Resonant Elastic and Inelastic X-ray Scattering

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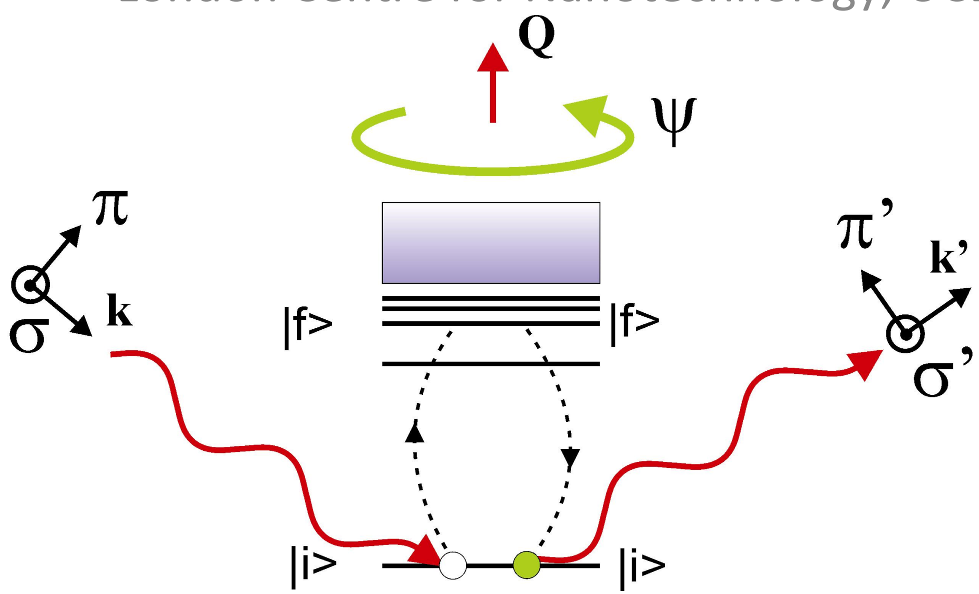
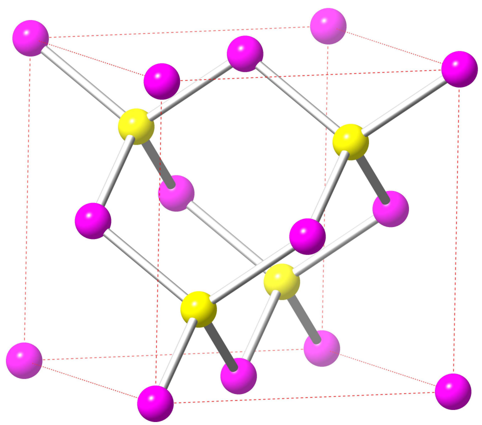


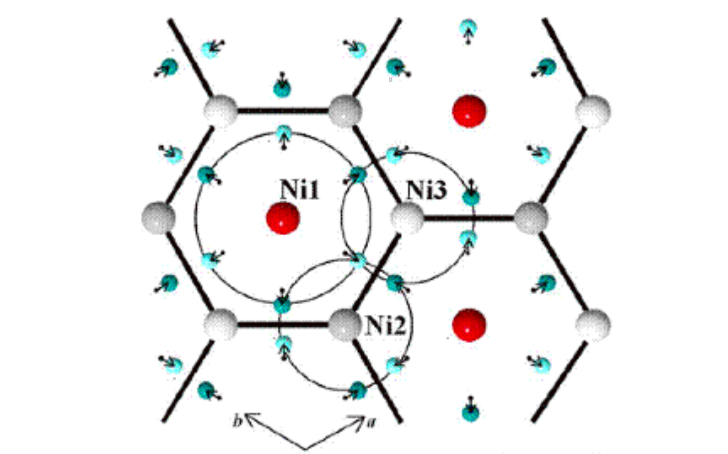
- Introduction
- Scattering cross-sections, refraction and absoprtion
- Resonant Elastic X-ray Scattering
    - Magnetic order: Novel MITs in 5d transition metal oxides
    - Mulitipolar order: Orbital ordering
- Resonant Inelastic X-ray Scattering
    - Magnons and crystal-field excitations: 5d transition metal oxides
- Summary

Elastic Scattering: groundstates and order

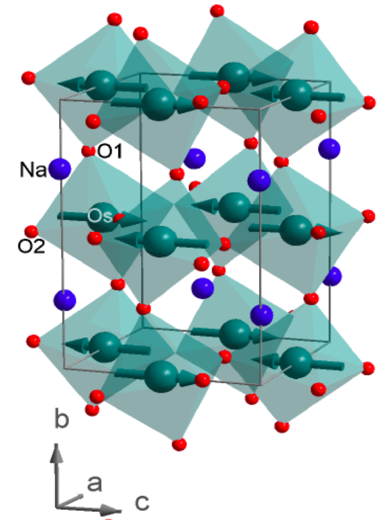
Charge density

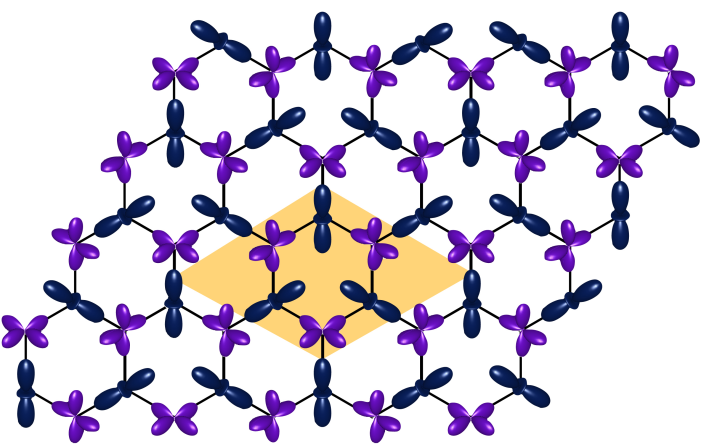


Charge order

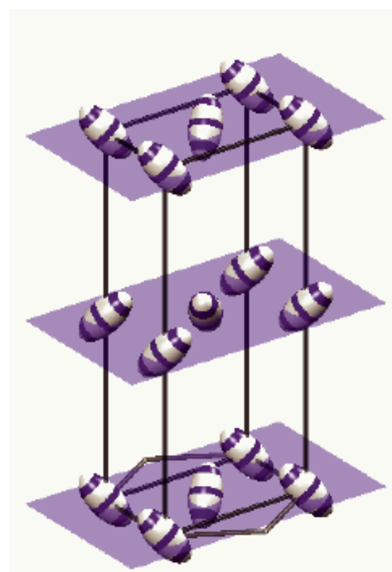


Magnetic order

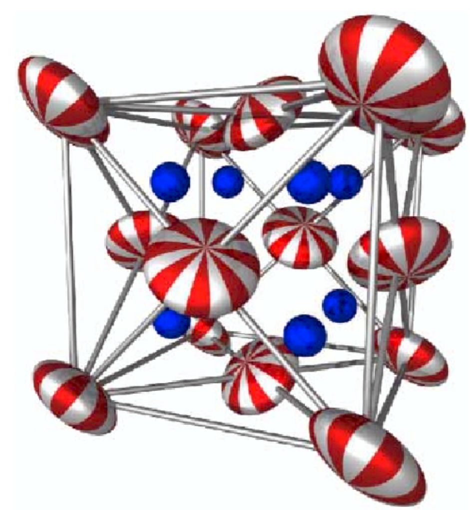




Orbital order



Quadrupolar order



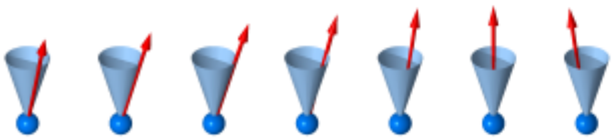
Octupolar order

Inelastic Scattering: excitations

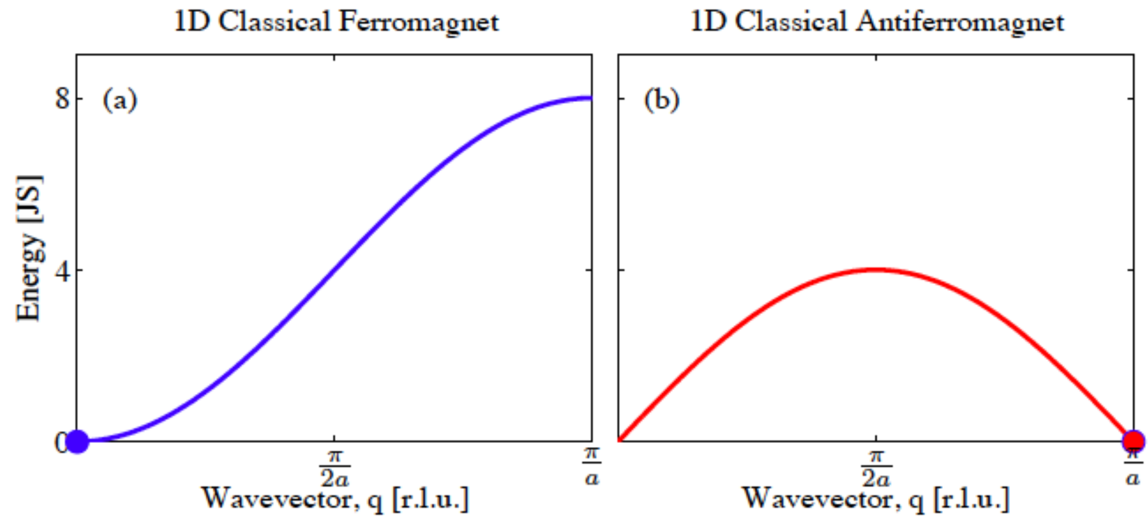
Interactions

$$\mathcal{H} = J \sum_{<ij>} \mathbf{S}_i \cdot \mathbf{S}_j$$

Collective Excitations

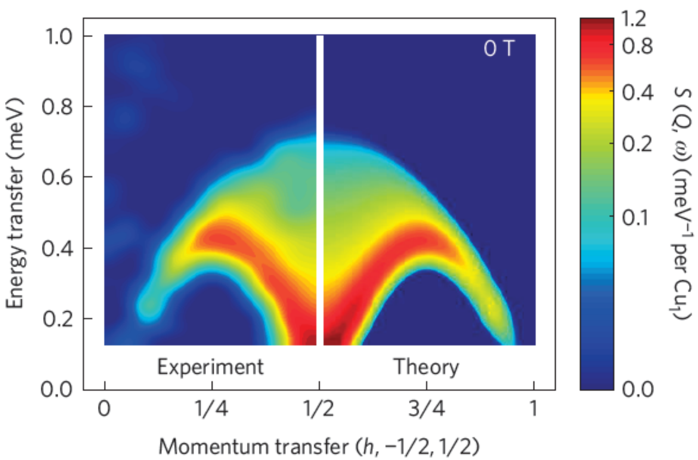


Dispersion Relations

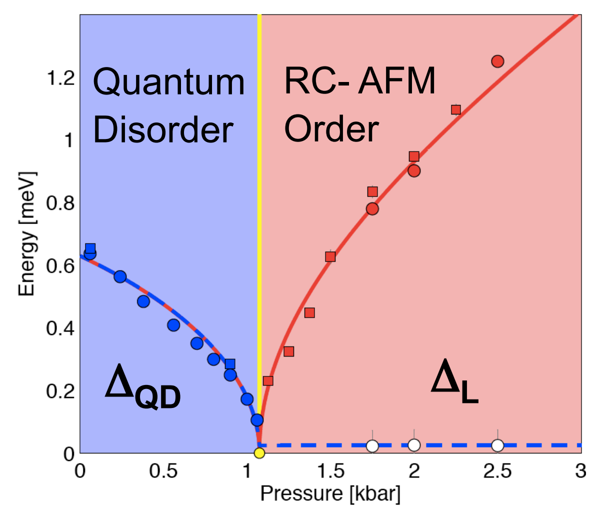


Excitation spectrum, direct measure of interactions: strength, range, symmetry

Quasi-particle spectroscopy



1D: Fractional spinon excitations in the quantum Heisenberg antiferromagnetic chain
Mourigal et al. Nature Physics (2013)



3D: Quantum and classical criticality in a dimerized quantum antiferromagnet
Merchant et al. Nature Physics (2014)

What do we measure in a scattering experiment?

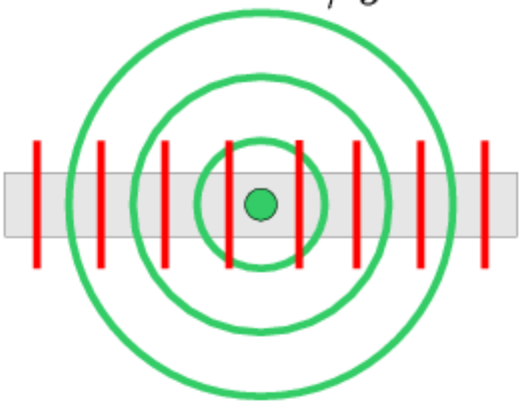
Cross-section and scattering length

$$\psi_0 = e^{i\,\mathbf{k}z}$$

$$\psi_s = -\,|b|\,\frac{e^{i\,\mathbf{k}\cdot\mathbf{r}}}{\mathbf{r}}$$

Incident plane wave

Outgoing spherical wave



$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{\text{Number of particles scattered per second into detector}}{\text{Incident Flux } \times \text{Detector solid Angle}} = \frac{I_{SC}}{\Phi_0\,\Delta\Omega}$$

$$I_{SC} = A_D \times \text{Flux of scattered particles} = A_D \times (\text{velocity } \times \text{density})$$

$$= A_D \times v \times |\psi_S|^2 = A_D \times v \times \frac{b^2}{R^2} = \Delta\Omega R^2 \times v \times \frac{b^2}{R^2} = \Delta\Omega v b^2$$

$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{\Delta\Omega v b^2}{\Phi_0\,\Delta\Omega} = \frac{\Delta\Omega v b^2}{v|\psi_0|^2\,\Delta\Omega} = b^2$$

$$\boxed{\left(\frac{d\sigma}{d\Omega}\right) = b^2}$$

The **Total Cross - section** is obtained by integrating over all solid angle

$$\sigma = \int \left(\frac{d\sigma}{d\Omega}\right) d\Omega = 4\pi b^2$$

X-rays and Neutrons

Basic properties and Scattering lengths

	Photon	Neutron
Charge:	0	0
Mass:	0	1.675×10^{-27} Kg
Spin:	1	½
Magnetic Moment:	0	$-1.913\ \mu_N$

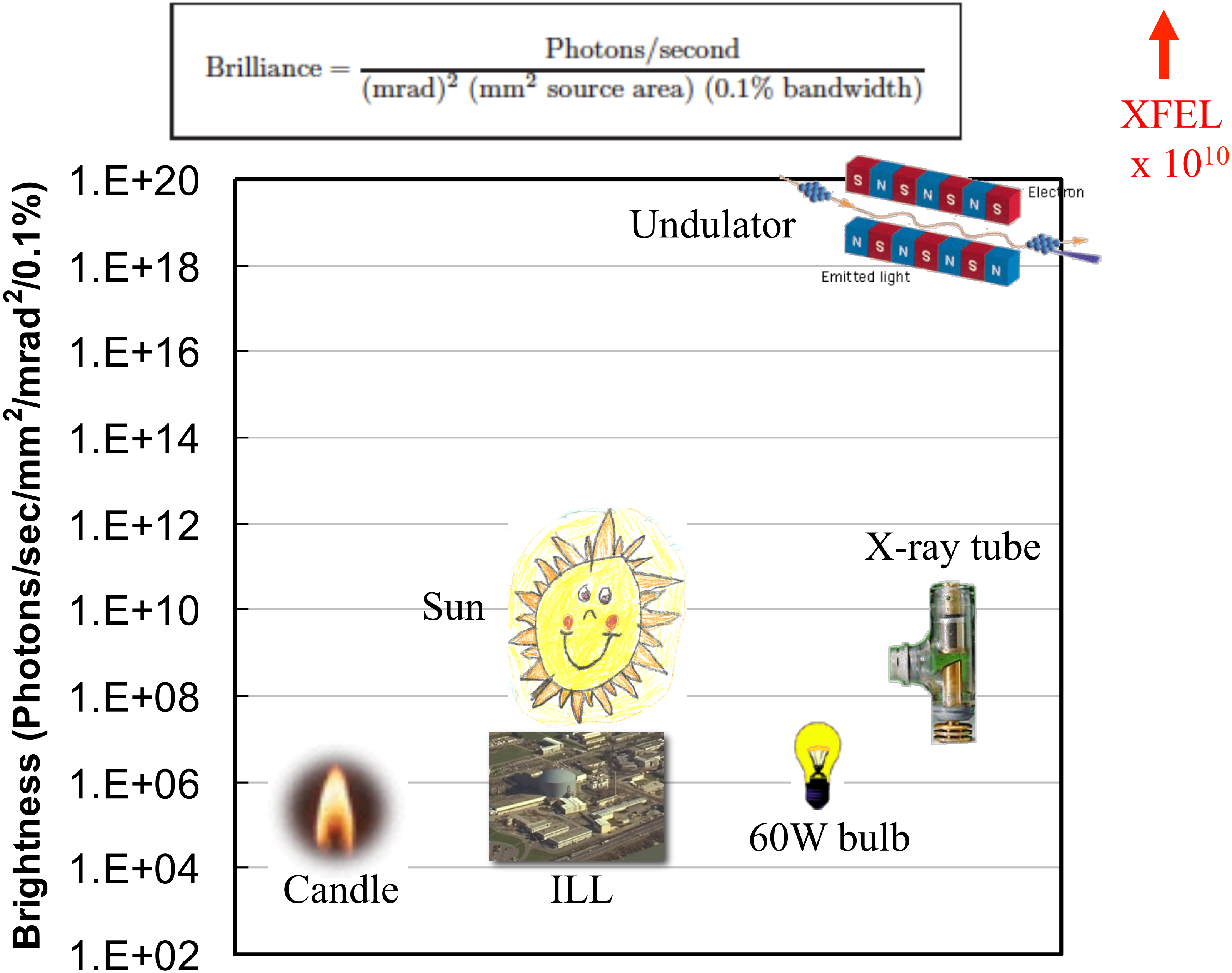
Scattering lengths:

	Photon	Neutron
Sensitivity to Structure:	$r_0 = 2.82 \times 10^{-5}$ Å (E field photon with e)	$b \sim r_0$ (Short range nuclear forces)
Sensitivity to Magnetism:	$r_0(\hbar\omega/mc^2)$ (E, H field photon with e and μ_B)	$b_{mag} \sim r_0$ ($\mu_n.B_{dipp}$)
Resonant Scattering:	100 r_0!	

$$r_0 = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{mc^2} = 2.82 \times 10^{-15} m$$

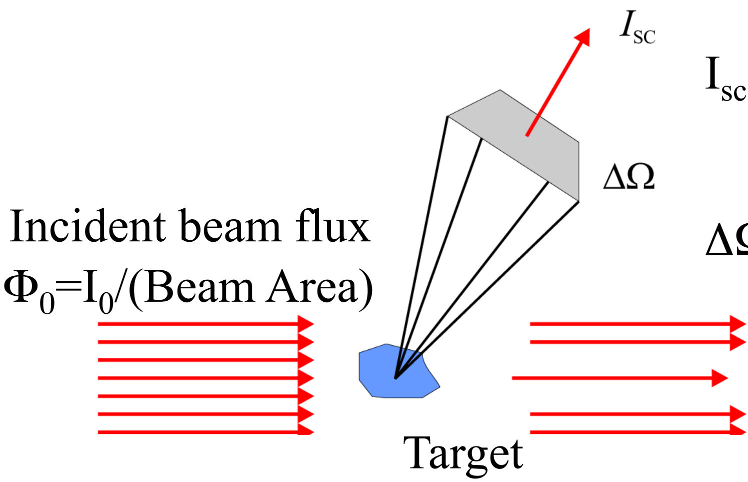
Source Brilliance (or spectral brightness)

$$\text{Brilliance} = \frac{\text{Photons/second}}{(\text{mrad})^2\ (\text{mm}^2\ \text{source area})\ (0.1\%\ \text{bandwidth})}$$



Scattering Cross-sections

Differential and partial differential



I_{sc} scattered beam intensity [particles/s]

$\Delta\Omega$ element of solid angle [(Area)/(distance)^2]

Quite generally we expect

$$I_{SC} = \Phi_0 \times \Delta\Omega \times \text{Scattering efficiency factor} = \Phi_0 \times \Delta\Omega \times \left(\frac{d\sigma}{d\Omega}\right)$$

This defines the **Differential Cross - section**

$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{\text{Number of particles scattered per second into detector}}{\text{Incident Flux } \times \text{ Detector solid Angle}} = \frac{I_{SC}}{\Phi_0 \Delta\Omega}$$

Elastic

The **Total Cross - section** is obtained by integrating over all solid angle

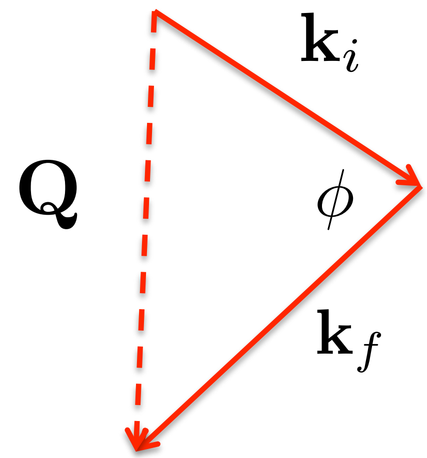
$$\sigma = \int \left(\frac{d\sigma}{d\Omega}\right) d\Omega$$

This **Partial Differential Cross - section**

$$\left(\frac{d\sigma}{d\Omega dE_f}\right) = \frac{\text{Particles scattered per second into detector in energy window } dE_f}{\text{Incident Flux } \times \text{ Detector solid Angle} \times \ dE_f}$$

Inelastic

Scattering kinematics



- Momentum transfer

$$\hbar\mathbf{Q} = \hbar\left(\mathbf{k}_i - \mathbf{k}_f\right)$$

- Energy transfer

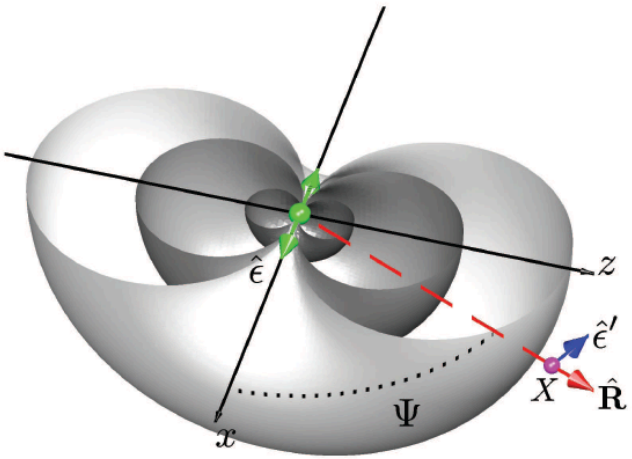
$$\hbar\omega = E_i - E_f$$

- Scattering event independent variables: (**Q**,ω)
  - Elastic Scattering $\hbar\omega = 0$ Crystallography
  - Inelastic Scattering $\hbar\omega \neq 0$ Spectroscopy
- FT conjugate variables
  - Q ~ 2π/(length)
  - ħω ~ 2πħ/(time)

Non-resonant charge scattering from unbound electrons

Thomson cross-section

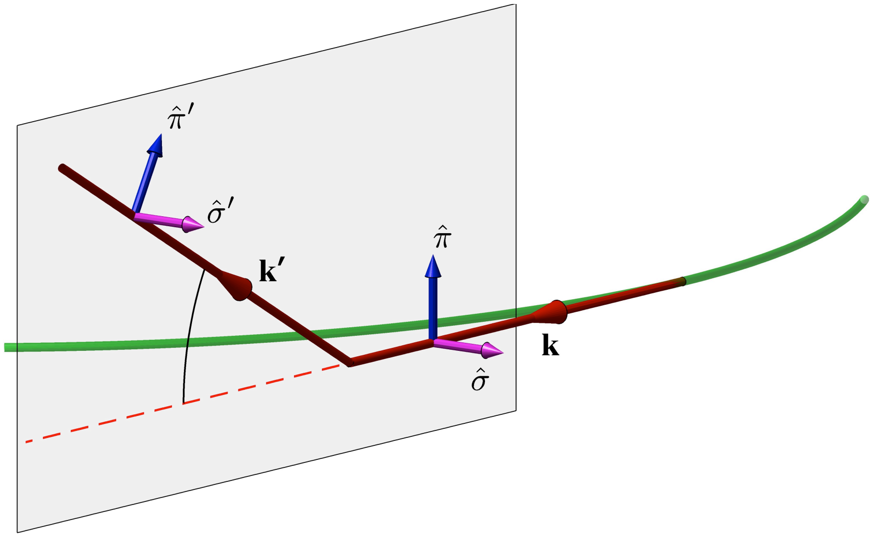
Classical calculation of the electric field reradiated from a free electron



$$\mathbf{E}_{rad} \propto \frac{-e}{R}\mathbf{a}_X(t')\sin\Psi \equiv \frac{e}{R}\mathbf{a}_X(t')\left(\hat{\boldsymbol{\epsilon}}\cdot\hat{\boldsymbol{\epsilon}}'\right)$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{Th.}} = r_0^2\left|\hat{\boldsymbol{\epsilon}}\cdot\hat{\boldsymbol{\epsilon}}'\right|^2$$

Single atom



$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{Th.}}^{atom} = r_0^2\left[f^0(\mathbf{Q})\right]^2\left|\hat{\boldsymbol{\epsilon}}\cdot\hat{\boldsymbol{\epsilon}}'\right|^2$$

$$f^0(\mathbf{Q}) = \int \rho(\mathbf{r})e^{i\mathbf{Q}\cdot\mathbf{r}}d\mathbf{r}$$

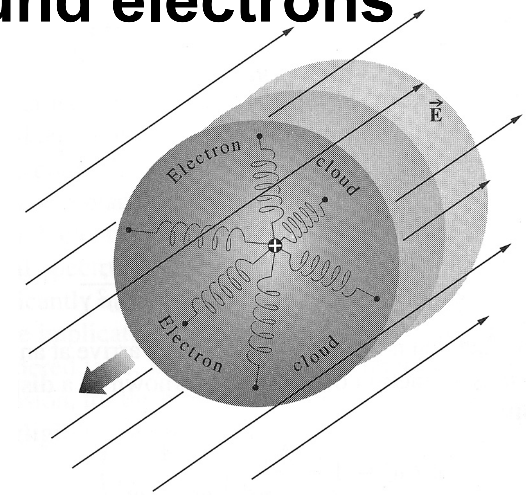
Atomic form factor

$$\mathbf{Q} = \mathbf{k} - \mathbf{k}'$$

Wave vector transfer

X-ray Resonant Scattering from bound electrons

Dispersion corrections



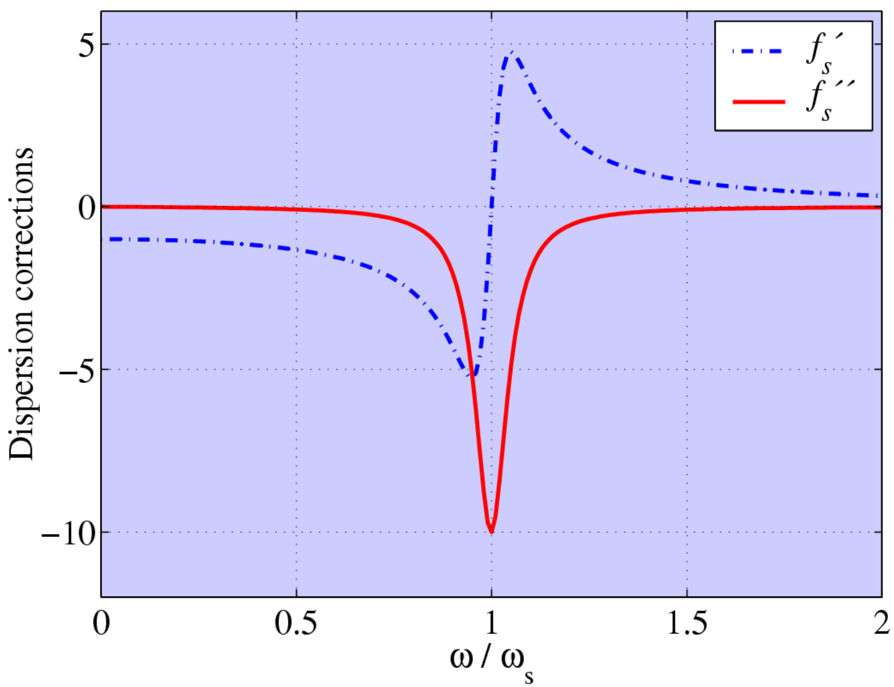
From electrons bound in atoms expect:

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

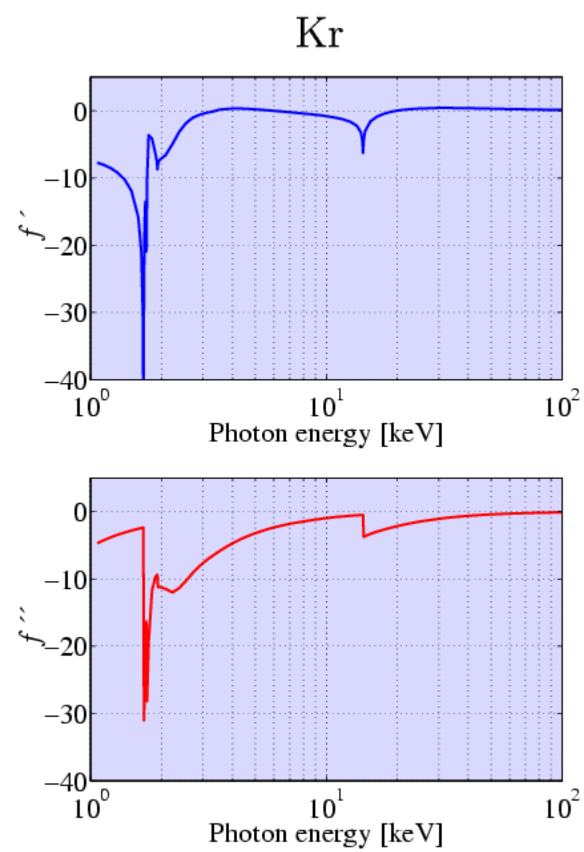
Forced, damped oscillator model

$$\ddot{x} + \Gamma\dot{x} + \omega_r^2 x = -\left(\frac{eE_0}{m}\right)e^{-i\omega t} \Rightarrow x(t) = \left(-\frac{e}{m}\right)\frac{E_0 e^{-i\omega t}}{(\omega_0^2 - \omega^2 - i\omega\Gamma)}$$

$$f_s' = \frac{\omega_0^2(\omega^2 - \omega_0^2)}{(\omega^2 - \omega_0^2)^2 + (\omega\Gamma)^2} \quad f_s' = -\frac{-\omega_0^2\omega\Gamma}{(\omega^2 - \omega_0^2)^2 + (\omega\Gamma)^2}$$



Dispersion corrections



Relationship between scattering and refraction

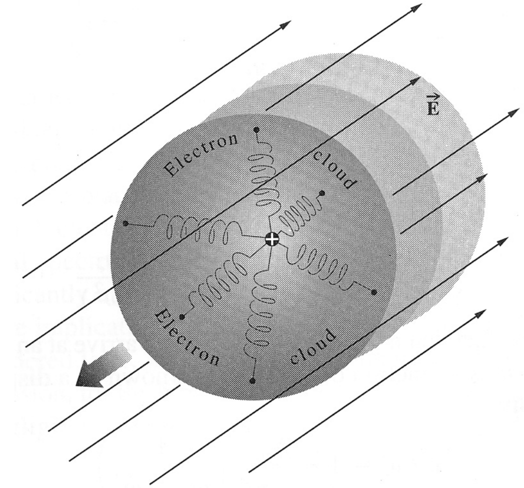
Electric field $\mathbf{E}(t)$=> $\mathbf{P}(t)$ (electric dipole/V)

$$\mathbf{P}(t) = \varepsilon_0 \chi \mathbf{E}(t) = (\varepsilon - \varepsilon_0)\mathbf{E}(t)$$

where

$$\mathrm{P}(t) = \frac{-Nex(t)}{V} = -\rho e x(t) = -\rho e\left(-\frac{e}{m}\right)\frac{\mathrm{E}_0 e^{-i\omega t}}{\left(\omega_0^2 - \omega^2 - i\omega\Gamma\right)}$$

$$\Rightarrow \frac{\mathrm{P}(t)}{\mathrm{E}(t)} = \varepsilon - \varepsilon_0 = \left(\frac{e^2\rho}{m}\right)\frac{1}{\left(\omega_0^2 - \omega^2 - i\omega\Gamma\right)}$$



The refractive index is defined by

$$n^2 = \frac{c^2}{v^2} = \frac{\varepsilon}{\varepsilon_0}$$

$$\Rightarrow n^2 = 1 + \left(\frac{e^2\rho}{\varepsilon_0 m}\right)\frac{1}{\left(\omega_0^2 - \omega^2 - i\omega\Gamma\right)}$$

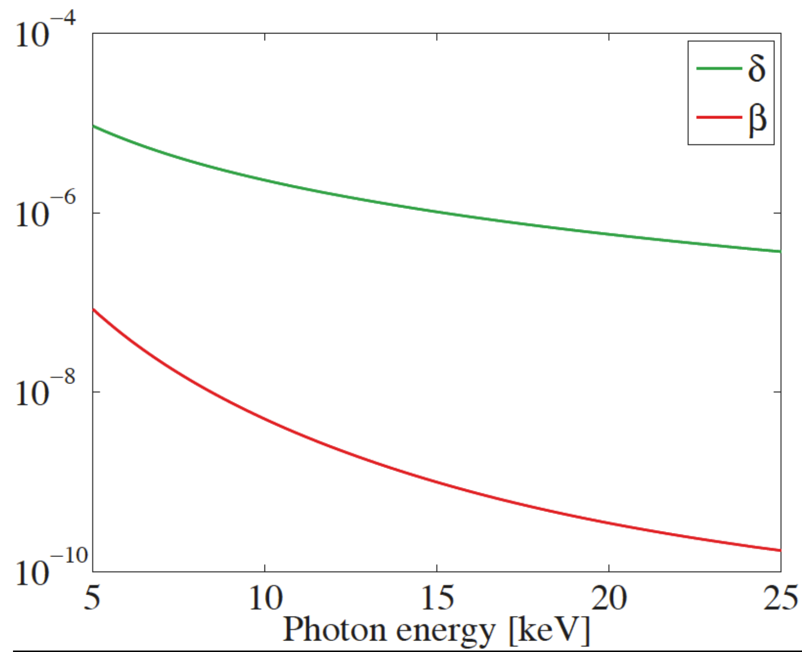
For X-rays, $\omega \gg \omega_0 \gg \Gamma$

$$n \approx 1 - \frac{1}{2}\left(\frac{e^2\rho}{\varepsilon_0 m\omega^2}\right) = 1 - \frac{2\pi\rho r_0}{k^2}$$

$$\boxed{n \approx 1 - \delta + i\beta}$$

Since $\rho = \rho_a f(0)$

$$\delta = \frac{2\pi\rho_a r_0\left(f^0(0) + f'(\hbar\omega)\right)}{k^2} \qquad \beta = -\frac{2\pi\rho_a r_0 f''(\hbar\omega)}{k^2}$$



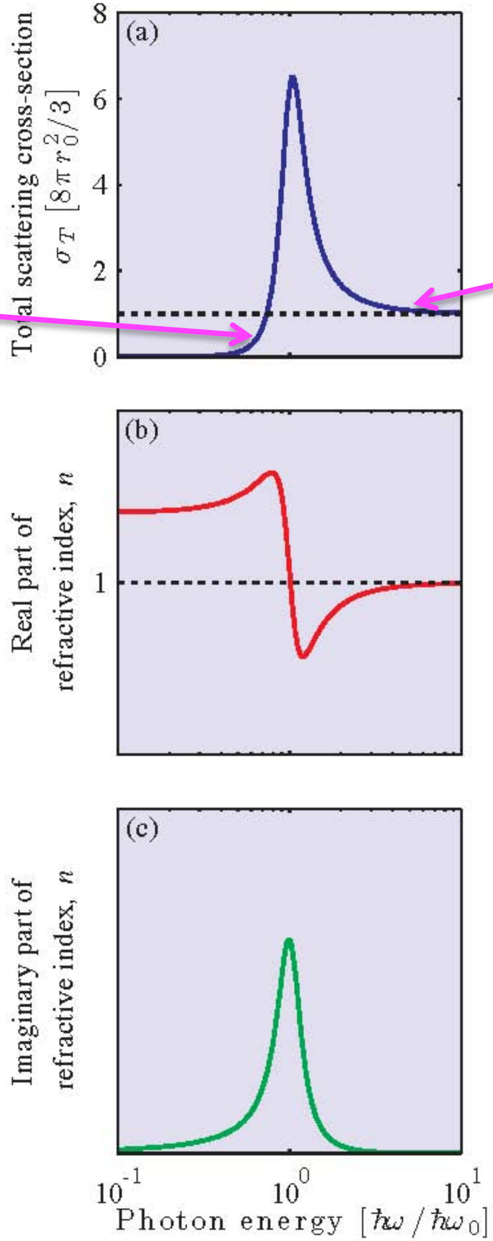
Relationship between scattering and refraction

Resonant scattering

$$f(Q,\hbar\omega) = f^0(Q) + f'(\hbar\omega) + if''(\hbar\omega)$$

Rayleigh scattering
Visible light

Thomson scattering
X-rays



Refractive index

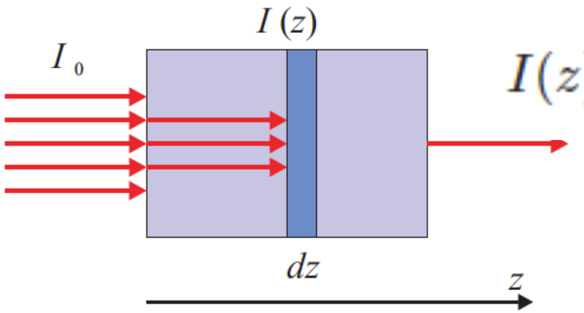
$$n = 1 - \delta + i\beta$$

$$\delta = (f^0(0) + f')\frac{2\pi\rho_a r_0}{k^2}$$

$$\beta = -f''\left(\frac{2\pi\rho_a r_0}{k^2}\right)$$

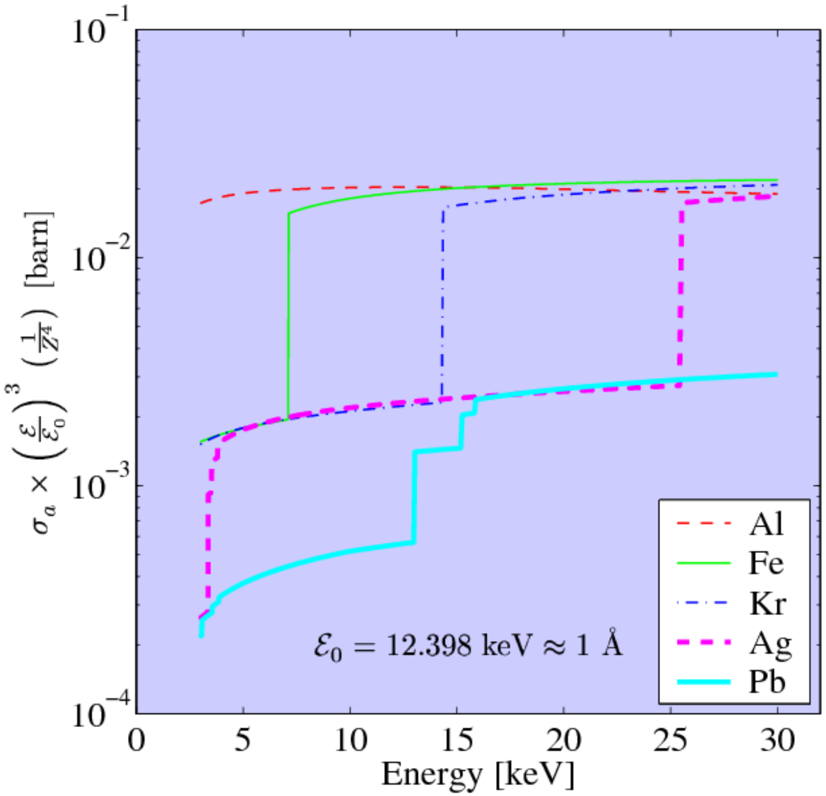
Scattering and refraction: different ways of understanding the same phenomena

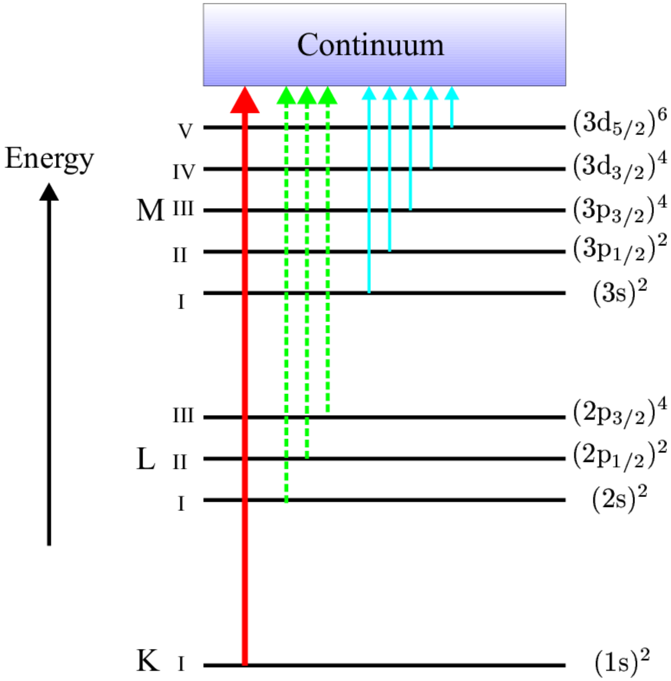
X-ray absorption edges



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

$$\mu = \rho_a \sigma_a = \left(\frac{\rho_m N_A}{A} \right) \sigma_a$$

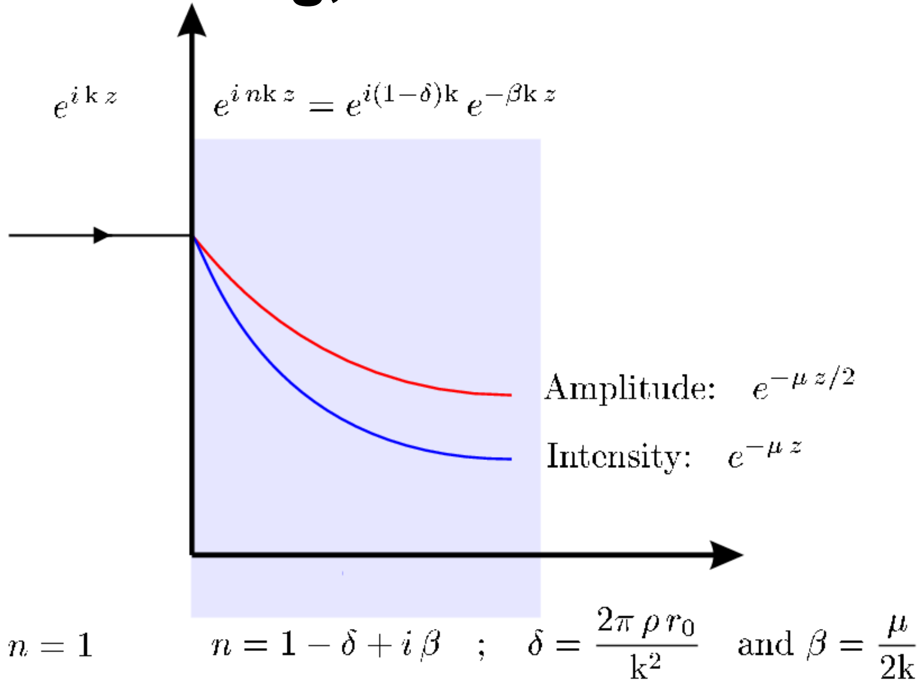




Absorption cross-section scales as

$$\sigma_{abs} \propto (\hbar\omega)^{-3} Z^4$$

Relationship scattering, refraction and absorption



$$n = 1 - \delta + i\beta \qquad \delta = \left(\frac{2\pi\rho_a (f^0(0) + f')r_0}{k^2} \right) \quad \beta = -\left(\frac{2\pi\rho_a f'' r_0}{k^2} \right)$$

Absorption coefficient μ defined by $I = I_0 e^{-\mu z}$ and absorption cross-section $\sigma_a = \mu / \rho_a$

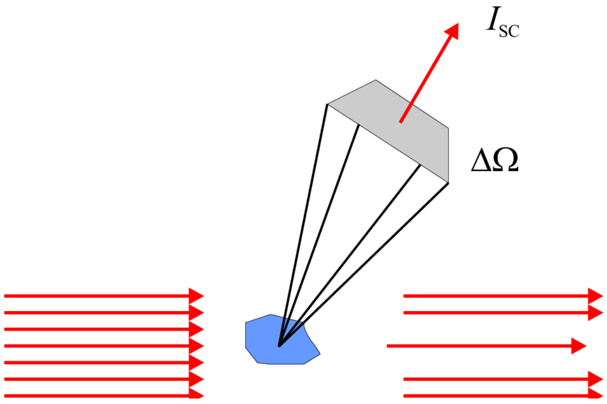
$$f'' = -\left(\frac{k^2}{2\pi\rho_a r_0} \right) \frac{\mu}{2k} = -\left(\frac{k}{4\pi r_0} \right) \sigma_a$$

Absorption is proportional to the imaginary part of the forward scattering amplitude (Optical Theorem)

Theoretical Framework

Cross-sections and the interaction Hamiltonian

Task is to determine the differential cross-section:



$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{\text{Number of particles scattered per second into detector}}{\text{Incident Flux } \times \text{ Detector solid Angle}}$$

$$= \frac{W}{\Phi_0(\Delta\Omega)}$$

The transition rate probability W to 2nd order

$$W = \frac{2\pi}{\hbar}\left|\langle f|H_I|i\rangle + \sum_n \frac{\langle f|H_I|n\rangle\langle n|H_I|i\rangle}{E_i - E_n}\right|^2 \rho(E_f)$$

Interaction Hamiltonian H_I: describes interaction between radiation and target

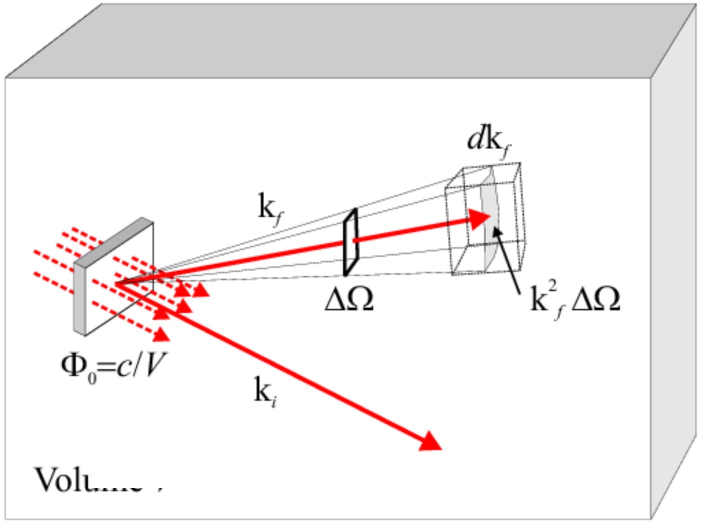
Density of final states

$$\rho(E_f)dE_f = \rho(\mathbf{k}_f)d\mathbf{k}_f$$

Box normalisation implies

$$\rho(E_f)dE_f = \rho(\mathrm{k}_f)\ \mathrm{k}_f^2\,\Delta\Omega\,d\mathrm{k}_f$$

$$\therefore \quad \rho(E_f) = \frac{V}{(2\pi)^3}\,\mathrm{k}_f^2\,\Delta\Omega\,\frac{d\mathrm{k}_f}{dE_f}$$



To first order

$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{1}{\Phi_0}\frac{2\pi}{\hbar}\left|\langle f|H_I|i\rangle\right|^2 \frac{V}{(2\pi)^3}\mathrm{k}_f^2\,\frac{d\mathrm{k}_f}{dE_f}$$

Valid for neutrons and X-rays

Non-resonant charge scattering from unbound electrons

Quantum mechanical calculation

Hamiltonian of single electron in an electromagnetic field:

$$\mathcal{H}_0 = \frac{p^2}{2m} + V \qquad \mathbf{p} \rightarrow \mathbf{p} + e\mathbf{A} \qquad \mathbf{B} = \nabla \times \mathbf{A}$$

Canonical momentum

$$\mathcal{H}_0 \rightarrow \mathcal{H}_0 + \mathcal{H}_I \qquad \mathcal{H}_I = \frac{e\mathbf{A}\cdot\mathbf{p}}{m} + \frac{e^2 \mathrm{A}^2}{2m}$$

Quantization of the electromagnetic field vector potential:

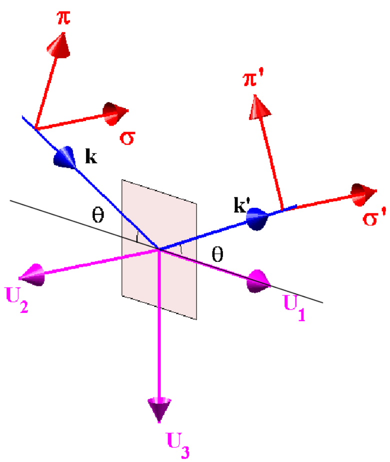
$$\mathbf{A}(\mathbf{r},t) = \sum_u \sum_{\mathbf{k}} \sqrt{\frac{\hbar}{2\epsilon_0 \omega V}} \hat{\boldsymbol{\epsilon}}_u \left[a_{u,\mathbf{k}} e^{i(\mathbf{k}\cdot r - \omega t)} + a^\dagger_{u,\mathbf{k}} e^{-i(\mathbf{k}\cdot r - \omega t)} \right]$$

$$a_{u,\mathbf{k}}|n\rangle = \sqrt{n}|n-1\rangle \qquad a^\dagger_{u,\mathbf{k}}|n\rangle = \sqrt{n+1}|n+1\rangle \qquad \rightarrow \mathcal{E}_{\mathrm{rad}} = \hbar\omega(a^\dagger_{u,\mathbf{k}} a_{u,\mathbf{k}} + 1/2)$$

1st order process: destroy photon from incident beam, create one in scattered beam

$$W = \frac{2\pi}{\hbar} |\langle f|\mathcal{H}_I|i\rangle|^2 \rho(E_f) = \frac{2\pi}{\hbar} |\langle f| \frac{e^2 \mathrm{A}^2}{2m} |i\rangle|^2 \rho(E_f)$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{Th.}} = \frac{W}{\Phi_0 \Delta\Omega} = r_0^2 \left|\hat{\boldsymbol{\epsilon}}_f \cdot \hat{\boldsymbol{\epsilon}}_i\right|^2$$



	$\hat{\varepsilon}_\perp \equiv \sigma$	$\hat{\varepsilon}_\parallel \equiv \pi$
$\hat{\varepsilon}'_\perp \equiv \sigma'$	1	0
$\hat{\varepsilon}'_\parallel \equiv \pi'$	0	$\cos 2\theta$

Thomson scattering

X-ray Scattering

Non-resonant elastic magnetic

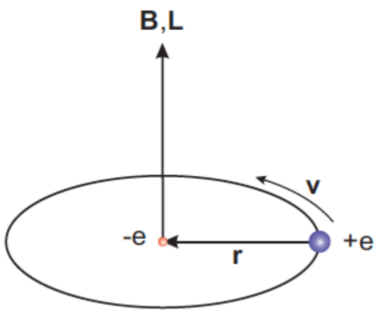
Single spin in electromagnetic field: identify leading order magnetic term

Zeeman $$\mathcal{H}_Z = g\mu_B \mathbf{s}\cdot\mathbf{B} = g\mu_B\mathbf{s}\cdot\nabla\times\mathbf{A}$$

Spin-orbit $$\mathcal{H}_{SO} = -\frac{1}{2}\mathbf{m}\cdot\mathbf{B} = \frac{1}{2}g\mu_B\mathbf{s}\cdot\frac{\mathbf{E}\times v}{c^2} = \frac{e\hbar}{2m^2c^2}\mathbf{s}\cdot\mathbf{E}\times p$$

$$= \frac{e\hbar}{2m^2c^2}\mathbf{s}\cdot(-\nabla\phi - \frac{\partial\mathbf{A}}{\partial t})\times(\mathbf{p}+e\mathbf{A})$$

$$\mathcal{H}_I = -\frac{e^2\hbar}{2m^2c^2}\mathbf{s}\cdot(\frac{\partial\mathbf{A}}{\partial t}\times\mathbf{A})$$



1st order scattering processes:

Charge

$$\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{Th.}} = r_0^2\left|\hat{\boldsymbol{\epsilon}}_f\cdot\hat{\boldsymbol{\epsilon}}_i\right|^2$$

Magnetic

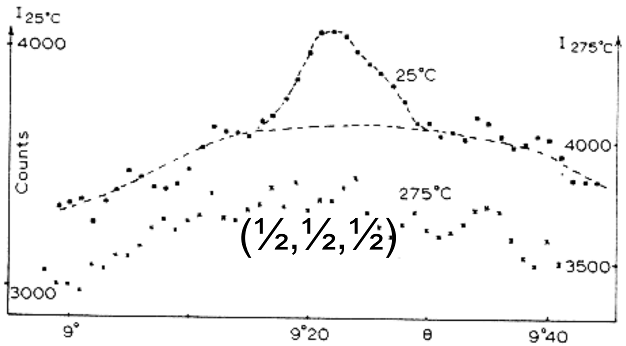
$$\left(\frac{d\sigma}{d\Omega}\right)^{\mathrm{1st\ order}}_{\mathrm{Mag.}} = r_0^2\left(\frac{\hbar\omega}{mc^2}\right)^2\left|\hat{\boldsymbol{\epsilon}}_f\times\hat{\boldsymbol{\epsilon}}_i\right|^2\langle\mathbf{s}\rangle^2$$

- Non-resonant magnetic scattering is weaker than charge by a factor of 0.0001 at 10 keV
- Non-resonant magnetic scattering (1st order) is proportional to <s>^{2} => Magnetic structures
- Magnetic scattering has a distinctive dependence on photon polarization

X-ray Magnetic Scattering

1st Non-resonant X-ray Magnetic Scattering

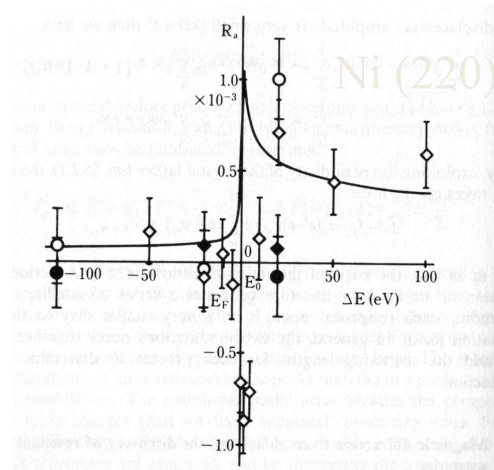
NiO, de Bergevin and Brunel (1972)



Tube source: Counts per 4 hours!

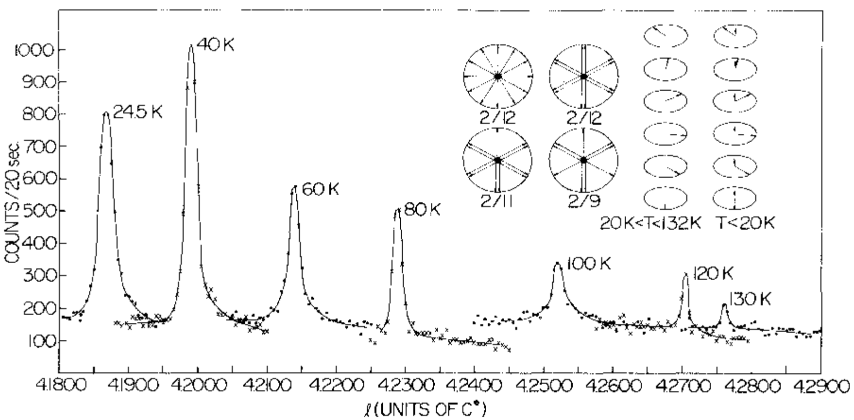
1st REXMS

Nickel, Namikawa (1985)

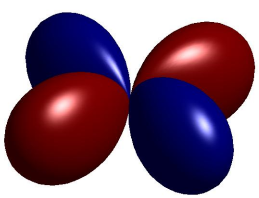


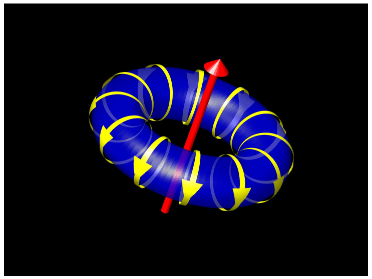
1st NREMXS Synchrotron Studies

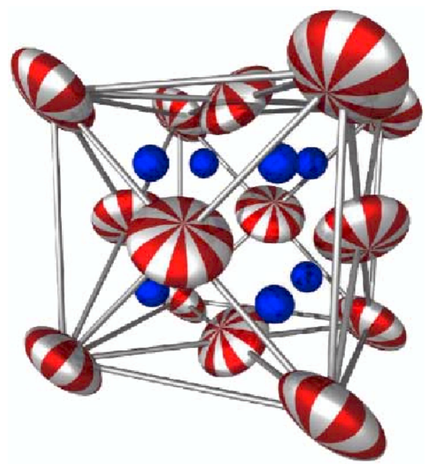
Holmium, Gibbs et al. (1985)



REXS Magnetic and multipolar ordering



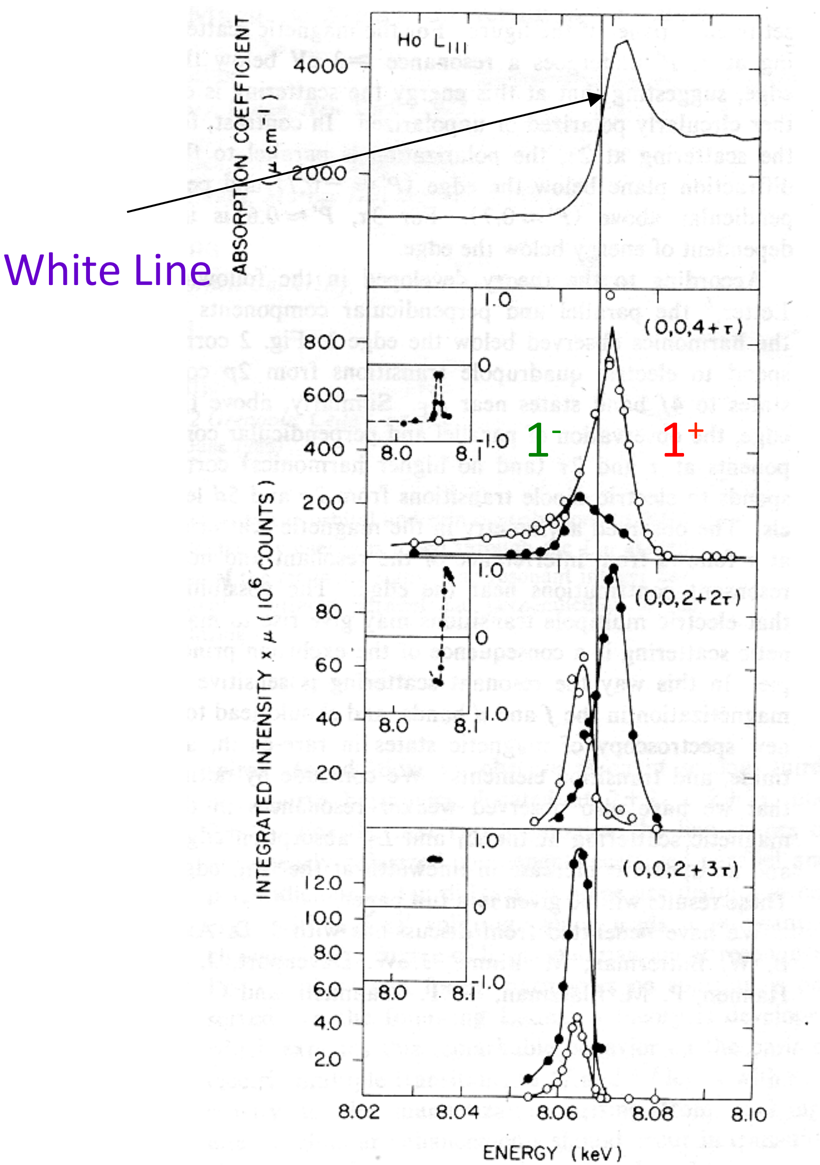




Resonant X-ray magnetic scattering (RXMS)

Large enhancement of XRS at L edges of Holmium

Gibbs, Harshman, Isaacs, McWhan, Mills and Vettier (1988)



- 100 fold increase when tuned to the L_3 edge
- Two distinct types of transition are observed: one above and one below the edge
- Higher order satellites up to 4th order
- Polarization state changes with order
  - 1^+: rotated, σ->π'
  - 1^- : unrotated, , σ->σ'
- Signal disappears at T_N
- Peaks arise from transitions to bound states
  - 1^+: 2p -> 5d Dipole
  - 1^-: 2p -> 4f Quadrupole

RXMS is Born: A New Element and Electron Shell Sensitive Probe!

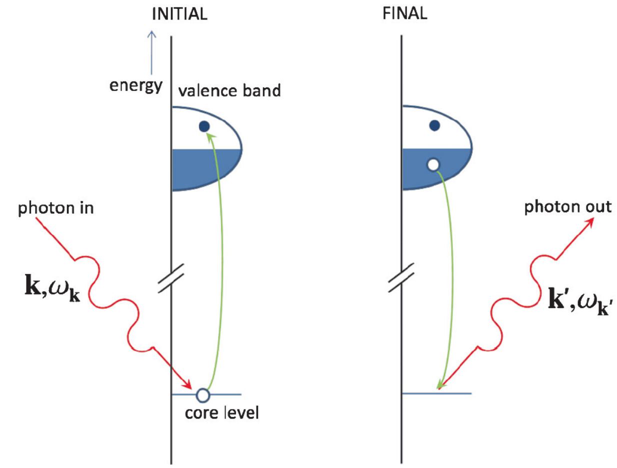
Resonant X-ray scattering

Theoretical Framework

Resonant inelastic X-ray scattering studies of elementary excitations
Ament et al. Rev. Mod. Phys. 83 705 (2011)

$$w = \frac{2\pi}{\hbar} \sum_{\mathrm{f}} |\langle \mathrm{f}|\mathcal{H}'|g\rangle + \sum_{n} \frac{\langle \mathrm{f}|\mathcal{H}'|n\rangle\langle \mathrm{n}|\mathcal{H}'|g\rangle}{E_g - E_n}|^2 \delta(E_{\mathrm{f}} - E_g)$$

$$E_g = E_{\mathrm{g}} + \hbar\omega_{\mathbf{k}} \qquad E_{\mathrm{f}} = E_f + \hbar\omega_{\mathbf{k}'}$$



When $E_g \sim E_n$ second term dominates. The interaction Hamiltonian to leading order is then

$$\mathcal{H}' = \frac{e\mathbf{A}\cdot\mathbf{p}}{m}$$

The Kramers-Heisenberg RIXS cross-section is:

$$I(\omega, \mathbf{k}, \mathbf{k}', \boldsymbol{\epsilon}, \boldsymbol{\epsilon}', \omega_{\mathbf{k}}, \omega_{\mathbf{k}'}) = r_0^2 m^2 \omega_{\mathbf{k}}^4 \sum_{\mathrm{f}} |\mathcal{F}_{f\mathrm{g}}(\mathbf{k}, \mathbf{k}', \boldsymbol{\epsilon}, \boldsymbol{\epsilon}', \omega_{\mathbf{k}}, \omega_{\mathbf{k}'})|^2 \delta(E_{\mathrm{g}} - E_f + \hbar\omega)$$

RIXS scattering amplitude:

$$\mathcal{F}_{f\mathrm{g}}(\mathbf{k}, \mathbf{k}', \boldsymbol{\epsilon}, \boldsymbol{\epsilon}', \omega_{\mathbf{k}}, \omega_{\mathbf{k}'}) = \sum_n \frac{\langle f|\mathcal{D}'|n\rangle\langle n|\mathcal{D}|\mathrm{g}\rangle}{E_{\mathrm{g}} + \hbar\omega_{\mathbf{k}} - E_n - i\Gamma_n}$$

Inelastic

Dipole transition operator $\mathcal{D} = \boldsymbol{\epsilon}\cdot\mathbf{D}$ $\qquad \langle n|\mathbf{D}|\mathrm{g}\rangle = \sum_{i=1}^{N} e^{i\mathbf{k}\cdot\mathbf{R}_i}\langle n|\mathbf{r}|\mathrm{g}\rangle$

REXS scattering amplitude:

$$\mathcal{F}_{\mathrm{gg}}(\boldsymbol{\epsilon}, \boldsymbol{\epsilon}', \omega_{\mathbf{k}}) = \sum_n \frac{\langle \mathrm{g}|\mathcal{D}'|n\rangle\langle n|\mathcal{D}|\mathrm{g}\rangle}{E_{\mathrm{g}} + \hbar\omega_{\mathbf{k}} - E_n - i\Gamma_n}$$

Elastic

Resonant elastic magnetic X-ray scattering

Scattering length for dipolar transitions: **Hill and McMorrow 1996**

$$\mathcal{F}_{E1} = \frac{1}{2}(\boldsymbol{\epsilon}' \cdot \boldsymbol{\epsilon})(F_{1,1} + F_{1,-1}) - \frac{i}{2}(\boldsymbol{\epsilon}' \times \boldsymbol{\epsilon}) \cdot \hat{\mathbf{z}}(F_{1,1} - F_{1,-1})$$

Dispersion corrections REMXS+XMCD

$$+ (\boldsymbol{\epsilon}' \cdot \hat{\mathbf{z}})(\boldsymbol{\epsilon} \cdot \hat{\mathbf{z}})(F_{1,0} - \frac{1}{2}F_{1,1} + \frac{1}{2}F_{1,-1})$$

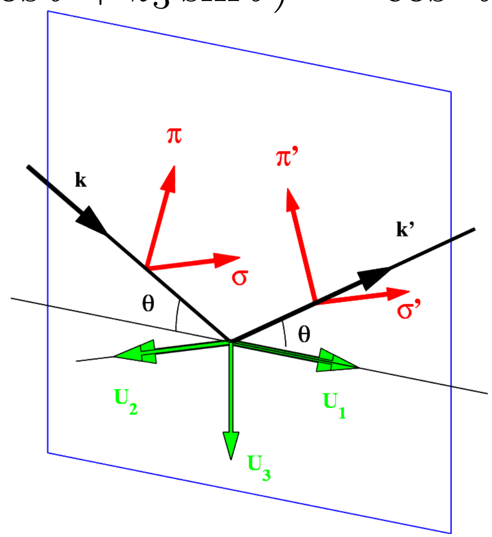
$F_{l,m}$ resonant amplitudes

REMXS+XMLD+Anisotropic Tensor Scattering (ATS)

Expressed in orthogonal photon polarization states:

$$\mathcal{F}_{E1} = F^0_{E1}\begin{pmatrix}1 & 0 \\ 0 & \cos 2\theta\end{pmatrix} - iF^1_{E1}\begin{pmatrix}0 & z_1\cos\theta + z_3\sin\theta \\ -z_1\cos\theta + z_3\sin\theta & -z_2\sin 2\theta\end{pmatrix}$$

$$+ F^2_{E1}\begin{pmatrix}z_2^2 & -z_2(z_1\cos\theta - z_3\sin\theta) \\ z_2(z_1\cos\theta + z_3\sin\theta) & -\cos^2\theta(z_1^2\tan^2\theta + z_3^2)\end{pmatrix}$$



M. Altarelli: *Resonant X-ray Scattering: A Theoretical Introduction*, Lect. Notes Phys. **697**, 201–242 (2006)

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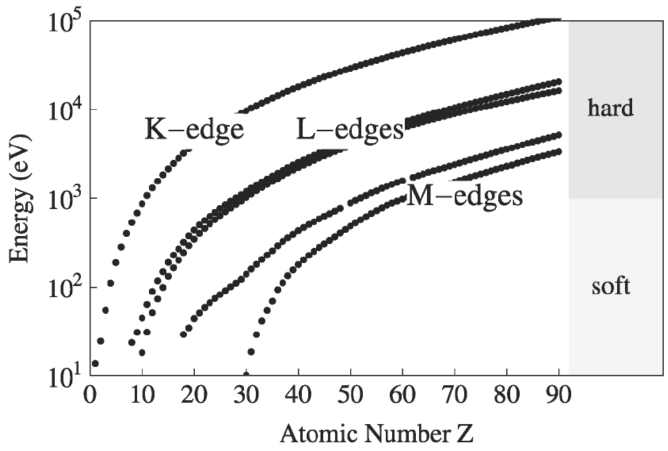
What controls the REXMS scattering length?

The scattering length depends on terms of the form

$$\langle n|\boldsymbol{r}|g\rangle \propto \int_0^\infty r^2\,dr\,\underbrace{R_{nl}(r)}_{\substack{core\\ electrons}}\,r\,\underbrace{R_{n'l'}(r)}_{\substack{valence\\ electrons}}$$

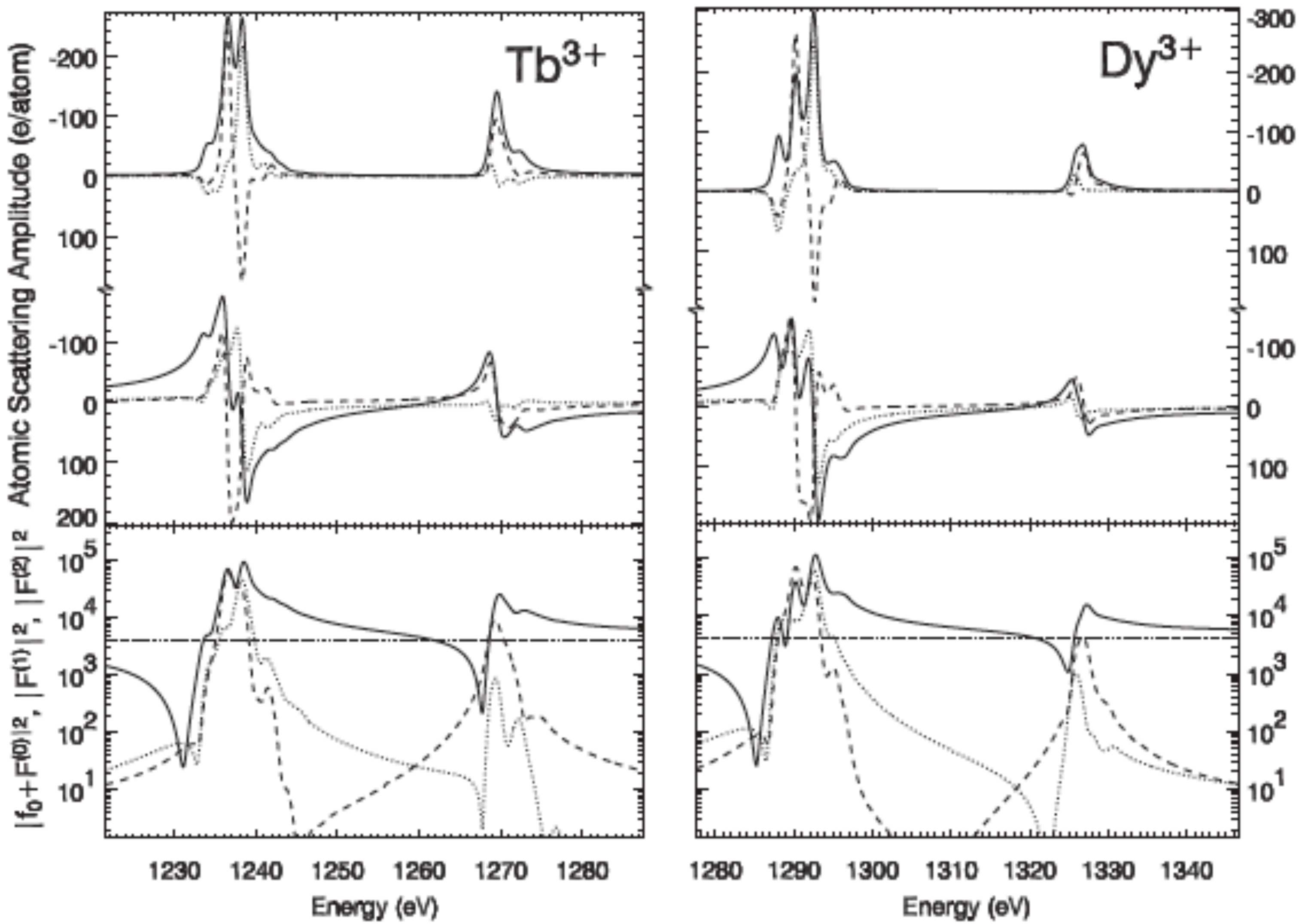
Large resonance are therefore expected when there is a large overalp between the core and valence electron radial wavefunctions.

Transition Metals 3d	L edges, 2p->3d c. 1 keV	Strong
Transition Metals 5d	L edges, 2p->5d c. 10 keV	medium
Rare-Earths 4f,5d	L edges, 2p->5d c. 10 keV	Weak
Rare-Earths 4f,5d	M edges, 3d->4f c. 1 keV	Strong
Actinides 5f	M edges, 3d->5f c. 3 keV	Strong

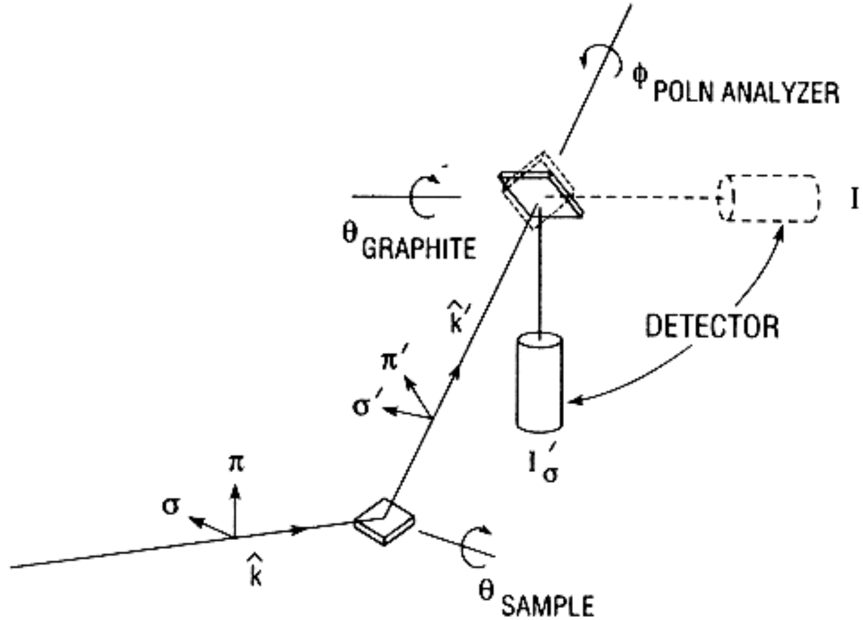


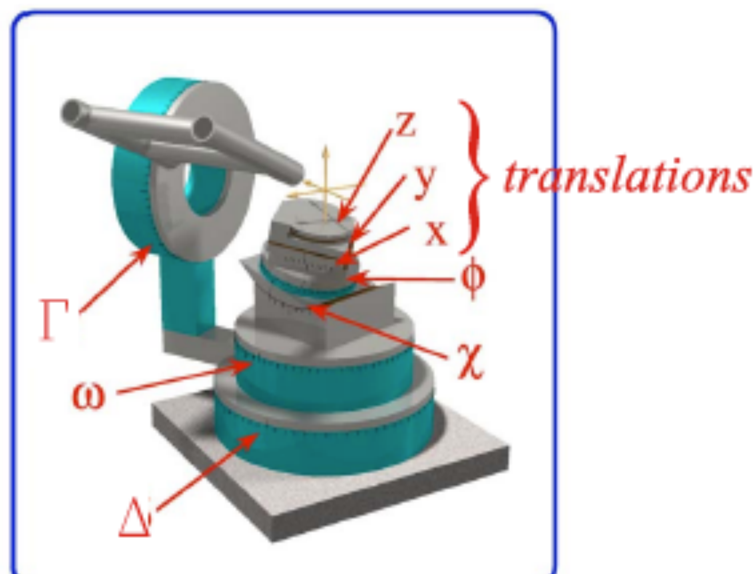
Giant resonances at the rare-earth $M_{4,5}$ edges (3p->4f)

J.M. Soriano, PhD thesis, University of Amsterdam



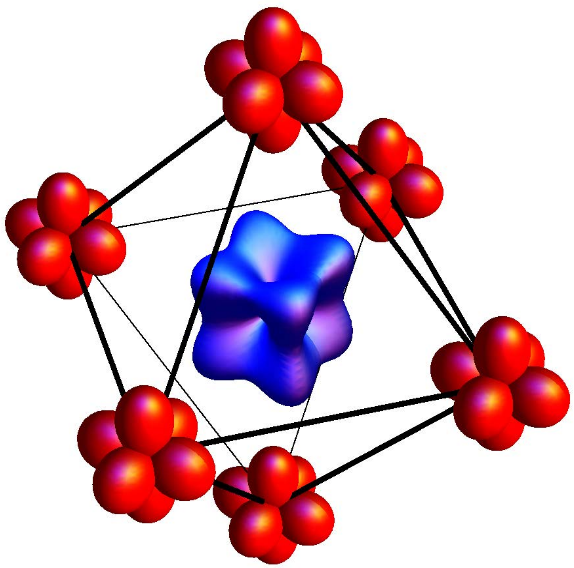
Experimental considerations





- High flux beamline
- Tunable photon energy, 1-15 keV
- Well defined and variable incident polarizatior
- Versatile diffractometer
- Azimuthal degree of freedom
- Polarization analysis

Resonant X-ray Studies of 5d Oxides



5d Oxides

- Strong Spin-Orbit Coupling Limit
- Spatially extended d orbitals
- Significant correlation energy
- Mott-Hubbard physics in strong SOC limit
  - Novel MITs
  - Wavefunctions formed from entanglement of S and L
  - Interaction Hamiltonian takes on unique character (bond directional "Kitaev")
  - Predictions for novel quantum groundstates and excitations

Overview:

- Correlated electron systems in the strong spin-orbit coupling limit
- Perovskite iridates and the realisation of the $J_{eff}=1/2$ state
- Evidence for Kitaev physics in honeycomb iridates
- Slater metal-insulator transitions (MITs) in osmates

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