UiO Department of Physics
University of Oslo

Inelastic form factors, scattering cross sections, dipole selection rules

FYS5310/FYS9320
Lecture 4

16.02.2016

FYS5310 teaching schedule

Preliminary schedule only! You should keep the class-times on Wednesdays and Thursdays open unless notified by email (or in this schedule) that there is no class

References to the textbook to Fultz & Howe unless stated otherwise.

Date		Time	Lecture/lab	Topic	Chapters	Homework
Wednesday	18.01.2017	14:15-16:00	Lecture	Introduction to the course. Derivation of the structure factor (01)	4.1, 4.3.1, 6.1	Exercise set 1 (handout)
Thursday	19.01.2017	12:15-14:00	Lecture	No class (SMN seminar)		
Wednesday	25.01.2017	13:15-16:00	Lab/Colloquium	Going through exercise set 1 + Lecture: The atomic form factor (02)	4.3	Excercise set 2 (handout)
Thursday	26.01.2017	12:15-14:00	Lecture	No class		
Wednesday	01.02.2017	14:15-16:00	Lab/colloquium	Going though exercise set 2		
Thursday	02.02.2017	12:15-14:00	Lecture	Uses of EELS and EELS instrumentation (03)	5.1, 5.2; W&C 37	Exercise set 3 (handout)
Wednesday	08.02.2017	14:15-16:00	Lab/colloquium	Going though exercise set 3		
Thursday	09.02.2017	12:15-14:00	Lecture	Inelastic form factors (04)	5.4.1-5.4.3 + primer on Dirac notation	
Wednesday	15.02.2017	12:15-16:00	Lab/colloquium	No class		
Thursday	16.02.2017	12:15-14:00	Lecture	Inelastic form factors, scattering cross sections, dipole selection rules (05)	5.4.4-5.4.7, W&C 39, plus Brehm and Mullin on parity and dipole selectrion rules	
Wednesday	22.02.2017	12:15-16:00	Lab/colloquium	No class		
Thursday	23.02.2017	12:15-14:00	Lecture	Core losses: Quantification and electronic structure (06)	5.4, W&C 39+40	Exercise set 4 (handout)
Wednesday	01.03.2017	12:15-16:00	Lab/colloquium	Going through excercise set 4		
Thursday	02.03.2017	12:15-14:00	Lecture	Low energy loss; electronic structure and dielectric properties pt 1 (07)		
Wednesday	08.03.2017	12:15-16:00	Lab/colloquium	Computer lab?		
Thursday	09.03.2017	12:15-14:00	Lecture	Low energy loss; electronic structure and dielectric properties pt 2 (08)	5.3, W&C 38	
Wednesday	15.03.2017	12:15-16:00	Lab/colloquium	No class		
Thursday	16.03.2017	12:15-14:00	Lecture	No class		
Wednesday	22.03.2017	12:15-16:00	Lab/colloquium	Computer lab?		

This lecture

- Recap from last time
  - The inelastic form factor
- Cross section of a single scattering event
- Cross section for several possible final states
- GOS
- Dipole selection rules

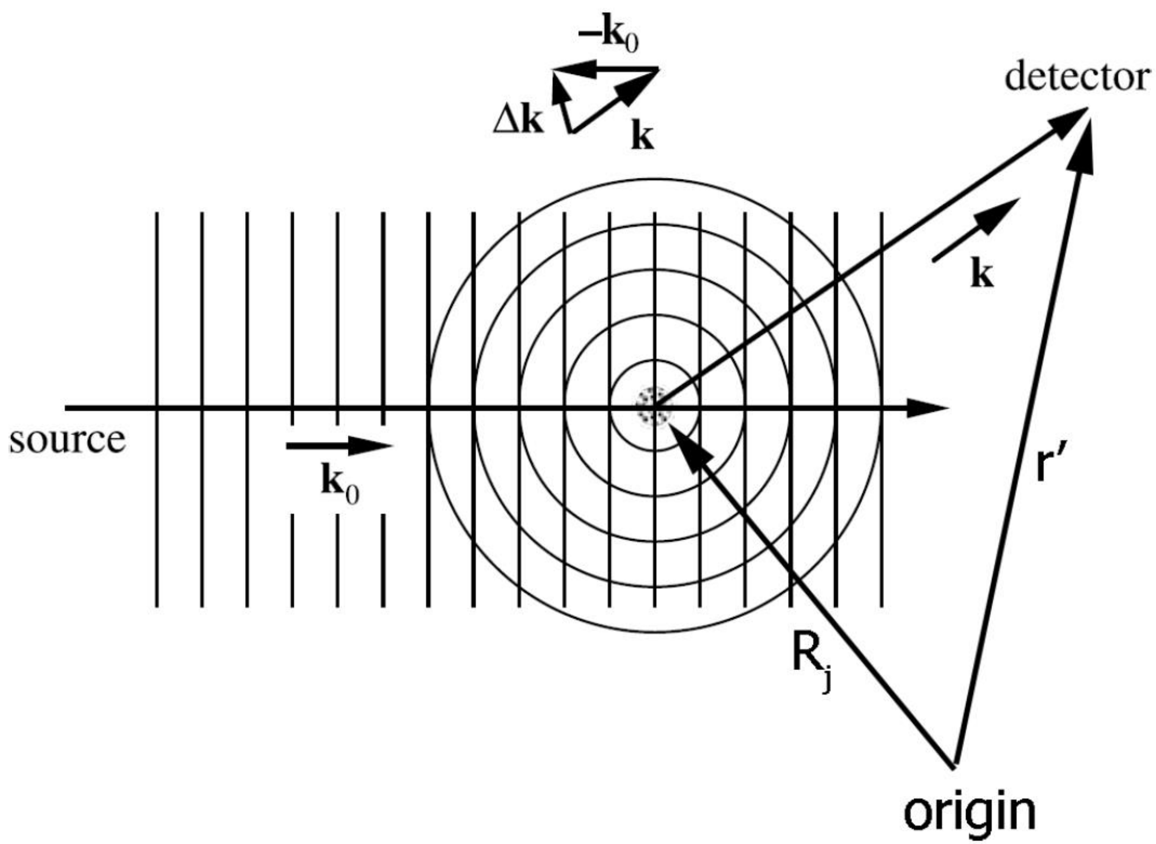


Figure 1: Sketch showing a plane wave scattered by atom in $\mathbf{R}_j$.

$$
\begin{aligned}
f(\mathbf{k},\mathbf{k}_0) &= \frac{-m_e}{2\pi\hbar^2}\langle\beta|\langle\mathbf{k}|\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}+V(\mathbf{r}_1)|\mathbf{k}_0\rangle|\alpha\rangle \\
&= \frac{-m_e}{2\pi\hbar^2}\left[\langle\beta|\langle\mathbf{k}|\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}|\mathbf{k}_0\rangle|\alpha\rangle+\langle\beta|\langle\mathbf{k}|V(\mathbf{r}_1)|\mathbf{k}_0\rangle|\alpha\rangle\right] \\
&= \frac{-m_e}{2\pi\hbar^2}\left[\langle\beta|\langle\mathbf{k}|\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}|\mathbf{k}_0\rangle|\alpha\rangle+\langle\beta|\alpha\rangle\langle\mathbf{k}|V(\mathbf{r}_1)|\mathbf{k}_0\rangle\right] \\
&= \frac{-m_e}{2\pi\hbar^2}\left[\langle\beta|\langle\mathbf{k}|\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}|\mathbf{k}_0\rangle|\alpha\rangle\right]
\end{aligned}
$$

Fermi golden rule – scattering between two distict states

$$\frac{\mathrm{d}\sigma(\boldsymbol{\Delta}\mathbf{k})}{\mathrm{d}\Omega} = |f(\mathbf{k},\mathbf{k}_0)|^2 = \frac{4}{a_0^2\Delta k^4}\left|\int_{-\infty}^{\infty}\Psi_\beta^*(\mathbf{r}_2)e^{-i\boldsymbol{\Delta}\mathbf{k}\cdot\mathbf{r}_2}\Psi_\alpha(\mathbf{r}_2)\mathrm{d}^3\mathbf{r}_2\right|^2$$

$\Delta\mathbf{k}$ – scattering vector $\Delta\mathbf{k} = \mathbf{k}_0 - \mathbf{k}$
Ψ_α – initial state of target electron
Ψ_β – final state of target electron
$\mathbf{r}_2$ – position of scattering event

<u>Assumption 1</u>
Only one scattering event at a time

<u>Assumption 2</u>
Separation of the electronic and atomic degrees of freedom

Double differential cross section

$$\frac{d\sigma}{\Delta\mathbf{k}} \rightarrow \frac{d^2\sigma(\Delta\mathbf{k}, E)}{\Delta\mathbf{k}\, dE}$$

We want to consider all possible transistions from Ψ_α with energy *E*

$$\left|\langle\beta|e^{-i\boldsymbol{\Delta}\mathbf{k}\cdot\mathbf{r}}|\alpha\rangle\right|^2$$

Several possible final states with same energy

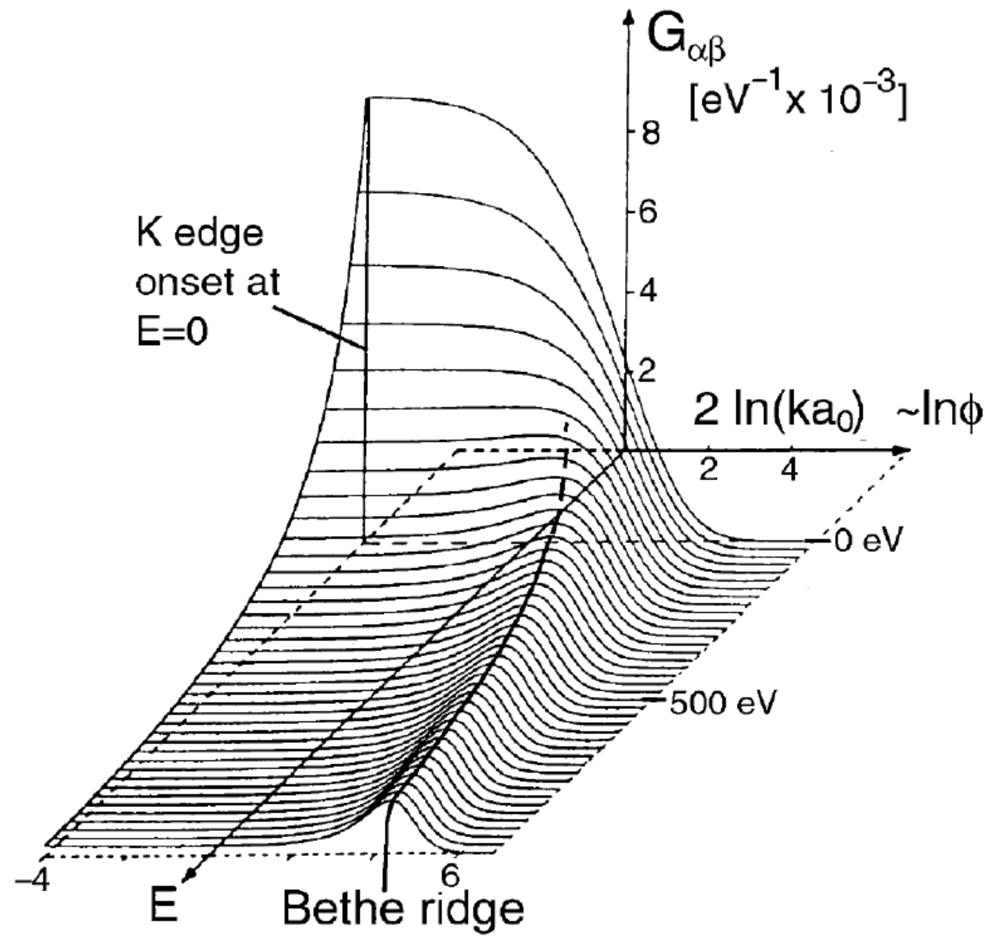
$$\frac{\mathrm{d}^2\sigma(\boldsymbol{\Delta}\mathbf{k}, E)}{\mathrm{d}\Omega\mathrm{d}E} = \frac{4}{a_0^2\Delta k^4}\rho(E)\left|\langle\beta|e^{-i\boldsymbol{\Delta}\mathbf{k}\cdot\mathbf{r}}|\alpha\rangle\right|^2$$

<u>Assumption 3</u>
Matrix element is a constant for all β under consideration

$$G_{\alpha\beta}(\Delta k, E) = E_{\alpha\beta}\frac{2m_e}{\hbar^2 \Delta k^2}\left|\int_{-\infty}^{\infty} \Psi_\beta^*(\mathbf{r}) e^{-i\mathbf{\Delta k}\cdot\mathbf{r}_2}\Psi_\alpha(\mathbf{r}_2)\mathrm{d}^3\mathbf{r}\right|^2$$

$$\frac{\mathrm{d}^2\sigma(\phi, E)}{\mathrm{d}\phi\mathrm{d}E} = \frac{2\pi\hbar^4}{a_0^2 m_2^2 E_{\alpha\beta} T} \overbrace{\frac{\phi}{\phi^2 + \phi_E^2}}^{\text{exp. scatt. angles}} \underbrace{\rho(E)}_{\text{sol. state eff.}} \overbrace{G_{\alpha\beta}(\Delta k, E)}^{\text{atomic osci. str.}}$$

Bethe surface for K-shell ionization of C, calculated using a hydrogenic model. The GOS is zero for energy losses below the ionization threshold $E_K = E_{\alpha\beta}$, or $E < 0$. The horizontal coordinate increases with scattering angle. The Bethe ridge is most distinct at large E towards the front of the figure. After [5.5]



Small scattering angles – the dipole selection rule

Most of the scattering is at small angles

Can be further limited by selecting small β

$\Delta\mathbf{k}\cdot\boldsymbol{r} \ll 1 \qquad e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots$

$$e^{i\boldsymbol{q}\cdot\boldsymbol{r}} = 1 + i\Delta\mathbf{k}\cdot\boldsymbol{r} + \frac{(i\Delta\mathbf{k}\cdot\boldsymbol{r})^2}{2!} + \frac{(i\Delta\mathbf{k}\cdot\boldsymbol{r})^3}{3!} + \ \ldots \qquad \frac{d\sigma}{d\Delta\mathbf{k}} = \frac{4}{a_0\Delta\mathbf{k}^4}\left|\left\langle\beta\middle|e^{i\Delta\mathbf{k}\cdot\boldsymbol{r}}\middle|\alpha\right\rangle\right|^2$$

$$\frac{d\sigma}{d\Delta\mathbf{k}} \approx \frac{4}{a_0\Delta\mathbf{k}^4}|\langle\beta|1 + i\Delta\mathbf{k}\cdot\boldsymbol{r}|\alpha\rangle|^2 = \frac{4}{a_0\Delta\mathbf{k}^4}|\langle\underbrace{\beta|i\Delta\mathbf{k}\cdot\boldsymbol{r}|\alpha\rangle|^2}$$

Matrix element dependent on spatial overlap of states
The scattering is dominated by *local* states

Under these assumtions, the core loss EELS spectrum probes the

- local density of states around the excited atom…
- with symmetry *l±1…*
- above the Fermi-level

The site and symmetry selected DOS

$$\frac{\mathrm{d}^2\sigma(\mathbf{\Delta k}, E)}{\mathrm{d}\Omega\mathrm{d}E} = \frac{4}{a_0^2\Delta k^4}\rho(E)\left|\langle\beta|e^{-i\mathbf{\Delta k}\cdot\mathbf{r}}|\alpha\rangle\right|^2$$

Direct comparison with calculated density of states (DOS)

$$\frac{\mathrm{d}^2\sigma(\mathbf{\Delta k}, E)}{\mathrm{d}\Omega\mathrm{d}E} = \frac{4}{a_0^2 \Delta k^4}\rho(E)\left|\langle\beta|e^{-i\mathbf{\Delta k}\cdot\mathbf{r}}|\alpha\rangle\right|^2$$

- The transition matrix determines the underlying edge shape
- Usually slowly varying with energy
- The density of states gives more rapid variations on top of this
- Allows comparison with calculated DOS, e.g. from density functional theory (DFT)

Next time

- More on comparisons of EELS spectra with DOS
- Elemental quantification with EELS