\pi c} \frac{e^{ik'r}}{r} [\mathbf{k}'_0 \times \mathbf{m}(t)]$$

$$E'(t) = i \frac{1}{4\pi\epsilon_0} \frac{e^2}{m_e c^2} \frac{\hbar\omega}{m_e c^2} \frac{e^{ik'r}}{r} [\mathbf{s} \times (\mathbf{k}_0 \times \mathbf{E}(t))] \times \mathbf{k}'_0$$

Electric dipole scattering



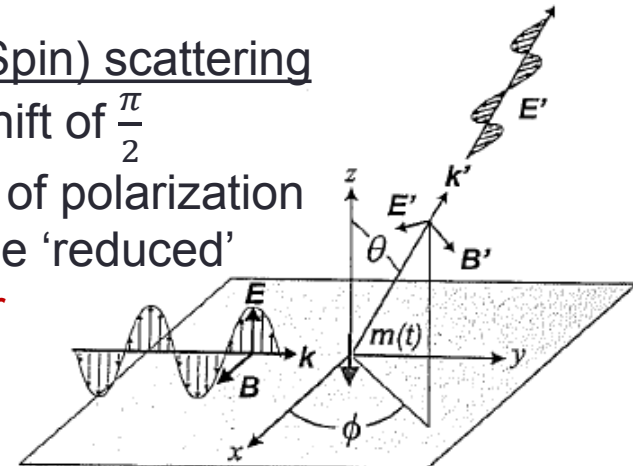
Charge scattering

- Phase shift of π
- Conservation of polarization

Magnetic dipole scattering

Magnetic (Spin) scattering

- Phase shift of $\frac{\pi}{2}$
- Rotation of polarization
- Amplitude 'reduced' by factor



Interaction of polarized photons with matter

➤ Scattering by a single electron (also consider Spin of electron)

Polarization dependent scattering lengths: $f(\epsilon, \epsilon') = -\frac{r_e e^{-ik'r}}{E} \mathbf{E}' \cdot \epsilon'$

$$f_e(\epsilon, \epsilon') = \frac{1}{4\pi\epsilon_0} \frac{e^2}{m_e c^2} \epsilon \cdot \epsilon' = r_0 \underbrace{\epsilon \cdot \epsilon'} \quad f_s(\epsilon, \epsilon') = -i r_0 \frac{\hbar\omega}{m_e c^2} \mathbf{s} \cdot (\mathbf{k}_0 \times \epsilon) \times (\mathbf{k}'_0 \times \epsilon')$$

Remember: Polarization factor $P = \sin\theta$

Differential scattering cross-section: $\frac{d\sigma}{d\Omega} = |f(\epsilon, \epsilon')|^2 = r_0^2 \sin^2\theta$ für $f = f_e$

Total cross-section: $\sigma_e = \int |f(\epsilon, \epsilon')|^2 d\Omega = r_0^2 \int_0^{2\pi} d\varphi \int_0^\pi d\theta \sin^2\theta$

$$\sigma_e = \frac{8\pi}{3} r_0^2 = 0.665 \times 10^{-28} \text{ m}^2 = 0.665 \text{ barn}$$

$$\sigma_s = \frac{8\pi}{3} \frac{1}{4} \left(\frac{\hbar\omega}{m_e c^2} \right)^2 r_0^2 = \frac{\sigma_e}{4} \left(\frac{\hbar\omega}{m_e c^2} \right)^2$$

$E = 10 \text{ keV} \rightarrow \frac{\sigma_s}{\sigma_e} = 0.0004$ Only weak spin-scattering signal



Main Messages:

- Charge scattering causes a phase shift of π ('-') between incident and scattered field
- Spin scattering causes a phase shift of $\frac{\pi}{2}$ ('i') between incident and transmitted field
- The spin-scattering amplitude is reduced by a factor $\frac{\hbar\omega}{m_e c^2}$ relative to charge scattering amplitude, with $m_e c^2 = 511\text{keV}$, i.e., for extremely high photon energies spin scattering is stronger (these energies are [usually] not relevant for x-ray physics)
- Charge scattering conserves the polarization while spin scattering causes a rotation of the polarization

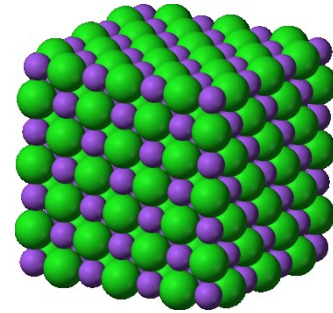
Spin scattering is generally weak and can only be measured in special circumstances



Interaction of polarized photons with matter

➤ Scattering by a single electron (also consider Spin of electron)

Example: magnetic XRD of antiferromagnetic NiO



Volume 39A, number 2

PHYSICS LETTERS

24 April 1972

OBSERVATION OF MAGNETIC SUPERLATTICE PEAKS BY X-RAY DIFFRACTION ON AN ANTIFERROMAGNETIC NiO CRYSTAL

F. De BERGEVIN and M. BRUNEL
 Laboratoire de rayons-X, Cédex 166, 38-Grenoble-Gare, France

Received 14 February 1972

intensity of the (111) reflection. We have searched and measured in the zone $\{hhh\}$ the first two superlattice magnetic reflections $(\frac{1}{2} \frac{1}{2} \frac{1}{2})$ and $(\frac{3}{2} \frac{3}{2} \frac{3}{2})$ and the first ordinary reflection (111). If an equal amount of all possible magnetic domains or twins is supposed to form the crystal, the formula (1) applied to these reflections gives a ratio R between magnetic and ordinary (111) intensities, approximately equal to 4×10^{-8} . Such a small value obliges to take an unusual care of obtaining a maximum intensity and a minimum background. The r

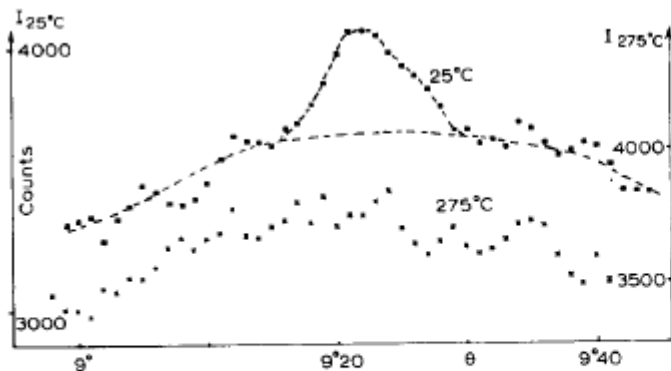


Fig. 1. Intensity $I_f(\theta)$ near the $(\frac{1}{2} \frac{1}{2} \frac{1}{2})$ position at $t = 25^\circ \text{C}$ and 275°C in counts/225 min. The hump which cover the interval could be due to some impurity.

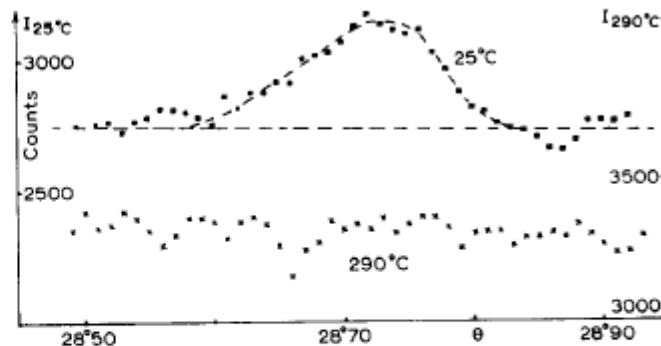


Fig. 2. Intensity $I_f(\theta)$ near the $(\frac{3}{2} \frac{3}{2} \frac{3}{2})$ position at $t = 25^\circ \text{C}$ and 290°C in counts/225 min.



Interaction of polarized photons with matter

- > Recap: Absorption and Resonant Scattering (classical concept)

Picture: Electrons are bound to atoms

→ Forced oscillator model with resonances ω_s and damping Γ to describe equation of motion of electrons

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

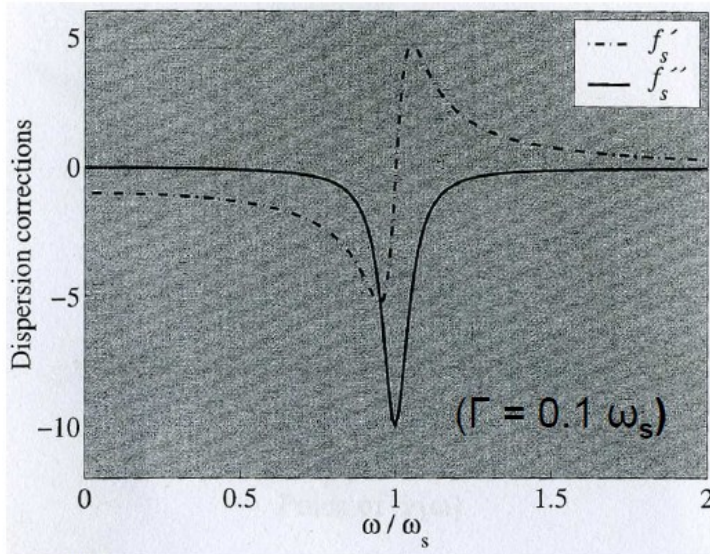
atomic scattering length f_s (in units of $-r_0$) for bound electron
 note: $f_s \rightarrow 1$ ($\omega \gg \omega_s$)

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

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

Interaction of polarized photons with matter

> Recap: Absorption and Resonant Scattering (classical concept)



$$f'' = -(k/4\pi) \sigma_a (E) \quad (\text{optical theorem } 2k\beta = \mu = \rho\sigma_a)$$

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

Measure absorption cross-section in experiment

Use Kramers-Kronig relations to obtain f'

with:

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

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

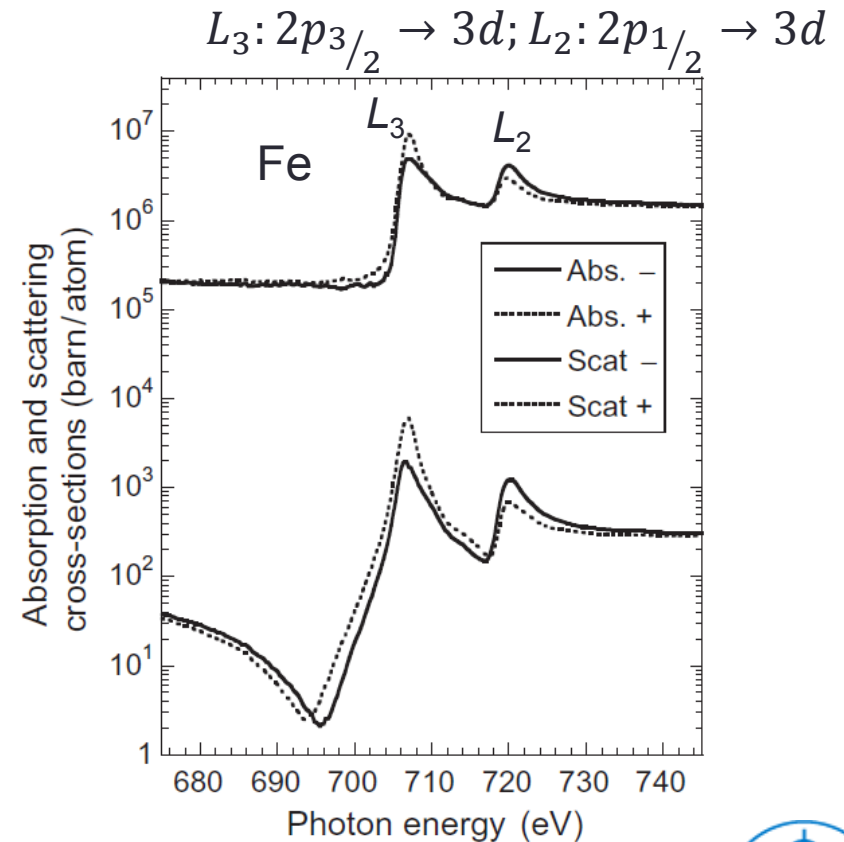
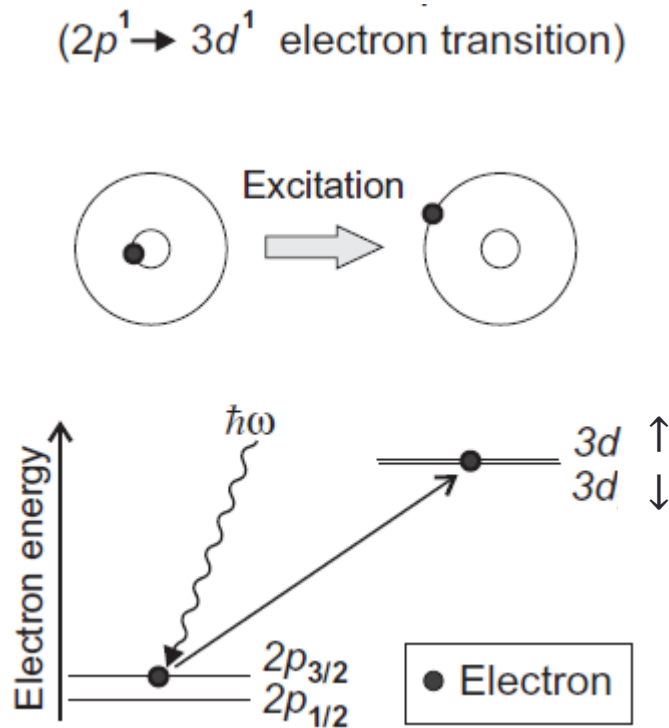
$$f'(\omega) = \frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{f''(\omega')}{(\omega' - \omega)} d\omega'$$

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

Interaction of polarized photons with matter

- > Absorption & Resonant scattering (qm concept, Fermi's Golden rule)

Motivation: Understand polarization dependent $2p \rightarrow 3d$ transition in ferromagnets, i.e., XMCD effect



Interaction of polarized photons with matter

> Absorption & Resonant scattering (qm concept, Fermi's Golden rule)

- Time-dependent perturbation theory (up to second order) = „Fermi's Golden rule“

$$T_{if} = \frac{2\pi}{\hbar} \left| \langle f | \mathcal{H}_{\text{int}} | i \rangle + \sum_n \frac{\langle f | \mathcal{H}_{\text{int}} | n \rangle \langle n | \mathcal{H}_{\text{int}} | i \rangle}{\varepsilon_i - \varepsilon_n} \right|^2 \delta(\varepsilon_i - \varepsilon_f) \rho(\varepsilon_f)$$

T_{if} : transition rate from state i to f ; $[T_{if}] = \text{s}^{-1}$;
 i and f are initial and final states of the combined electron and photon system

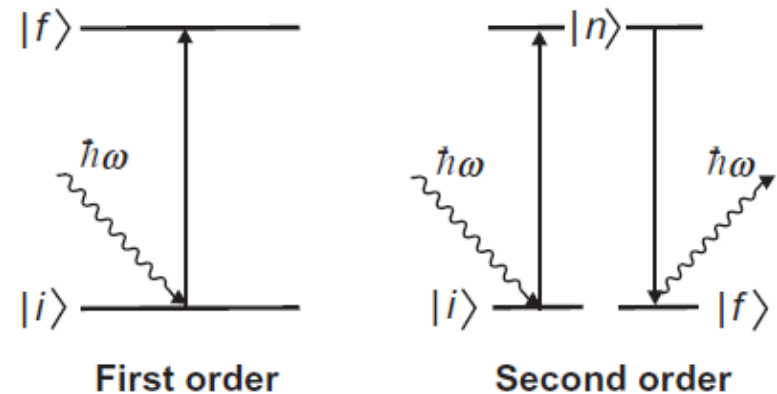
$\rho(\varepsilon_f)$: density of final states

ε_n : energy of all possible intermediate states n

- Total cross-section given by $\sigma = \frac{T_{if}}{\Phi_0}$

Incident photon flux

(a) X-Ray absorption (b) Resonant scattering



Interaction of polarized photons with matter

> Absorption & Resonant scattering (qm concept, Fermi's Golden rule)

- Time-dependent perturbation theory (up to second order)

$$T_{if} = \frac{2\pi}{\hbar} \left| \langle f | \mathcal{H}_{\text{int}} | i \rangle + \sum_n \frac{\langle f | \mathcal{H}_{\text{int}} | n \rangle \langle n | \mathcal{H}_{\text{int}} | i \rangle}{\varepsilon_i - \varepsilon_n} \right|^2 \delta(\varepsilon_i - \varepsilon_f) \rho(\varepsilon_f)$$

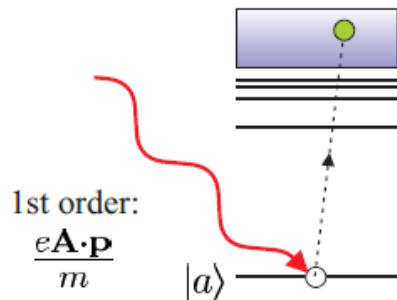
- Interaction Hamiltonian

(derivation again via force on "atom in electric and magnetic field")

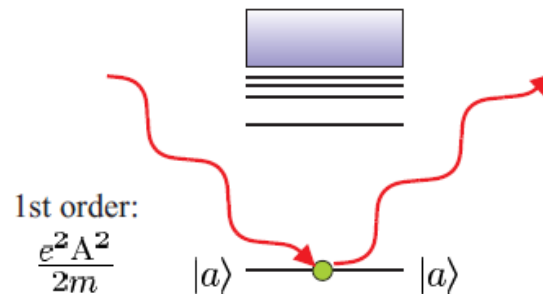
$$\mathcal{H}_e^{\text{int}} = \frac{e}{m_e} \mathbf{p} \cdot \mathbf{A} + \cancel{\frac{e^2 A^2}{2m_e}}$$

p : momentum of electrons
 A : vector potential

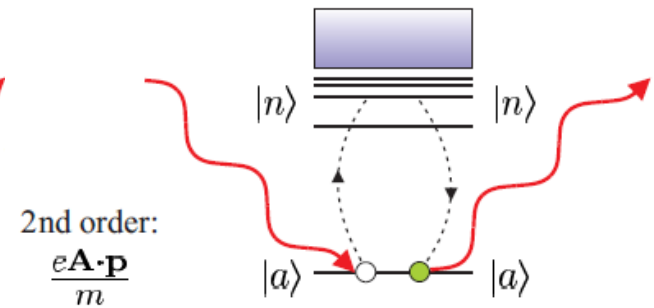
(a) Photoelectric absorption



(b) Thomson scattering



(c) Resonant scattering



Interaction of polarized photons with matter

> Absorption & Resonant scattering (qm concept, Fermi's Golden rule)

- Time-dependent perturbation theory (up to second order)

$$T_{if} = \frac{2\pi}{\hbar} \left| \underbrace{\langle f | \mathcal{H}_{\text{int}} | i \rangle}_M + \sum_n \frac{\langle f | \mathcal{H}_{\text{int}} | n \rangle \langle n | \mathcal{H}_{\text{int}} | i \rangle}{\varepsilon_i - \varepsilon_n} \right|^2 \delta(\varepsilon_i - \varepsilon_f) \rho(\varepsilon_f)$$

- Interaction Hamiltonian

(derivation again via force on "atom in electric and magnetic field")

$$\mathcal{H}_e^{\text{int}} = \frac{e}{m_e} \mathbf{p} \cdot \mathbf{A}$$

p : momentum of electrons
 A : vector potential

- Consider only the much stronger impact of electric field component of EM wave on electrons (begin of lecture: Charge scattering >> Spin scattering)

$$\vec{E} = -\frac{\partial A}{\partial t}$$

$$\vec{E}(\vec{r}) = \vec{\epsilon} E_0 \cdot e^{i\vec{k}\vec{r}}$$

$$M = \langle b | \vec{p} \vec{\epsilon} e^{i\vec{k}\vec{r}} | a \rangle, \quad |a\rangle, |b\rangle \text{ atomic states}$$



Interaction of polarized photons with matter

- > Absorption & Resonant scattering (qm concept, Fermi's Golden rule)

Matrix elements for atomic transitions between states a and b

$$\mathcal{M} = \langle b | \mathbf{p} \cdot \boldsymbol{\epsilon} e^{i\mathbf{k} \cdot \mathbf{r}} | a \rangle$$

Dipole-Approximation: eliminate the k dependence in M

Expansion of $e^{i\vec{k}\vec{r}} = 1 + i\vec{k}\vec{r} - \frac{(\vec{k}\vec{r})^2}{2} + \dots$

Size of r : $|\vec{r}| \approx 0.1\text{\AA} = \ell$ for $2p$ core shells

Soft X rays : $E_\gamma \leq 1\text{keV} \rightarrow \lambda \geq 1\text{nm} \approx 100 \cdot \ell$; $|\vec{k}| = \frac{2\pi}{\lambda} \leq 5 \cdot 10^9 \text{ m}^{-1}$

$$|\vec{k}| \cdot |\vec{r}| \leq 0.05 \ll 1 \rightarrow e^{i\vec{k}\vec{r}} \approx 1$$

$\rightarrow M = \langle b | \vec{p} \cdot \vec{\epsilon} | a \rangle$ is the dipole approximation



Interaction of polarized photons with matter

- > Absorption & Resonant scattering (qm concept, Fermi's Golden rule)

Matrix elements for atomic transitions between states a and b

$$\mathcal{M} \simeq \langle b | \mathbf{p} \cdot \boldsymbol{\epsilon} | a \rangle$$

Reformulation of Matrix-elements

$$\begin{aligned}
 M &= \langle b | \vec{p} \vec{\epsilon} | a \rangle = \frac{im_e}{\hbar} \langle b | [H_0, \vec{r}] \vec{\epsilon} | a \rangle \\
 &= \frac{im_e}{\hbar} (\langle b | H \cdot \vec{r} \vec{\epsilon} | a \rangle - \langle b | r \cdot H \cdot \vec{\epsilon} | a \rangle) \\
 &= \frac{im_e}{\hbar} (E_b \langle b | \vec{r} \vec{\epsilon} | a \rangle - E_a \langle b | \vec{r} \cdot \vec{\epsilon} | a \rangle) \\
 &= \frac{im_e}{\hbar} (E_b - E_a) \langle b | \vec{r} \vec{\epsilon} | a \rangle = im_e \omega \langle b | \vec{r} \vec{\epsilon} | a \rangle
 \end{aligned}$$

Absorption cross-section in dipole approximation

$$\sigma^{\text{abs}} = \text{[redacted]} \delta[\hbar\omega - (E_b - E_a)] \rho(E_b)$$



Interaction of polarized photons with matter

- > Absorption & Resonant scattering (qm concept, Fermi's Golden rule)

Polarization dependent Dipole Operator

$$P = \epsilon \cdot r$$

Electron position vector or length operator

$$r = x e_x + y e_y + z e_z$$

Linear polarized light

$$\epsilon_x^0 = \epsilon_x = e_x$$

$$\epsilon_y^0 = \epsilon_y = e_y$$

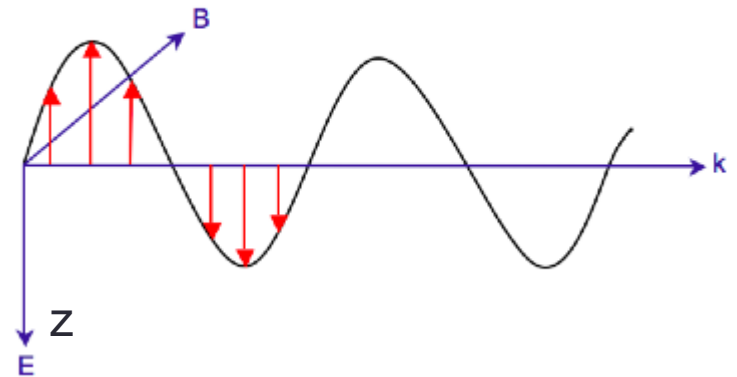
$$\epsilon_z^0 = \epsilon_z = e_z$$

(extreme cases')

$$\begin{aligned}
 P_z^0 &= \vec{\epsilon}_z \cdot \vec{r} = z = r \cos \theta \\
 &= r \sqrt{\frac{4\pi}{3}} \cdot Y_{1,0}
 \end{aligned}$$

$Y_{l,m}$: spherical harmonics = Kugelflächenfunktion

Linearly polarized



Interaction of polarized photons with matter

- > Absorption & Resonant scattering (qm concept, Fermi's Golden rule)

Polarization dependent Dipole Operator $P = \epsilon \cdot r$

Circular polarized light $(\vec{k} || z)$

$\vec{\epsilon} = \pm \frac{1}{\sqrt{2}} \epsilon_x \pm i\vec{\epsilon}_y$, i.e., supposition of linear light with a phase shift of $\frac{\pi}{2}$

Definition of Helicity

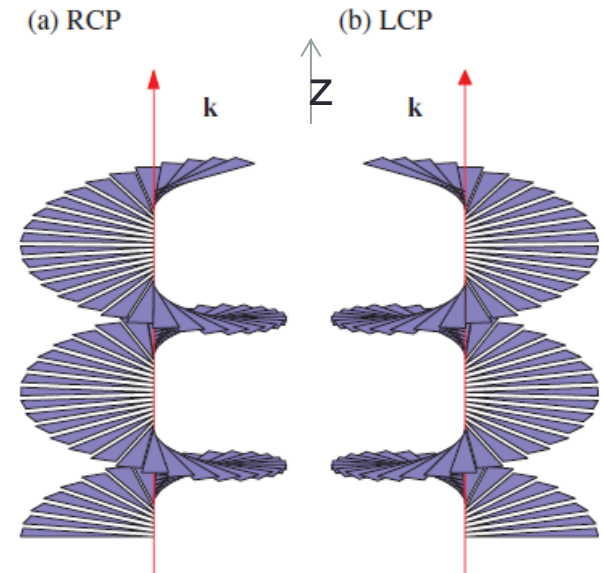
(photon angular momentum or spin $\mathbf{L}_{ph,z} || \mathbf{z}$):

$$|\mathbf{L}_{ph,z}| = \pm q h$$

“+”: $q = +1$ right circularly polarized light (RCP)

“-”: $q = -1$ left circularly polarized light (LCP)

(“0”: $q = 0$ lin. pol. Light)



Interaction of polarized photons with matter

> Absorption & Resonant scattering (qm concept, Fermi's Golden rule)

→ Polarization dependent Dipole Operator for circularly polarized light:

$$\begin{aligned}
 P_z^\pm &= \vec{\epsilon}_z^\pm \cdot \vec{r} = \mp \frac{1}{\sqrt{2}} (x + iy) = \mp r \cdot \sin\theta e^{\pm i\phi} \\
 &= r \sqrt{\frac{4\pi}{3}} Y_{1,\pm 1} = r \sqrt{\frac{4\pi}{3}} Y_{\ell,m_\ell}
 \end{aligned}$$

Racah's spherical tensor operators are defined as [181],

$$C_m^{(l)} = \sqrt{\frac{4\pi}{2l+1}} Y_{l,m}(\theta, \phi), \quad \left(C_m^{(l)}\right)^* = (-1)^m C_{-m}^{(l)}.$$

Dipol operator: $P_z^0 = rC_0^{(1)}$ for linear polarization
 $P_z^\pm = rC_{\pm 1}^{(1)}$ for RCP (+) and LCP (-)



Interaction of polarized photons with matter

> Absorption (qm concept, Fermi's Golden rule)

→ Transition-Matrix-Elements with atomic wave functions (non-relativistic approx.)

$$|a\rangle = |R_{n,l}(r); l, m_l, s, m_s\rangle = R_{n,l}(r) Y_{l,m_l} \chi_{s,m_s}$$

$$|b\rangle = |R_{n',l'}(r); l', m_{l'}, s', m'_{s'}\rangle$$

$$\langle b | P_Z^q | a \rangle = \underbrace{\delta(m'_{s'}, m_s)}_{\text{Spin}} \cdot \underbrace{\langle R_{n',l'}(\vec{r}) | r | R_{n,l}(\vec{r}) \rangle}_{\text{Radial}} \cdot \underbrace{\sum_{m_l, m'_{l'}, q} e_{\alpha,p}^q \langle l', m'_{l'} | C_q^{(1)} | l, m_l \rangle}_{\text{Angular}}$$

Spin:	Electron-spin direction is conserved
Radial transition strength:	the same transition strength for all $2p \rightarrow 3d$ transitions
Angular:	Contains polarization dependence

Note: as core electrons are strongly localized, absorption spectroscopy is sensitive to the valence shell properties within the atomic volume



Interaction of polarized photons with matter

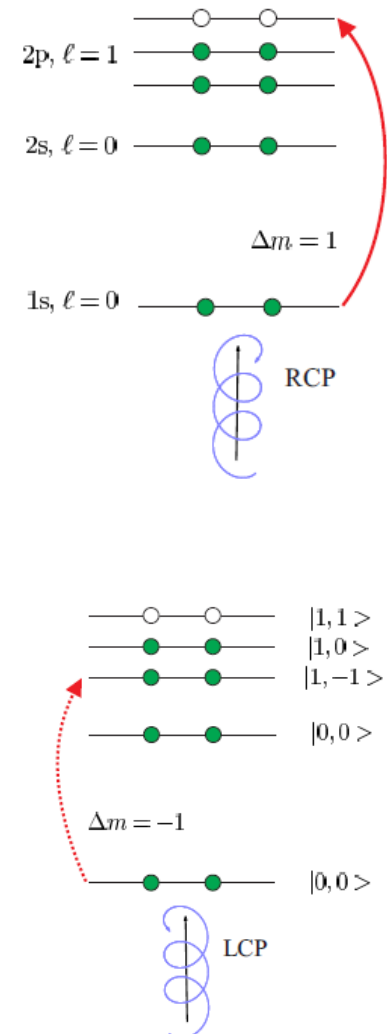
> Absorption (qm concept, Fermi's Golden rule)

Non-vanishing matrix elements (use in today's exercise)

Table 1 Nonvanishing angular momentum dipole matrix elements $\langle L, M | C_q^{(1)} | l, m \rangle$. The matrix elements are real, so that $\langle L, M | C_q^{(1)} | l, m \rangle^* = \langle L, M | C_q^{(1)} | l, m \rangle = (-1)^q \langle l, m | C_{-q}^{(1)} | L, M \rangle$. Nonlisted matrix elements are zero.^a

$\langle l + 1, m C_0^{(1)} l, m \rangle = \sqrt{\frac{(l + 1)^2 - m^2}{(2l + 3)(2l + 1)}}$	Lin. pol
$\langle l - 1, m C_0^{(1)} l, m \rangle = \sqrt{\frac{l^2 - m^2}{(2l - 1)(2l + 1)}}$	
$\langle l + 1, m + 1 C_1^{(1)} l, m \rangle = \sqrt{\frac{(l + m + 2)(l + m + 1)}{2(2l + 3)(2l + 1)}}$	RCP
$\langle l - 1, m + 1 C_1^{(1)} l, m \rangle = -\sqrt{\frac{(l - m)(l - m - 1)}{2(2l - 1)(2l + 1)}}$	
$\langle l + 1, m - 1 C_{-1}^{(1)} l, m \rangle = \sqrt{\frac{(l - m + 2)(l - m + 1)}{2(2l + 3)(2l + 1)}}$	LCP
$\langle l - 1, m - 1 C_{-1}^{(1)} l, m \rangle = -\sqrt{\frac{(l + m)(l + m - 1)}{2(2l - 1)(2l + 1)}}$	

(a) Simplified energy level diagram



Interaction of polarized photons with matter

> Absorption (qm concept, Fermi's Golden rule)

Dipole selection rules (for states of the form $|n, l, m_l, s, m_s\rangle$)

$$\Delta l = l' - l = \pm 1$$

$$\Delta m_l = m'_l - m_l = q = 0, \pm 1$$

$$\Delta s = s' - s = 0$$

$$\Delta m_s = m'_s - m_s = 0$$

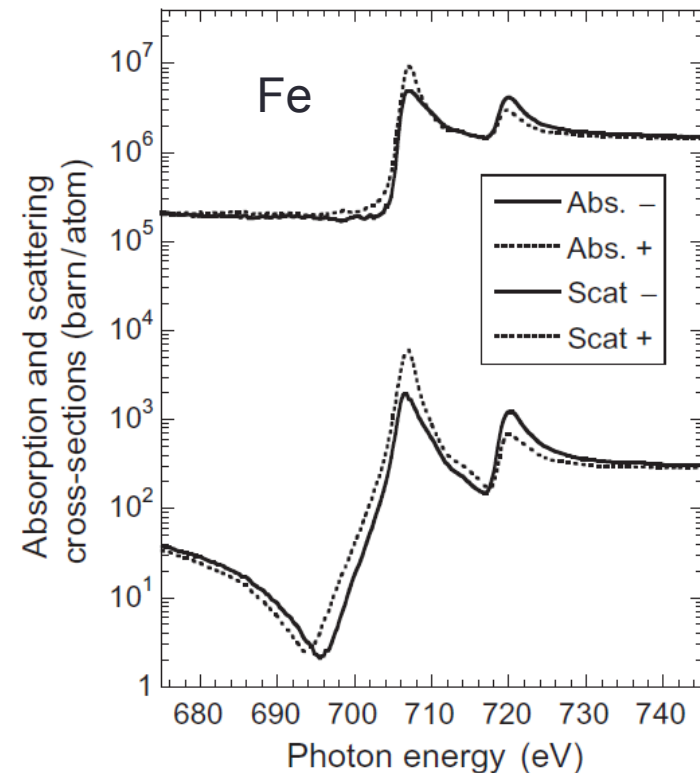
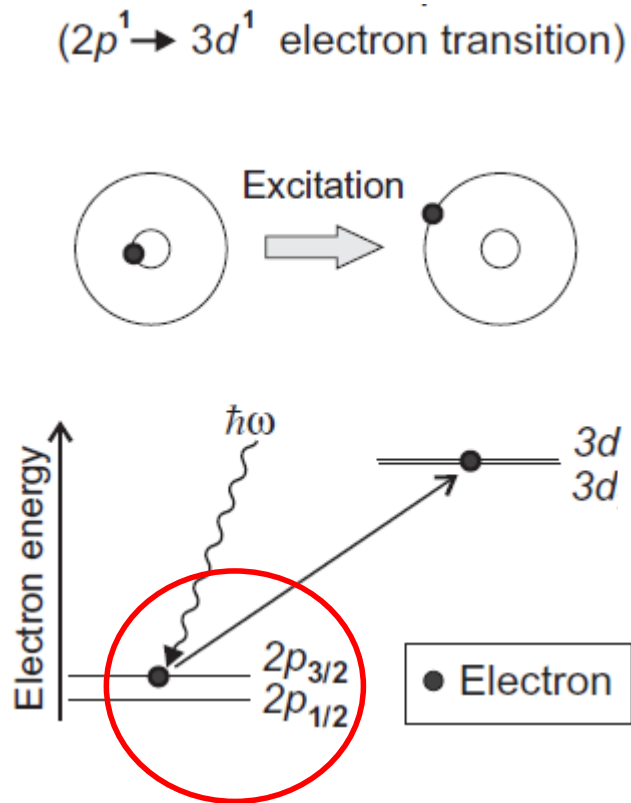
q = polarization (Lin, RCP, LCP)

Note: spin direction is conserved

Interaction of polarized photons with matter

- > Absorption & Resonant scattering (qm concept, Fermi's Golden rule)

Motivation: Understand polarization dependent $2p \rightarrow 3d$ transition in ferromagnets, i.e., XMCD effect



Interaction of polarized photons with matter

> Absorption (qm concept, Fermi's Golden rule)

Atomic core shell states are split due to spin-orbit split interaction (use in next lecture)
 → Clebsch-Gordon coefficients C

$$|l, s, j, m_j\rangle = \sum_{m_l, m_s} C_{m_l, m_s; j, m_j} |l, s, m_l, m_s\rangle$$

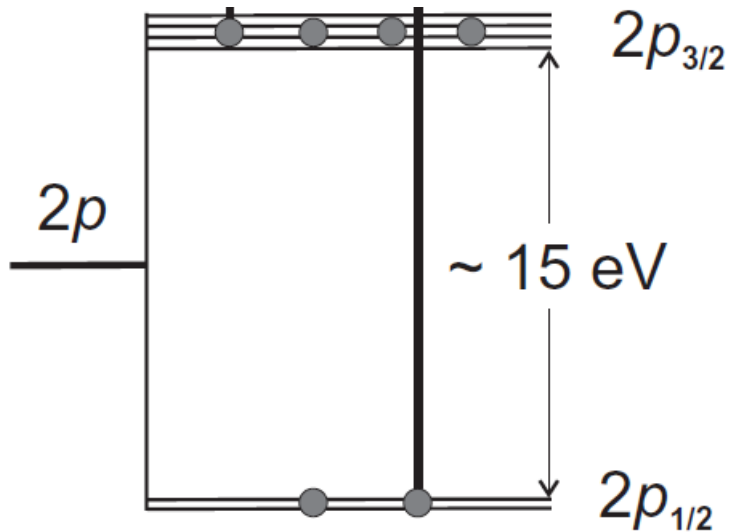


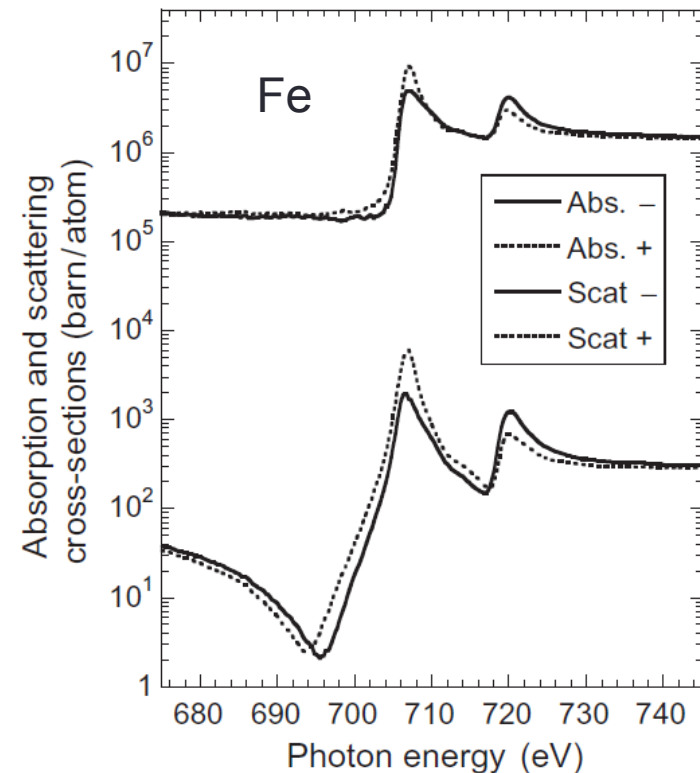
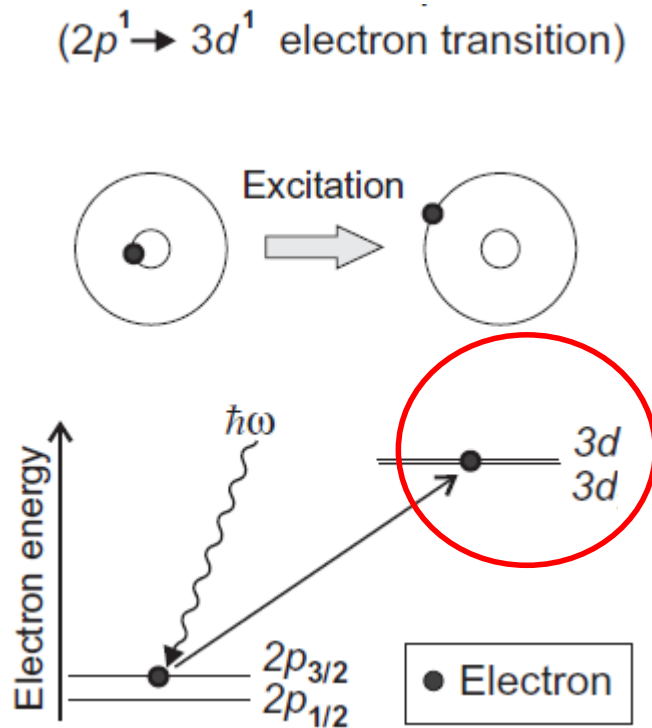
Table 2

$ l, s, j, m_j\rangle$ basis		$ l, m_l, s, m_s\rangle$ basis
j	m_j	$Y_{l, m_l} \chi^\pm$
$\frac{1}{2}$	$+\frac{1}{2}$	$\frac{1}{\sqrt{3}}(-Y_{1,0} \alpha + \sqrt{2} Y_{1,+1} \beta)$
	$-\frac{1}{2}$	$\frac{1}{\sqrt{3}}(-\sqrt{2} Y_{1,-1} \alpha + Y_{1,0} \beta)$
$\frac{3}{2}$	$+\frac{3}{2}$	$Y_{1,+1} \alpha$
	$+\frac{1}{2}$	$\frac{1}{\sqrt{3}}(\sqrt{2} Y_{1,0} \alpha + Y_{1,+1} \beta)$
	$-\frac{1}{2}$	$\frac{1}{\sqrt{3}}(Y_{1,-1} \alpha + \sqrt{2} Y_{1,0} \beta)$
	$-\frac{3}{2}$	$Y_{1,-1} \beta$

Interaction of polarized photons with matter

- > Absorption & Resonant scattering (qm concept, Fermi's Golden rule)

Motivation: Understand polarization dependent $2p \rightarrow 3d$ transition in ferromagnets, i.e., XMCD effect

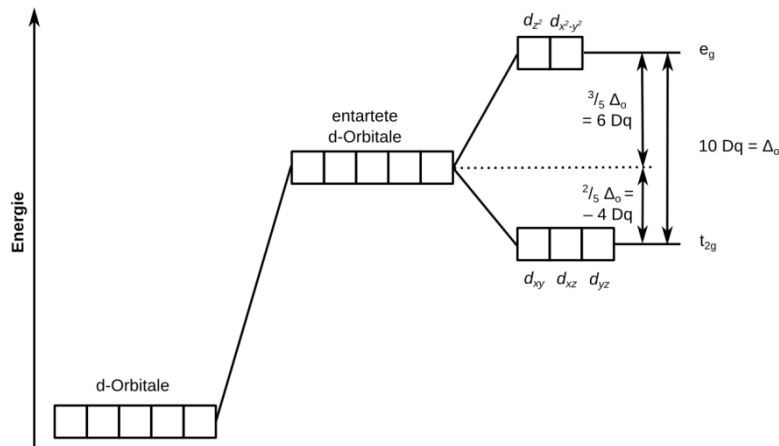
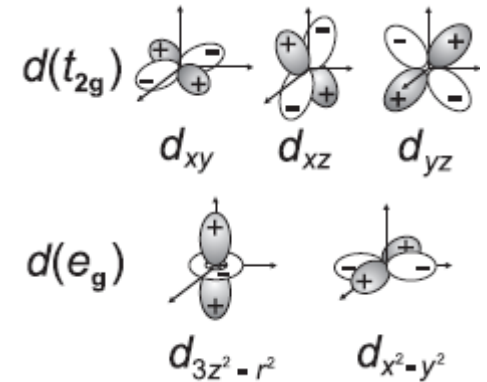


For d-states the spin-orbit coupling is small but there is crystal-field splitting

Interaction of polarized photons with matter

> Absorption (qm concept, Fermi's Golden rule)

Itinerant *d*-states are split due to crystal field
(can be neglected to a good approximation as splitting is small
→ use atomic wave functions without SOC; next lecture)



$$\begin{aligned}
 d_{xy} &= \sqrt{\frac{15}{4\pi}} \frac{xy}{r^2} = \frac{i}{\sqrt{2}} (Y_{2,-2} - Y_{2,+2}) \\
 d_{xz} &= \sqrt{\frac{15}{4\pi}} \frac{xz}{r^2} = \frac{1}{\sqrt{2}} (Y_{2,-1} - Y_{2,+1}) \\
 d_{yz} &= \sqrt{\frac{15}{4\pi}} \frac{yz}{r^2} = \frac{i}{\sqrt{2}} (Y_{2,-1} + Y_{2,+1}) \\
 d_{x^2-y^2} &= \sqrt{\frac{15}{16\pi}} \frac{(x^2 - y^2)}{r^2} = \frac{1}{\sqrt{2}} (Y_{2,-2} + Y_{2,+2}) \\
 d_{3z^2-r^2} &= \sqrt{\frac{5}{16\pi}} \frac{(3z^2 - r^2)}{r^2} = Y_{2,0}
 \end{aligned}$$

