

PHYS 570 - Introduction to Synchrotron Radiation

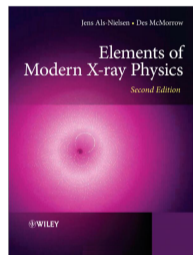


Term: Fall 2024
Meetings: Monday & Wednesday 17:00-18:15
Location: 102 Rettaliata Engineering

Instructor: Carlo Segre
Office: 166d/172 Pritzker Science
Phone: 312.567.3498
email: segre@iit.edu

Book: *Elements of Modern X-Ray Physics, 2nd ed.*,
J. Als-Nielsen and D. McMorrow (Wiley, 2011)

Web Site: <http://csrri.iit.edu/~segre/phys570/24F>





- Describe the means of production of synchrotron x-ray radiation

Course objectives



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- Describe the function of various components of a synchrotron beamline

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- Describe the physics behind a variety of experimental techniques
- Prepare and deliver an oral presentation of a synchrotron radiation research topic
- Write a General User Proposal in the format used by the Advanced Photon Source



- Focus on applications of synchrotron radiation

Course syllabus



- Focus on applications of synchrotron radiation
- Homework assignments



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- In-class student presentations on research topics
 - Choose a research article which features a synchrotron technique
 - Timetable will be posted



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- Homework assignments
- In-class student presentations on research topics
 - Choose a research article which features a synchrotron technique
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- Final project - writing a General User Proposal
 - Start thinking about a suitable project right away
 - Synchrotron technique must differ from journal article used in final presentation
 - Make proposal and get approval before starting



- Visits to Advanced Photon Source
 - All students who plan to attend will need to request badges from APS
 - Go to the APS User Portal and register as a new user:
https://beam.aps.anl.gov/pls/apsweb/ufr_main_pkg.usr_start_page
 - Use MRCAT (Sector 10) as location of experiment
 - Use Carlo Segre as local contact
 - State that your beamtime will be in the **second week of March**
 - Schedule to be determined



- Hands on data analysis training
 - GSAS for Rietveld refinement of powder diffraction data
<https://subversion.xray.aps.anl.gov/trac/pyGSAS>
 - Demeter: XAS processing and analysis
<https://bruceravel.github.io/demeter/>
 - Larch: Data analysis tools for x-ray spectroscopy
<https://xraypy.github.io/xraylarch/>



33% – Homework assignments

Course grading



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Weekly or bi-weekly

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Grading scale

A	–	80%	to	100%
B	–	65%	to	80%
C	–	50%	to	65%
E	–	0%	to	50%

Topics to be covered (at a minimum)



Topics to be covered (at a minimum)



- X-rays and their interaction with matter

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- X-rays and their interaction with matter
- Sources of x-rays

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- Photoelectric absorption

Topics to be covered (at a minimum)



- X-rays and their interaction with matter
- Sources of x-rays
- Refraction and reflection from interfaces
- Kinematical diffraction
- Diffraction by perfect crystals
- Small angle scattering
- Photoelectric absorption
- Resonant scattering

Topics to be covered (at a minimum)

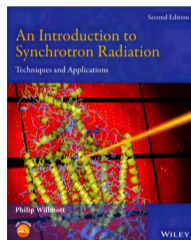


- X-rays and their interaction with matter
- Sources of x-rays
- Refraction and reflection from interfaces
- Kinematical diffraction
- Diffraction by perfect crystals
- Small angle scattering
- Photoelectric absorption
- Resonant scattering
- Imaging

Resources for the course



Introduction to Synchrotron Radiation: Techniques and Applications, 2nd ed., P. Willmott
(Wiley, 2019)

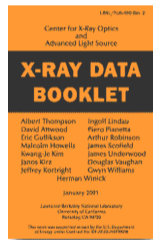
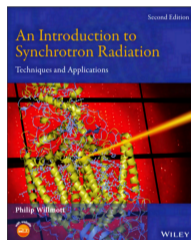


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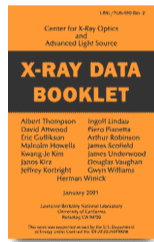
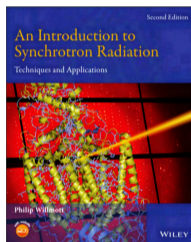


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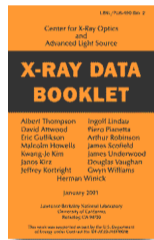
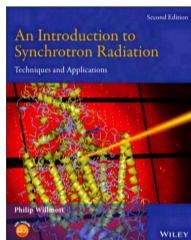




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<http://bruceravel.github.io/demeter>

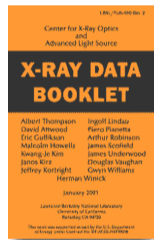
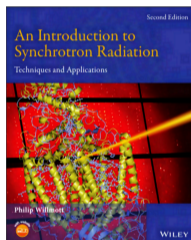


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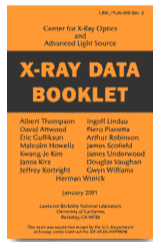
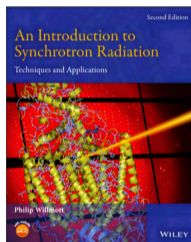




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- X-ray Oriented Programs: <https://www.aps.anl.gov/Science/Scientific-Software/XOP>



Today's outline - August 19, 2024





- The big picture

Today's outline - August 19, 2024



- The big picture
- History of x-ray sources

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- History of x-ray sources
- X-ray interactions with matter

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Reading Assignment: Chapter 1.1–1.6; 2.1–2.2

Why synchrotron radiation?



X-rays are the ideal structural probe for interatomic distances with wavelengths of $\sim 1 \text{ \AA}$

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The broad range of techniques make synchrotron x-ray sources to nearly any science or engineering field

The classical x-ray



The classical plane wave representation of x-rays is:

The classical x-ray



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



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$$\begin{aligned} \lambda &= hc/\mathcal{E} \\ &= (4.1357 \times 10^{-15} \text{ eV} \cdot \text{s})(2.9979 \times 10^8 \text{ m/s})/\mathcal{E} \\ &= (4.1357 \times 10^{-18} \text{ keV} \cdot \text{s})(2.9979 \times 10^{18} \text{ \AA/s})/\mathcal{E} \\ &= 12.398 \text{ \AA} \cdot \text{keV}/\mathcal{E} \quad \text{to give units of \AA} \end{aligned}$$

Interactions of x-rays with matter



For the purposes of this course, we care most about the interactions of x-rays with matter.

There are four basic types of such interactions:

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4. Pair production

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2. Inelastic scattering
3. Absorption
4. Pair production

We will only discuss the first three.

Elastic scattering

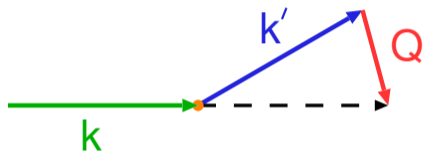


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Elastic scattering



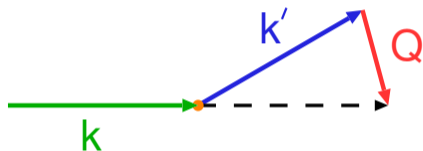
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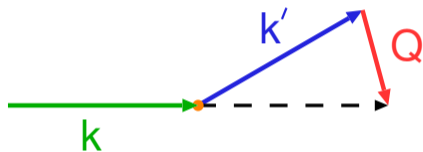


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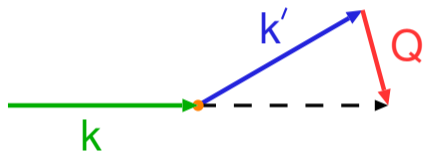


where an incident x-ray of wave number k
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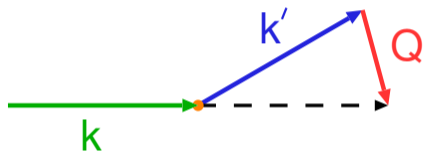


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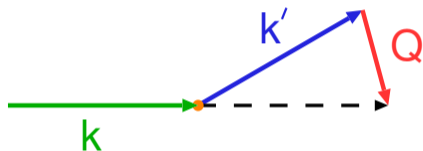
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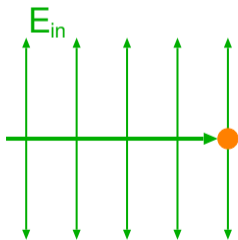
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Start with the scattering from a single electron, then build up to more complexity

Thomson scattering



Assumptions:

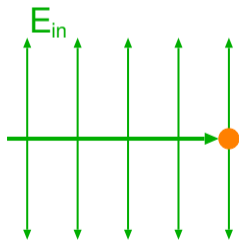


Thomson scattering



Assumptions:

incident x-ray plane wave



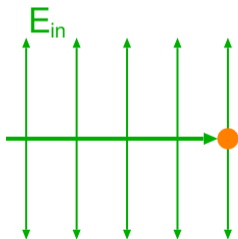
Thomson scattering



Assumptions:

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electron is a point charge

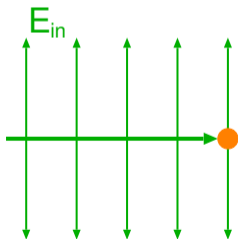


Thomson scattering



Assumptions:

incident x-ray plane wave
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Thomson scattering



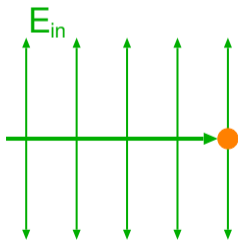
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scattered intensity $\propto 1/R^2$



Thomson scattering



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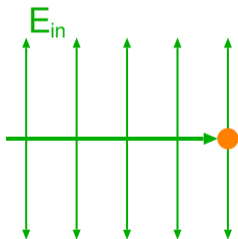
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The electron is exposed to the incident electric field $E_{in}(t')$ and is accelerated



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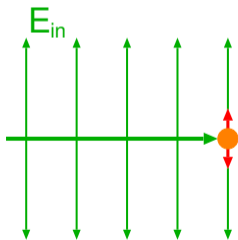
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The acceleration of the electron, $a_x(t')$, results in the radiation of a spherical wave with the same frequency



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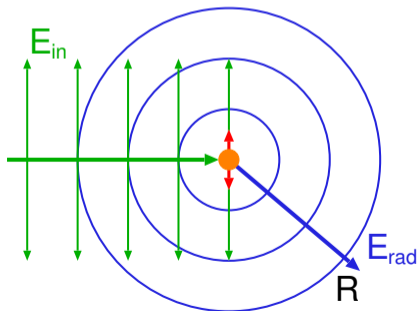
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Thomson scattering



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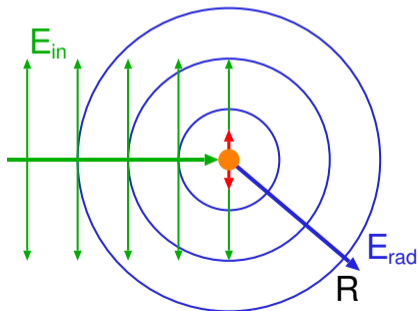
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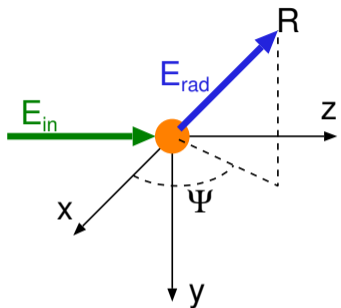
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Using this, calculate the elastic scattering cross-section

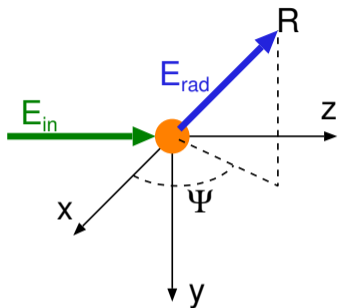


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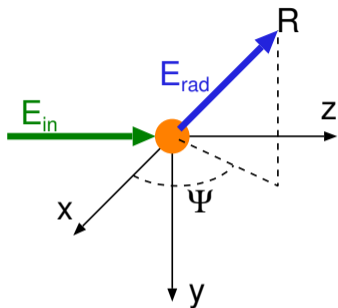
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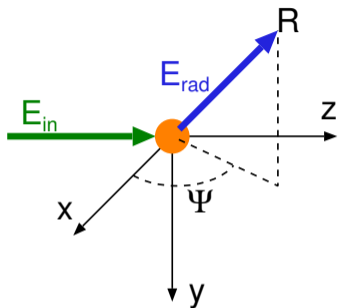
$$E_{rad}(R, t) = -\frac{-e}{4\pi\epsilon_0 c^2 R} a_x(t') \sin \Psi, \quad t' = t - R/c$$

Thomson scattering



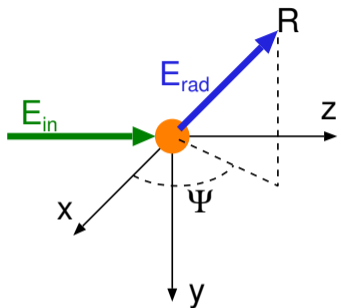
$$E_{rad}(R, t) = -\frac{-e}{4\pi\epsilon_0 c^2 R} a_x(t') \sin \Psi, \quad t' = t - R/c$$
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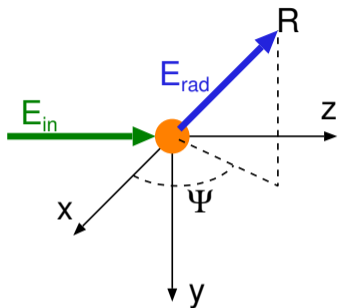


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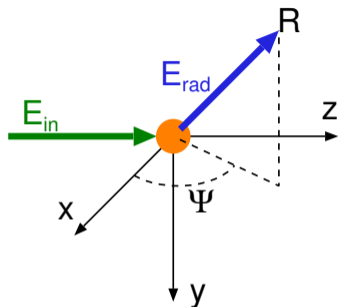
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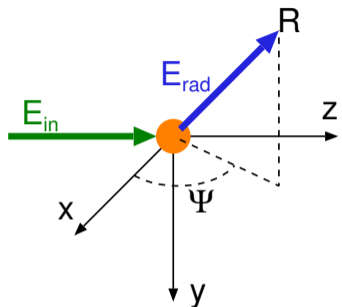
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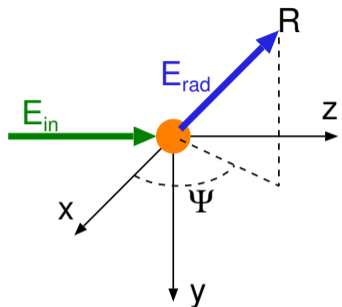
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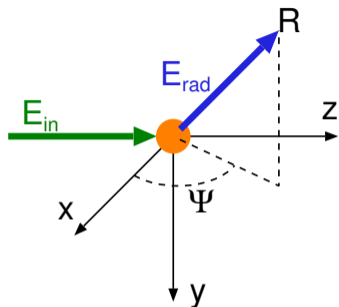
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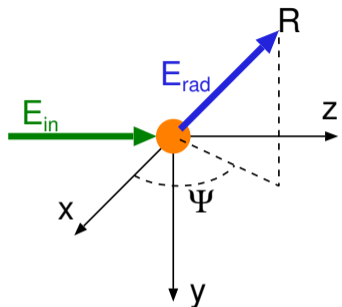
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$$r_0 = \frac{e^2}{4\pi\epsilon_0 mc^2} = 2.82 \times 10^{-5} \text{ \AA}$$

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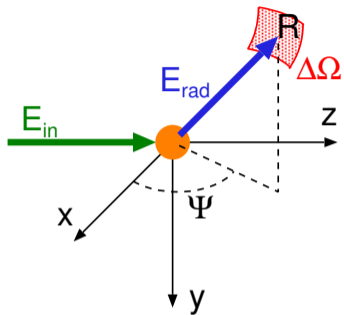
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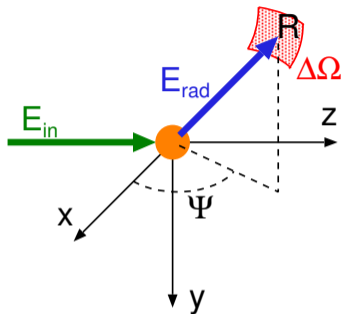
$$r_0 = \frac{e^2}{4\pi\epsilon_0 m c^2} = 2.82 \times 10^{-5} \text{ \AA}$$

r_0 is called the Thomson scattering length or the “classical” radius of the electron

Scattering cross-section

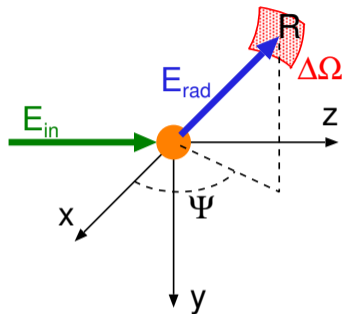


Scattering cross-section



detector of solid angle $\Delta\Omega$ located a distance R from electron

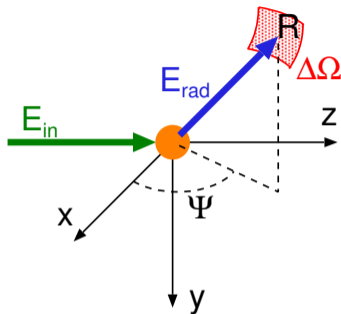
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incoming beam has cross-section A_0 so the flux, Φ_0 is

Scattering cross-section

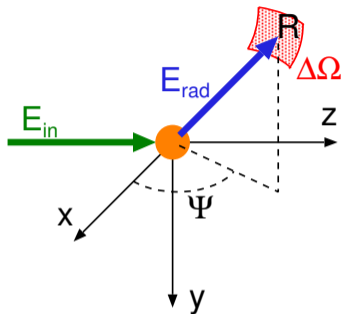


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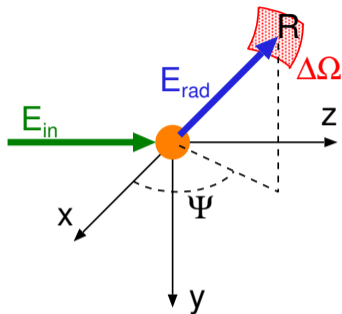
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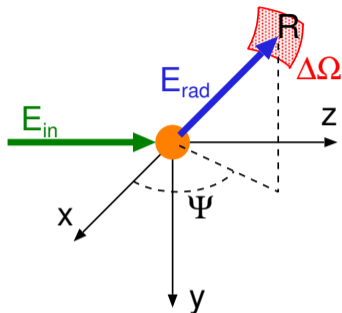
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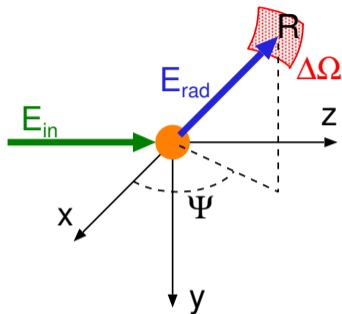
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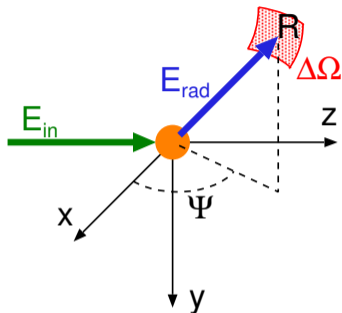
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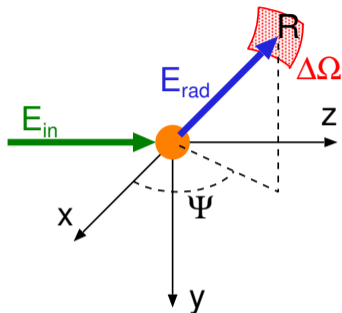
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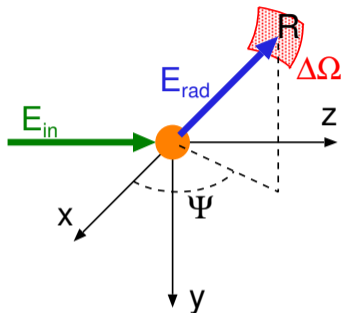
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$$\frac{d\sigma}{d\Omega}$$

Scattering cross-section



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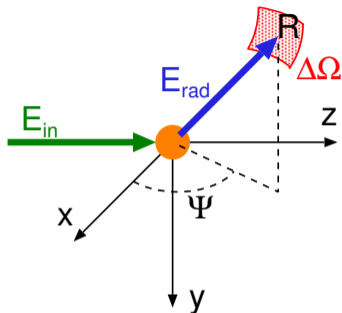
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Scattering cross-section



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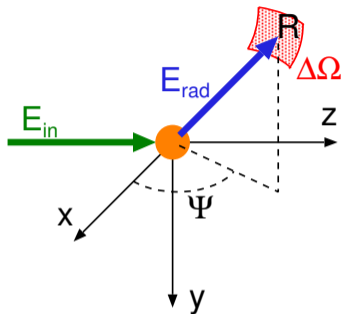
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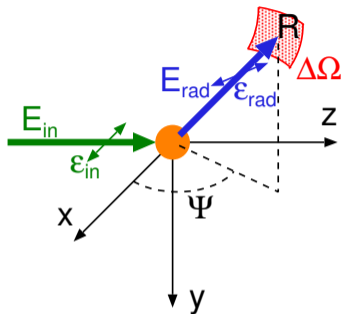
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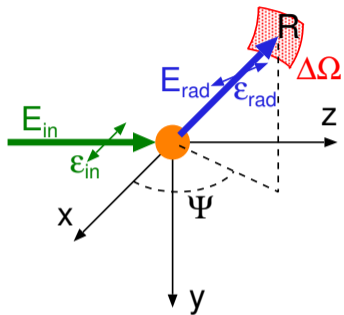
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Total cross-section

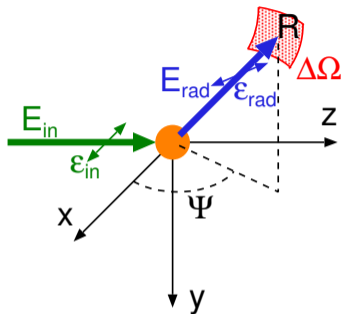


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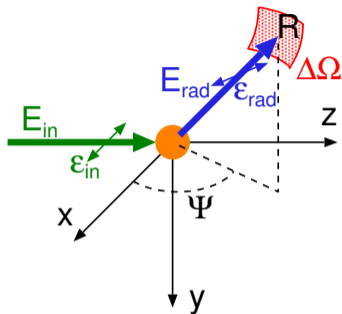
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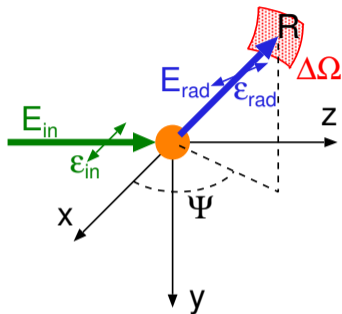
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Total cross-section



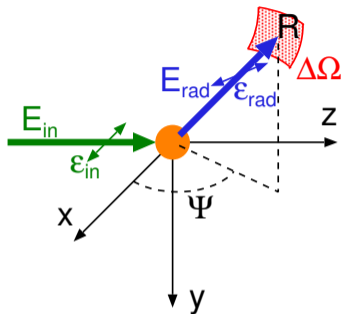
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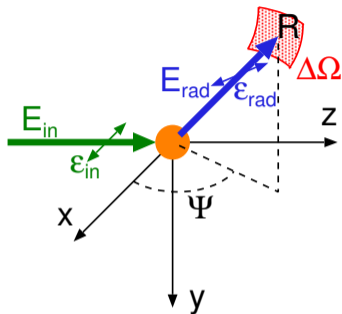


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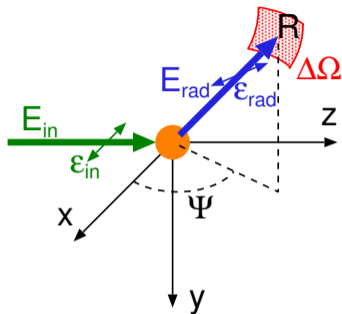
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Integrate to obtain the total Thomson scattering cross-section from an electron.

Total cross-section



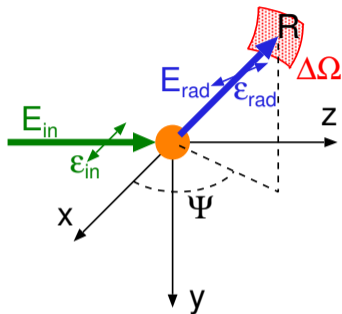
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Integrate to obtain the total Thomson scattering cross-section from an electron.

$$\sigma = \int r_0^2 \sin^2 \Psi d\Omega$$

Total cross-section



$$\frac{d\sigma}{d\Omega} = \frac{|E_{\text{rad}}|^2}{|E_{\text{in}}|^2} R^2 = r_0^2 \sin^2 \Psi$$

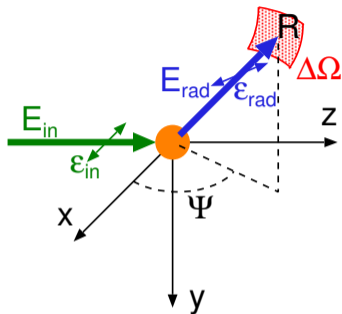
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$$\sigma = \int r_0^2 \sin^2 \Psi d\Omega = \frac{2}{3} 4\pi r_0^2$$

Total cross-section



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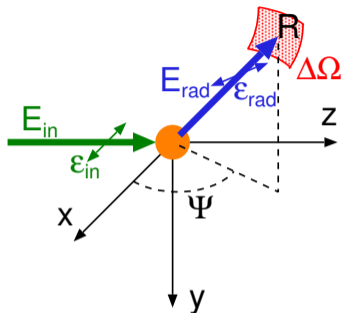
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$$\sigma = \int r_0^2 \sin^2 \Psi d\Omega = \frac{2}{3} 4\pi r_0^2 = \frac{8\pi}{3} r_0^2$$

Total cross-section



$$\frac{d\sigma}{d\Omega} = \frac{|E_{\text{rad}}|^2}{|E_{\text{in}}|^2} R^2 = r_0^2 \sin^2 \Psi$$

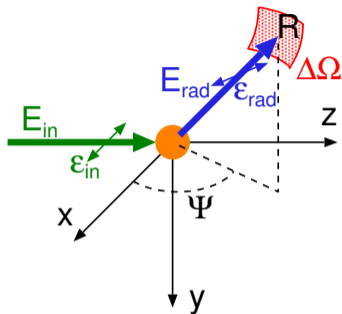
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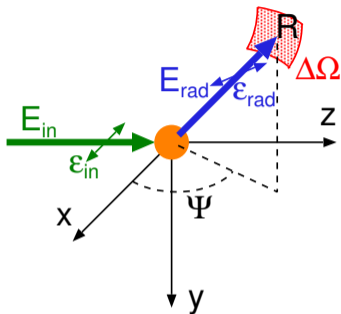
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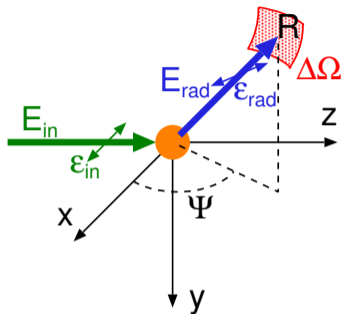
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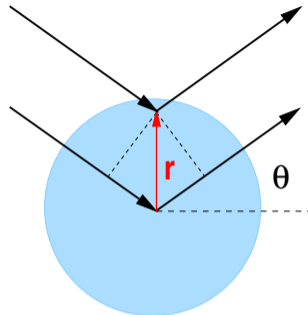
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Atomic scattering



If we have a charge distribution instead of a single electron, the scattering is more complex

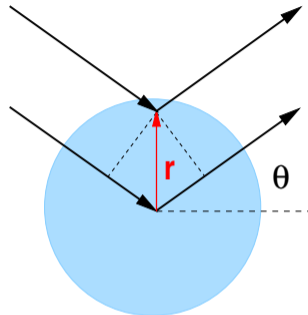


Atomic scattering



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A phase shift arises because of scattering from different portions of extended electron distribution



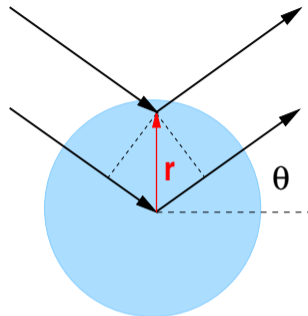
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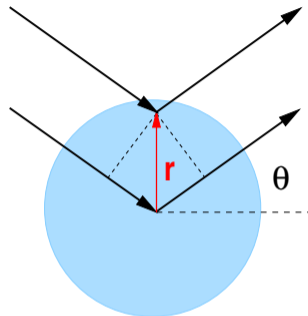
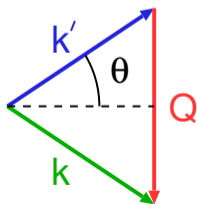
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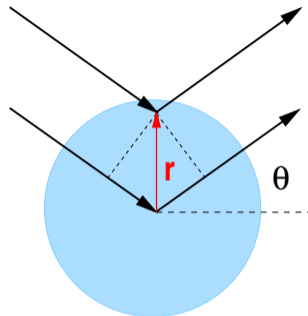
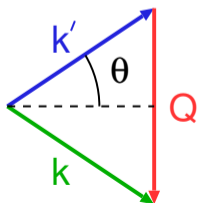
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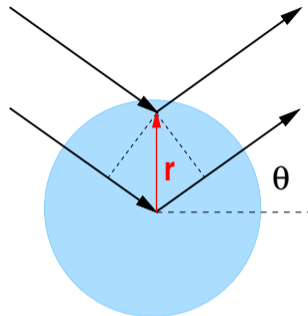
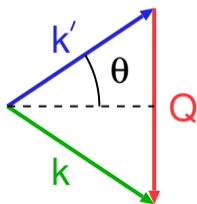
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Atomic form factor



The volume element at \mathbf{r} contributes $-r_0\rho(\mathbf{r})d^3r$ with phase factor $e^{i\mathbf{Q}\cdot\mathbf{r}}$

Atomic form factor



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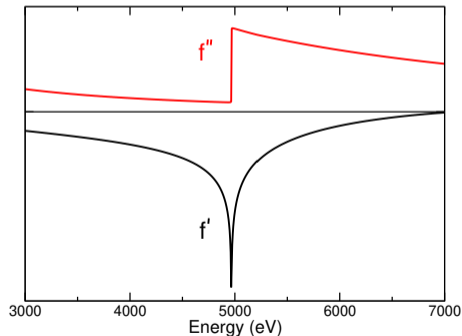
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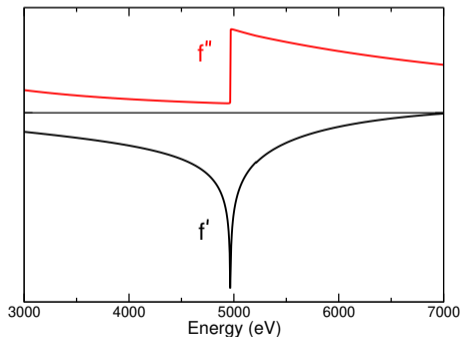


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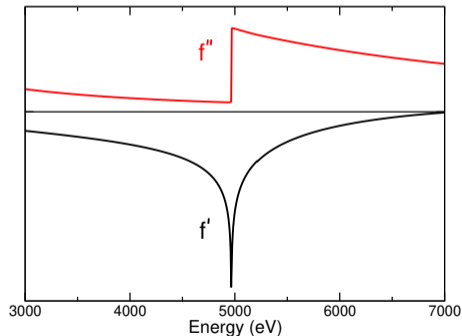
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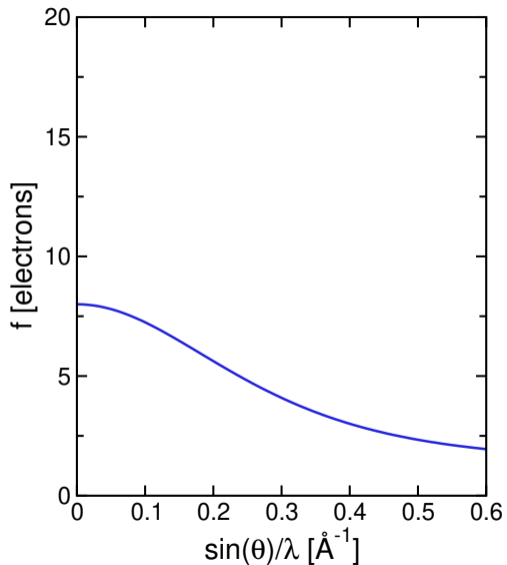
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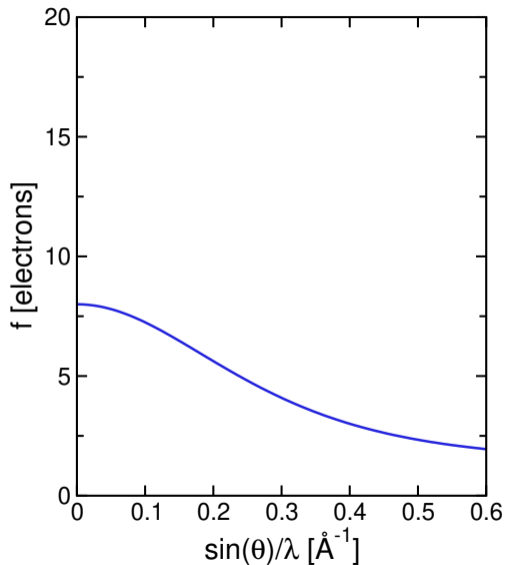


Atomic form factor



The atomic form factor has an angular dependence

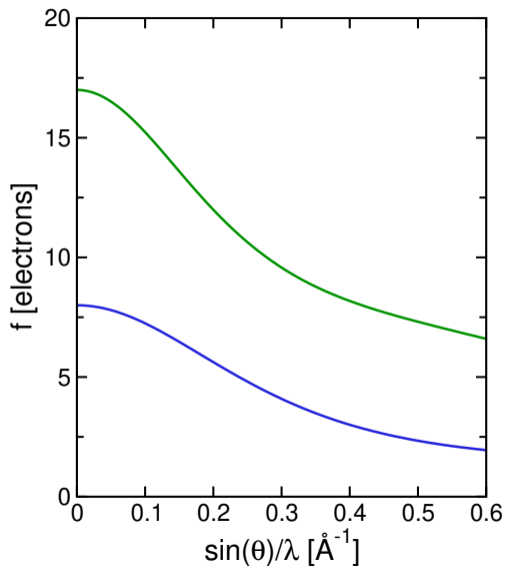
Atomic form factor



The atomic form factor has an angular dependence

$$Q = \frac{4\pi}{\lambda} \sin \theta$$

Atomic form factor

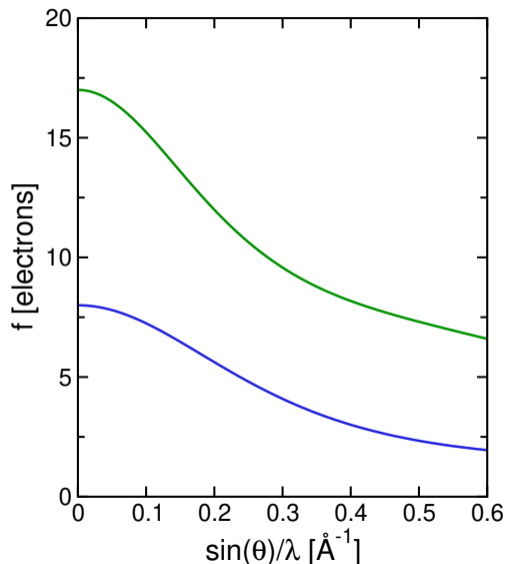


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lighter atoms have a broader form factor

Atomic form factor



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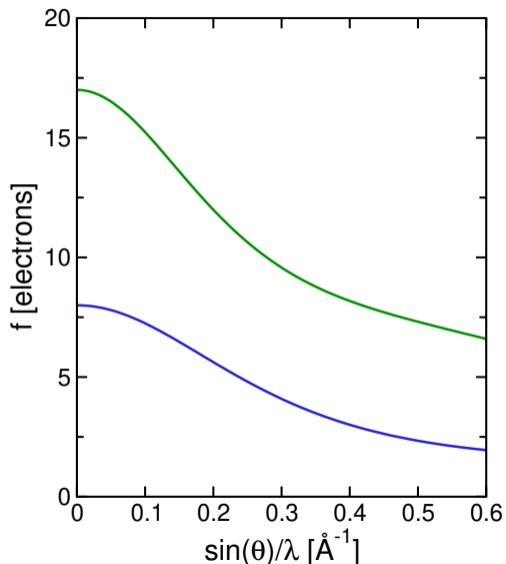
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forward scattering counts electrons

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Atomic form factor



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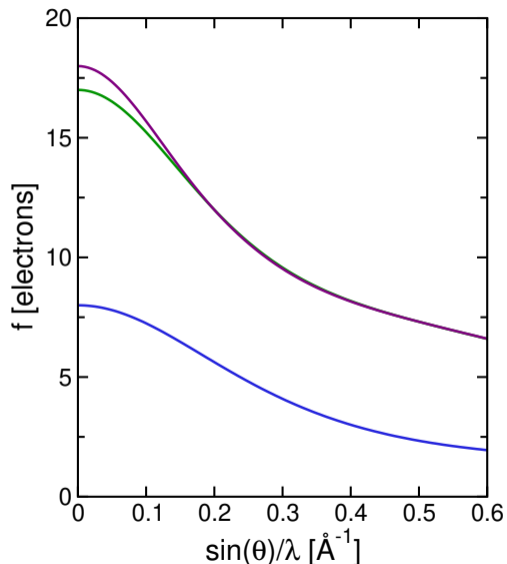
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Atomic form factor



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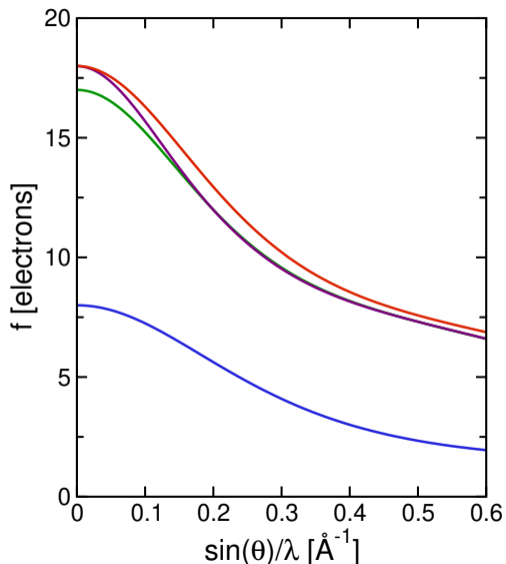
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