

PHYS 570 - Introduction to Synchrotron Radiation

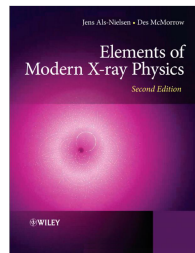


Term: Fall 2021
Meetings: Tuesday & Thursday 17:10-18:25
Location: 121 Pritzker Science

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/phys570/21F>





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



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- Describe the function of various components of a synchrotron beamline



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- Prepare and deliver an oral presentation of a synchrotron radiation research topic



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- Perform calculations in support of a synchrotron experiment
- 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



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- 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
 - Because of COVID-19 the APS is on Limited Operations status
 - Only 2 people per experiment can be on site
 - Over the course of the semester, we will hold virtual beamline sessions at 10-BM for any who wish to attend



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- 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



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Weekly or bi-weekly



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Weekly or bi-weekly
Due at beginning of class



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Course grading



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33% – Final Exam Presentation



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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

Topics to be covered (at a minimum)



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

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- Refraction and reflection from interfaces

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- Small angle scattering
- 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)

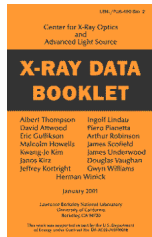


- X-rays and their interaction with matter
- Sources of x-rays
- Refraction and reflection from interfaces
- Kinematical diffraction
- Diffraction by perfect crystals
- Small angle scattering
- Photoelectric absorption
- Resonant scattering
- Imaging

Resources for the course



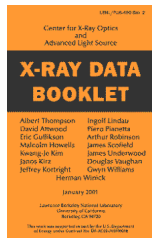
- Orange x-ray data booklet:
<http://xdb.lbl.gov/xdb-new.pdf>



Resources for the course



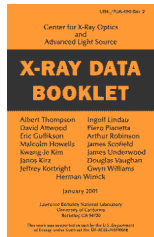
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Resources for the course



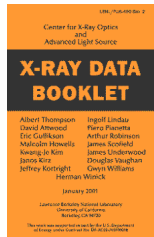
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- Hephaestus from the Demeter suite:
<http://bruceravel.github.io/demeter>



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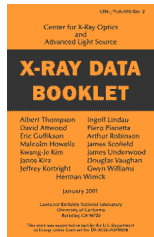
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- X-ray Oriented Programs: <https://www.aps.anl.gov/Science/Scientific-Software/XOP>



Today's outline - August 24, 2021



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- The big picture
- History of x-ray sources

Today's outline - August 24, 2021



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

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- Atomic form factor

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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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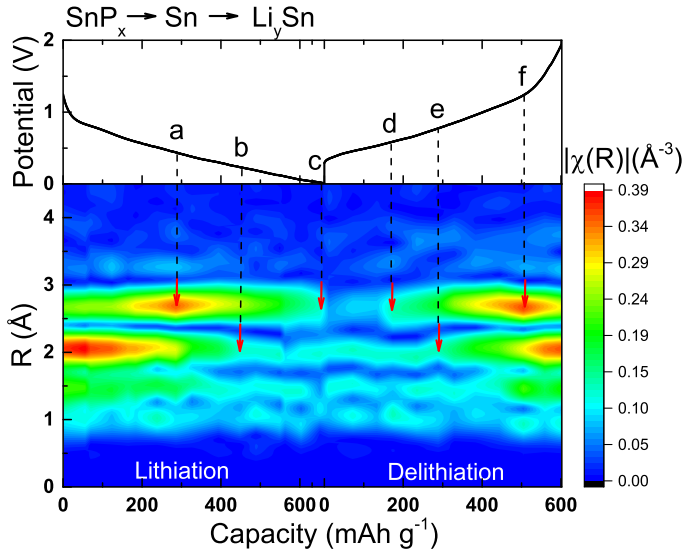
Synchrotron sources and particularly FELs produce coherent beams

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

A bit about my research. . .



A bit about my research...



“In situ EXAFS-derived mechanism of highly reversible tin phosphide/graphite composite anode for Li-ion batteries,” Y. Ding, Z. Li, E.V. Timofeeva, and C.U. Segre, *Adv. Energy Mater.* 1702134 (2017).

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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where $\hat{\mathbf{e}}$ is a unit vector in the direction of the electric field

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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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1. Elastic scattering
2. Inelastic scattering
3. Absorption
4. Pair production

We will only discuss the first three.

Elastic scattering

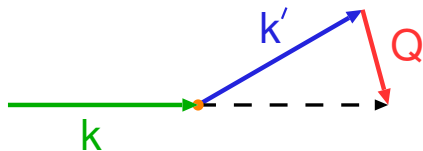


Most of the phenomena we will discuss can be treated classically as elastic scattering of electromagnetic waves (x-rays).

Elastic scattering



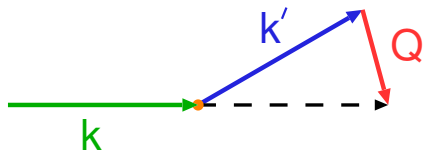
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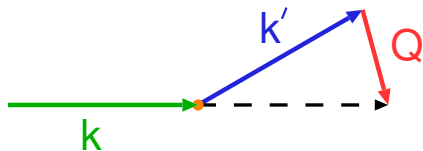


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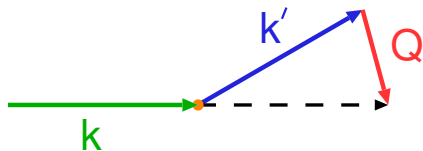


where an incident x-ray of wave number k
scatters elastically from an electron to k'

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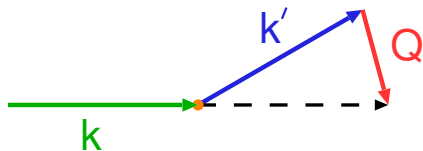


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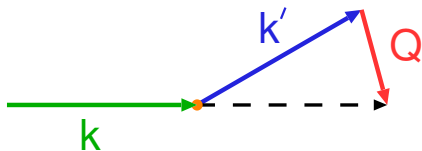
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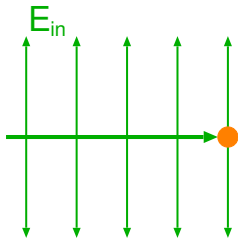
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Start with the scattering from a single electron, then build up to more complexity

Thomson scattering



Assumptions:

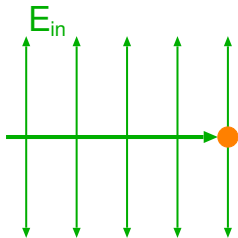


Thomson scattering



Assumptions:

incident x-ray plane wave



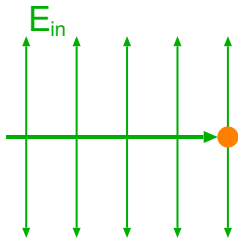
Thomson scattering



Assumptions:

incident x-ray plane wave

electron is a point charge

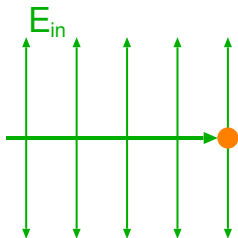


Thomson scattering



Assumptions:

incident x-ray plane wave
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Thomson scattering



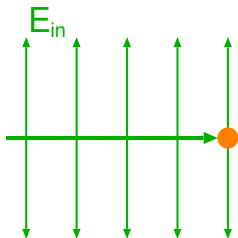
Assumptions:

incident x-ray plane wave

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scattering is elastic

scattered intensity $\propto 1/R^2$



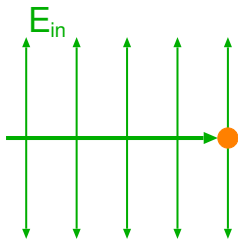
Thomson scattering



Assumptions:

incident x-ray plane wave
electron is a point charge
scattering is elastic
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The electron is exposed to the incident electric field $E_{in}(t')$ and is accelerated



Thomson scattering



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incident x-ray plane wave

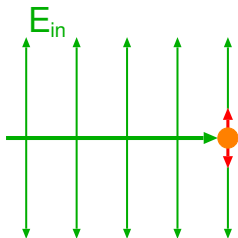
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The electron is exposed to the incident electric field $E_{in}(t')$ and is accelerated

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



Thomson scattering



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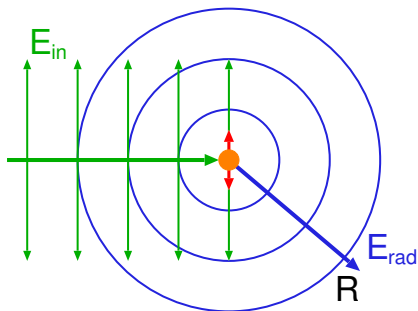
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The observer at R “sees” a scattered electric field $E_{rad}(R, t)$ at a later time $t = t' + R/c$



Thomson scattering



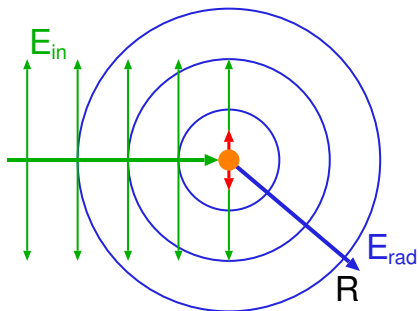
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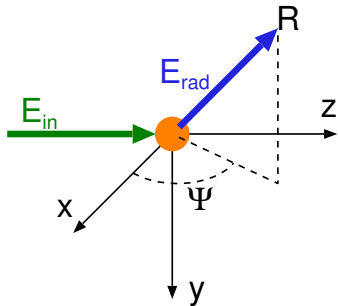
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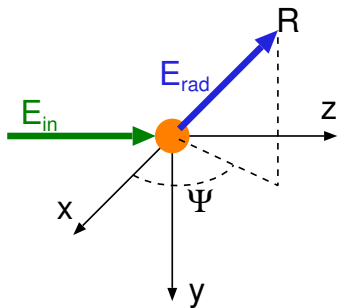
Using this, calculate the elastic scattering cross-section

Thomson scattering



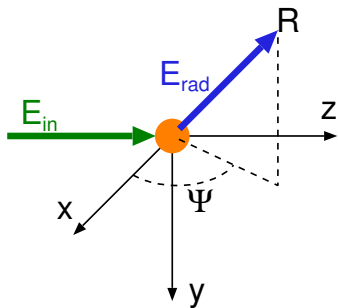
$$E_{rad}(R, t) = -\frac{-e}{4\pi\epsilon_0 c^2 R} a_x(t') \sin \Psi,$$

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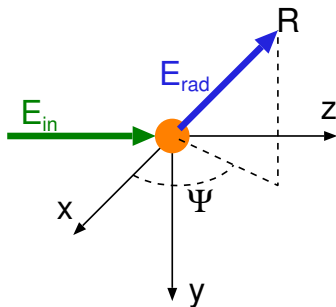
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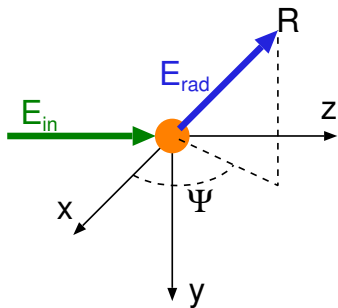
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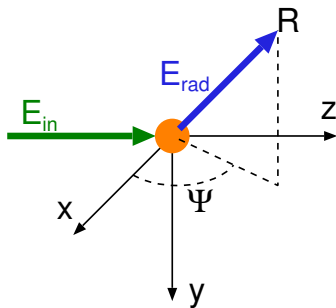


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$$a_x(t') = -\frac{e}{m} E_{in} e^{i\omega R/c}$$

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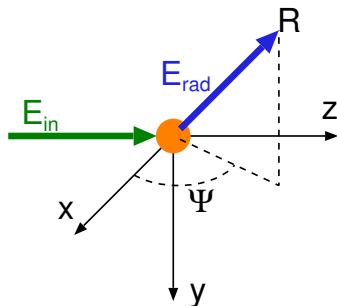
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Thomson scattering



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

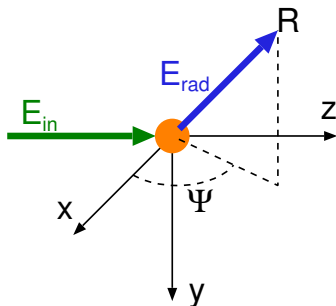
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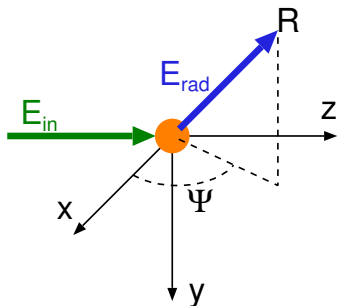
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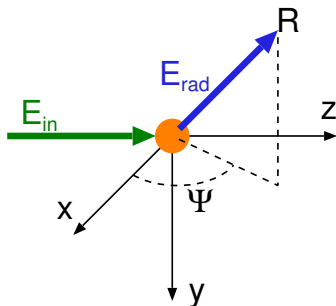
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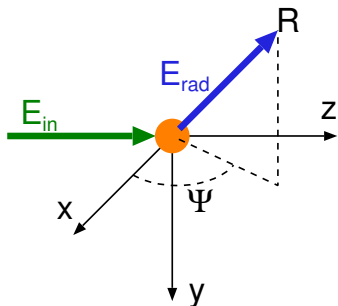
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$$r_0 = \frac{e^2}{4\pi\epsilon_0 m c^2} = 2.82 \times 10^{-5} \text{ \AA}$$

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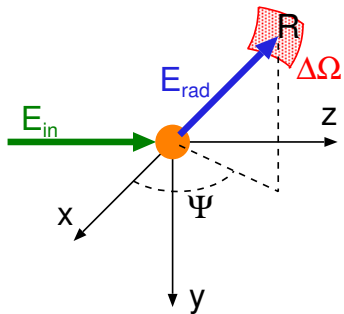
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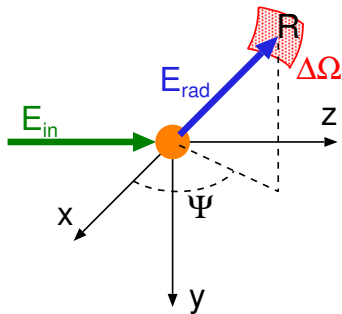
$$r_0 = \frac{e^2}{4\pi\epsilon_0 m c^2} = 2.82 \times 10^{-5} \text{ \AA}$$

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

Scattering cross-section

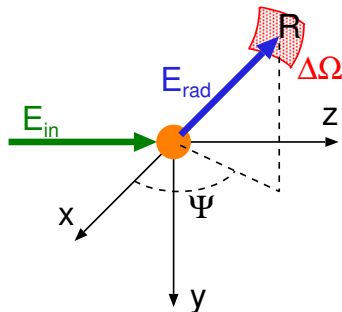


Scattering cross-section



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

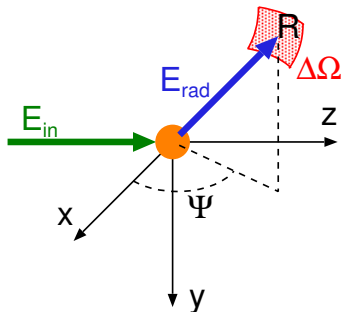
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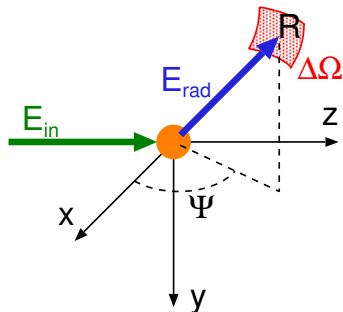


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Scattering cross-section



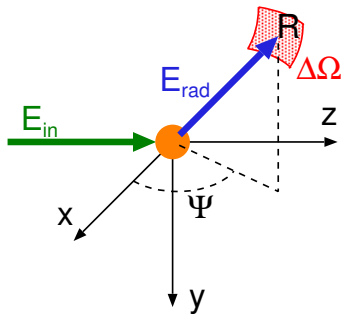
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Scattering cross-section



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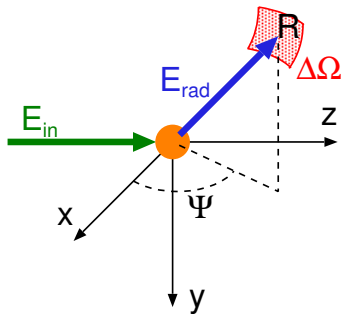
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Scattering cross-section



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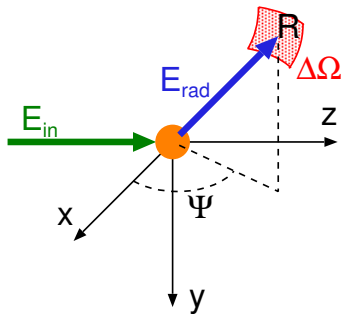
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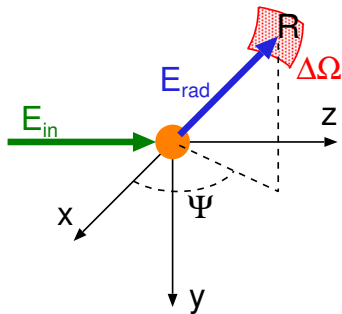
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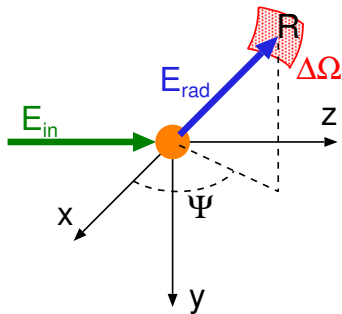
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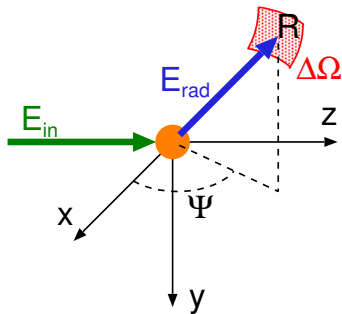
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Scattering cross-section



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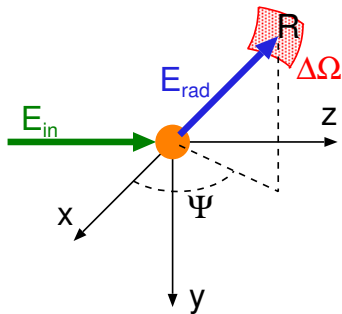
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Scattering cross-section



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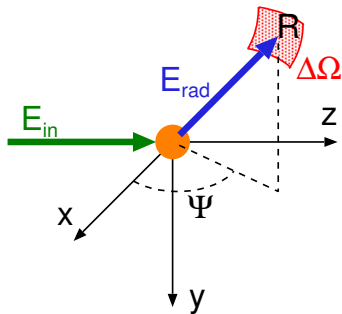
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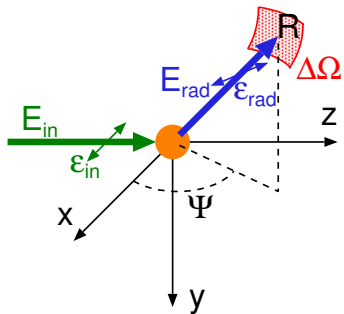
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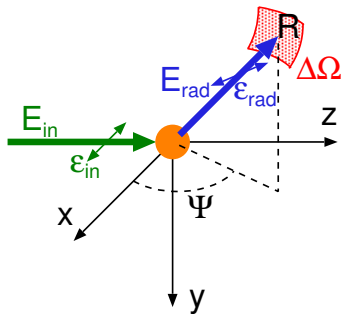
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Total cross-section

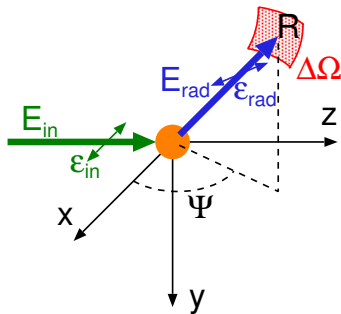


Total cross-section



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

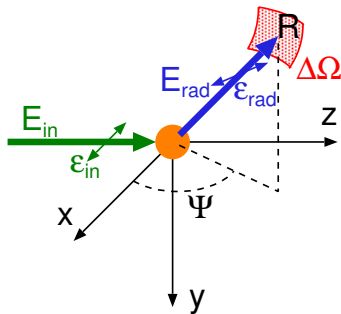
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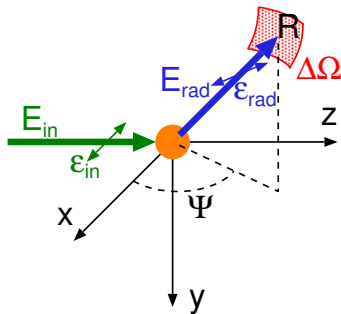
$$\frac{E_{rad}}{E_{in}} = -r_0 \frac{e^{ikR}}{R} |\hat{\epsilon}_{in} \cdot \hat{\epsilon}_{rad}|$$

Total cross-section



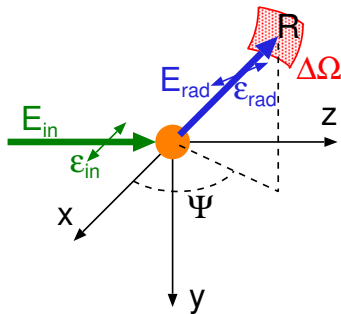
$$\begin{aligned}\frac{d\sigma}{d\Omega} &= \frac{|E_{\text{rad}}|^2}{|E_{\text{in}}|^2} R^2 \\ \frac{E_{\text{rad}}}{E_{\text{in}}} &= -r_0 \frac{e^{ikR}}{R} |\hat{\epsilon}_{\text{in}} \cdot \hat{\epsilon}_{\text{rad}}| \\ &= -r_0 \frac{e^{ikR}}{R} \left| \cos\left(\frac{\pi}{2} - \Psi\right) \right|\end{aligned}$$

Total cross-section



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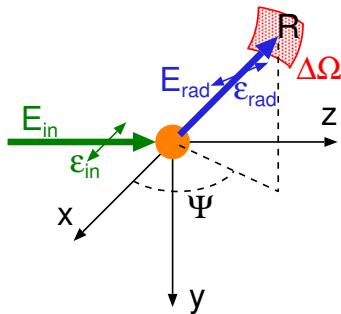
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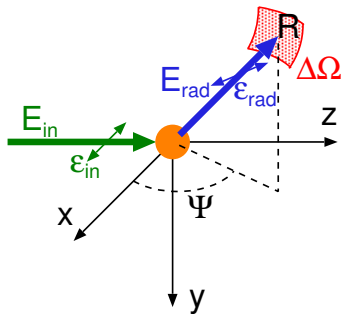


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Integrate to obtain the total Thomson scattering cross-section from an electron.

Total cross-section



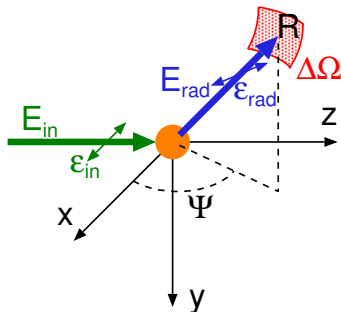
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Total cross-section



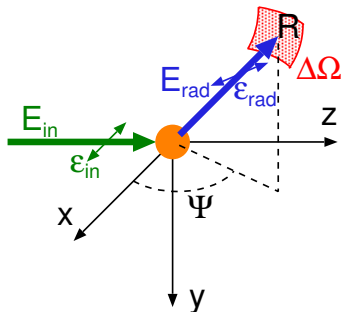
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Total cross-section



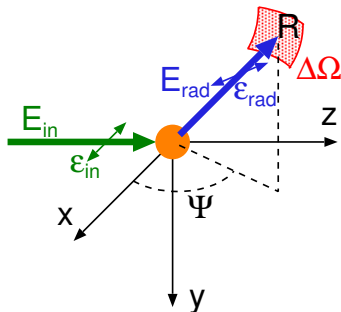
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$$\sigma = \int r_0^2 \sin^2 \psi d\Omega = \frac{2}{3} 4\pi r_0^2 = \frac{8\pi}{3} r_0^2$$

Total cross-section



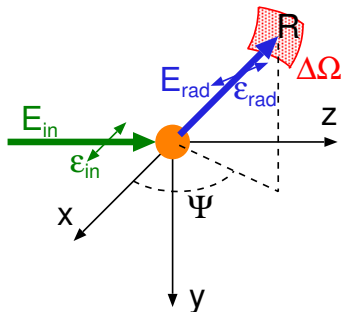
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$$\begin{aligned} \sigma &= \int r_0^2 \sin^2 \psi d\Omega = \frac{2}{3} 4\pi r_0^2 = \frac{8\pi}{3} r_0^2 \\ &= 0.665 \times 10^{-24} \text{ cm}^2 = 0.665 \text{ barn} \end{aligned}$$

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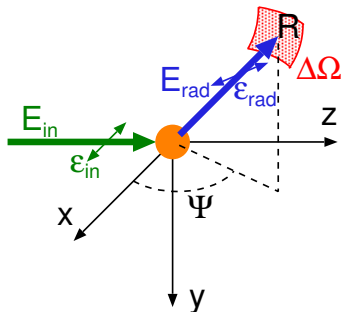
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$$P = \left\langle |\hat{\epsilon}_{in} \cdot \hat{\epsilon}_{rad}|^2 \right\rangle = \left\{ \left\langle \sin^2 \psi \right\rangle = \frac{2}{3} \right.$$

Total cross-section



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

$$\begin{aligned} \frac{E_{rad}}{E_{in}} &= -r_0 \frac{e^{ikR}}{R} |\hat{\epsilon}_{in} \cdot \hat{\epsilon}_{rad}| \\ &= -r_0 \frac{e^{ikR}}{R} \left| \cos \left(\frac{\pi}{2} - \Psi \right) \right| = -r_0 \frac{e^{ikR}}{R} \sin \Psi \end{aligned}$$

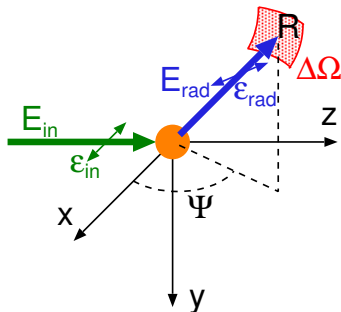
Integrate to obtain the total Thomson scattering cross-section from an electron.

If displacement is in vertical direction, $\sin \Psi$ term is replaced by unity

$$\begin{aligned} \sigma &= \int r_0^2 \sin^2 \Psi d\Omega = \frac{2}{3} 4\pi r_0^2 = \frac{8\pi}{3} r_0^2 \\ &= 0.665 \times 10^{-24} \text{ cm}^2 = 0.665 \text{ barn} \end{aligned}$$

$$P = \left\langle |\hat{\epsilon}_{in} \cdot \hat{\epsilon}_{rad}|^2 \right\rangle = \begin{cases} 1 \\ \langle \sin^2 \Psi \rangle = \frac{2}{3} \end{cases}$$

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If displacement is in vertical direction, $\sin \Psi$ term is replaced by unity and if the source is unpolarized, it is a combination.

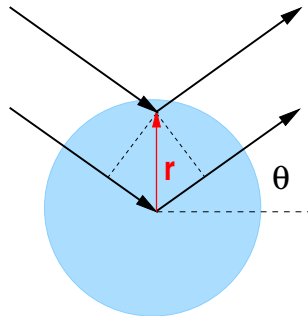
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Atomic scattering



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

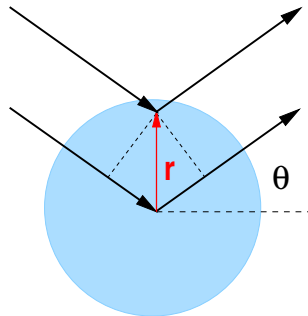


Atomic scattering



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

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



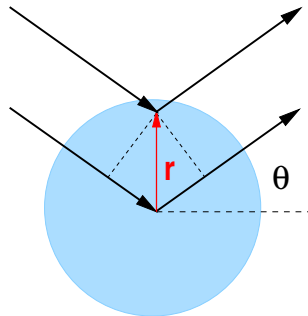
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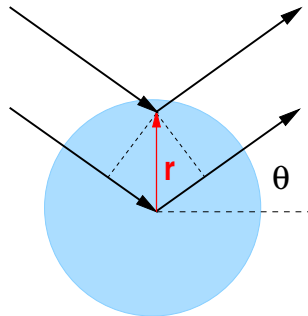
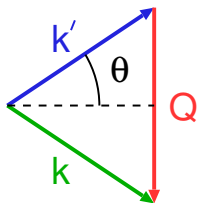
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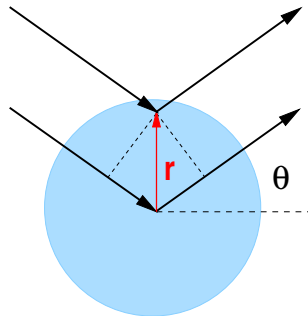
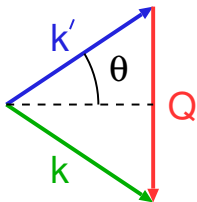
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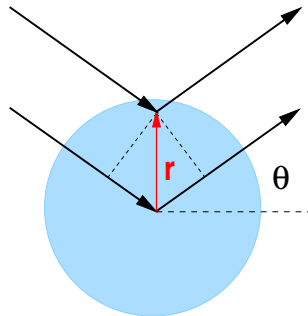
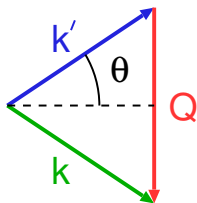
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Atomic form factor



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



The volume element at \mathbf{r} contributes $\rho(\mathbf{r})d^3r$ with phase factor $e^{i\mathbf{Q}\cdot\mathbf{r}}$ for an entire atom, integrate to get the atomic form factor $f^0(\mathbf{Q})$:

Atomic form factor



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Electrons which are tightly bound cannot respond like a free electron. This results in a depression of the atomic form factor, called f' and a lossy term near an ionization energy, called f'' . Together these are the “anomalous” corrections to the atomic form factor.

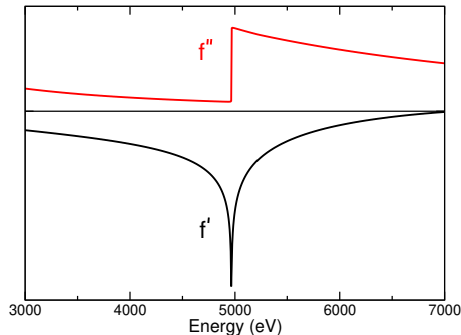
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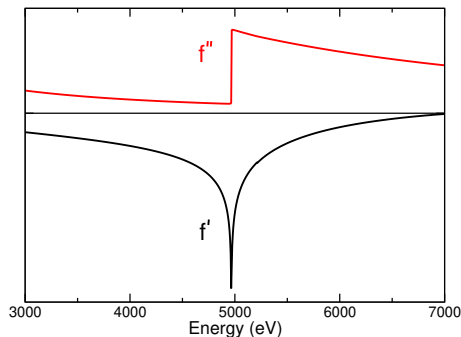


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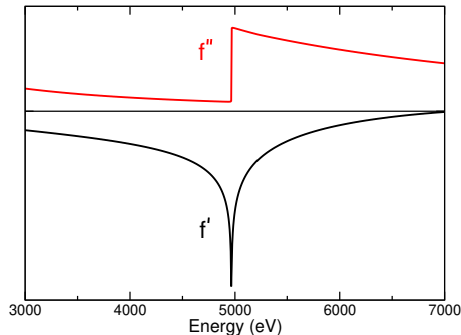
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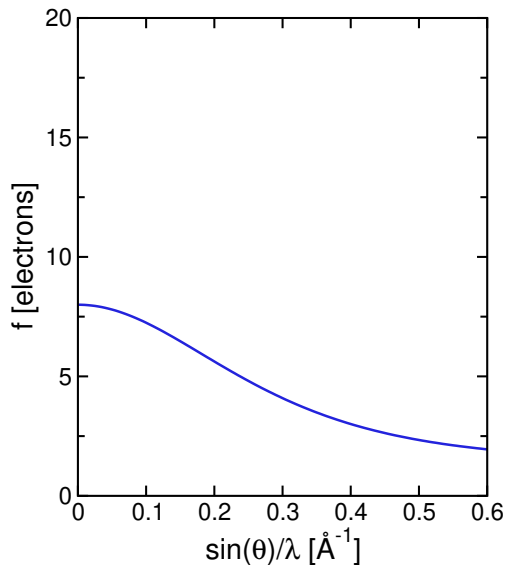
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$$f(\mathbf{Q}, \hbar\omega) = f^0(\mathbf{Q}) + f'(\hbar\omega) + if''(\hbar\omega)$$

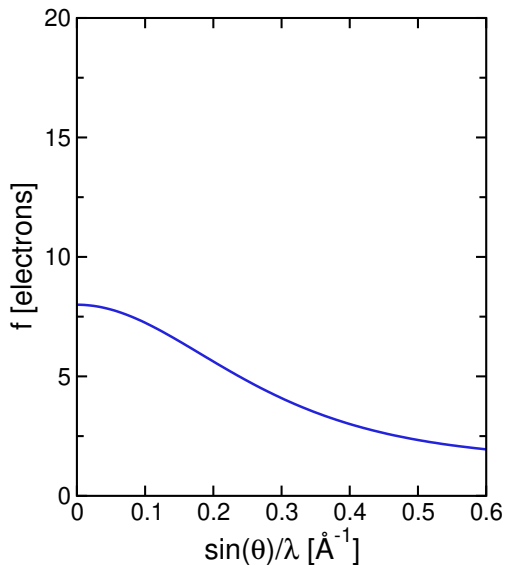


Atomic form factor



The atomic form factor has an angular dependence

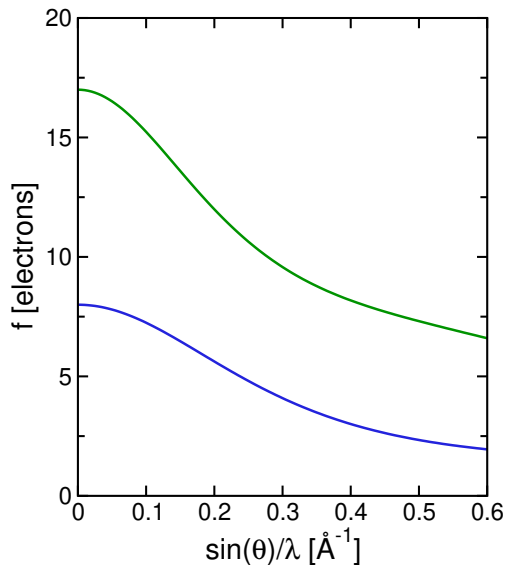
Atomic form factor



The atomic form factor has an angular dependence

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

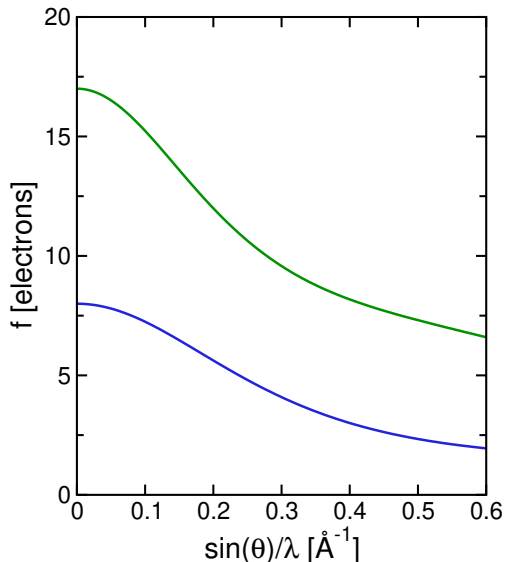
Atomic form factor



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lighter atoms have a broader form factor



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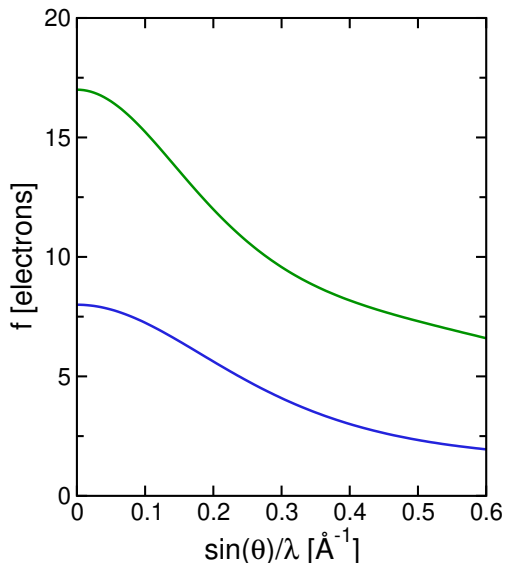
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forward scattering counts electrons

$$f(0) = Z$$

Atomic form factor



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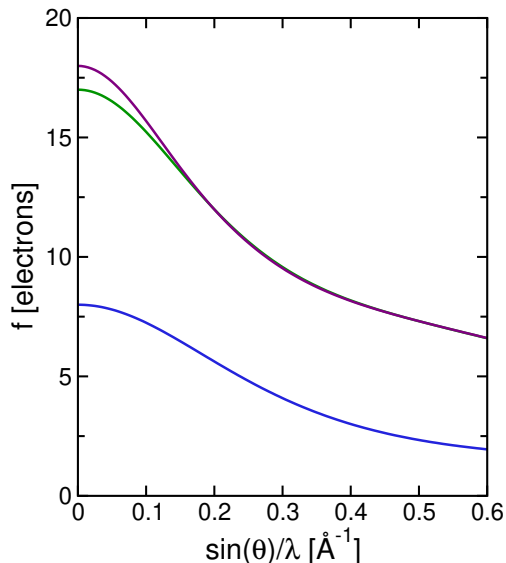
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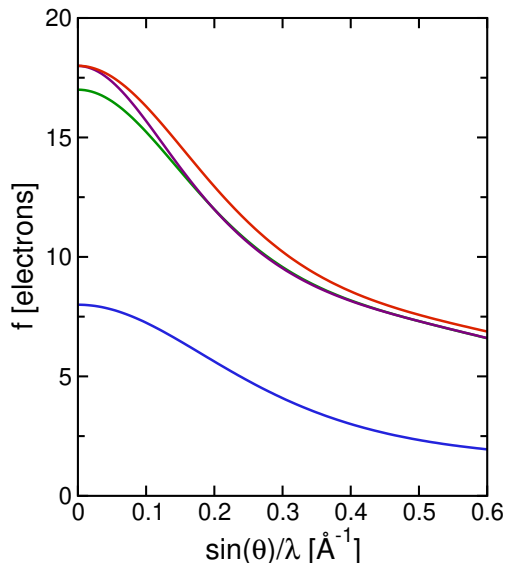
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