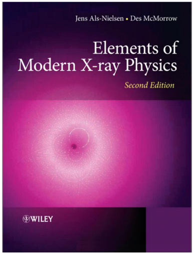
PHYS 570 - Introduction to Synchrotron Radiation

Term: Spring 2020
Meetings: Tuesday & Thursday 17:00-18:15
Location: 241 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, 2^{nd} ed.*, J. Als-Nielsen and D. McMorrow (Wiley, 2011)

Web Site: http://csrri.iit.edu/~segre/phys570/20S

Course objectives

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

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- Understand the physics behind a variety of experimental techniques
- Be able to make an oral presentation of a synchrotron radiation research topic
- Be able to write a General User Proposal in the format used by the Advanced Photon Source

Course syllabus

- Focus on applications of synchrotron radiation

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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

Optional activities

- 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 but will try to make it during the week of the Advanced Photon Source User Meeting (April 20-24, 2020)

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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
  - IFEFFIT suite for x-ray absorption spectroscopy analysis http://cars9.uchicago.edu/ifeffit

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)

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- Imaging

Resources for the course

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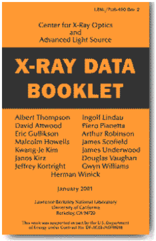

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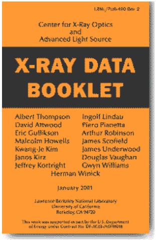

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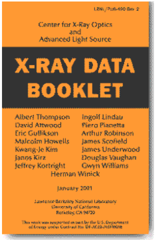

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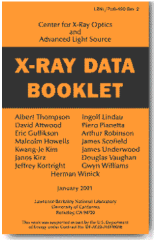

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- X-ray Oriented Programs:
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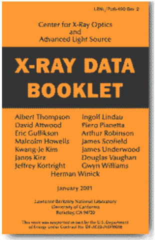

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Reading Assignment: Chapter 1.1–1.6; 2.1–2.2

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

A bit about my research…

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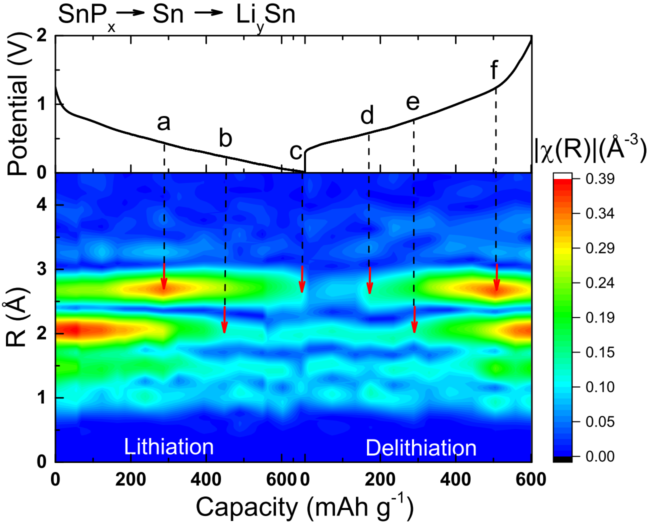

"In situ EXAFS-derived mechanism of highly reversible tin phosphide/graphite composite anode for Li-ion batteries," Y. Ding, Z. Li, E.V. Timofeeva, and C.U. Segre, *Adv. Energy Mater.* 1702134 (2017).

The classical x-ray

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

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We will only discuss the first three.

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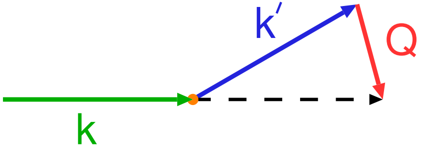

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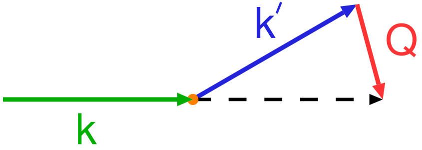

where an incident x-ray of wave number **k**

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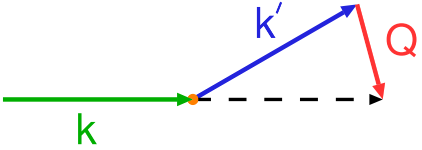

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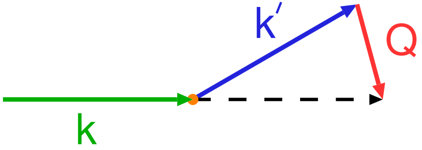

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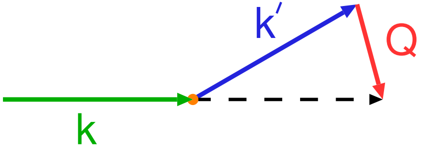

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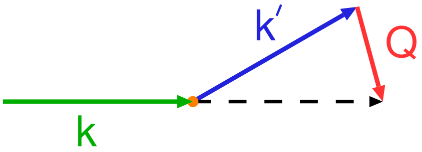

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Start with the scattering from a single electron, then build up to more complexity

Thomson scattering

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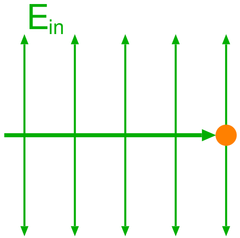

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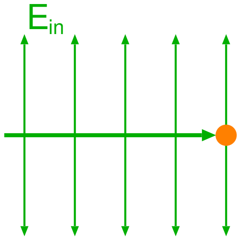

Thomson scattering

Assumptions:

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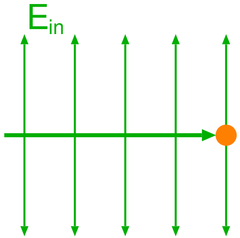
electron is a point charge



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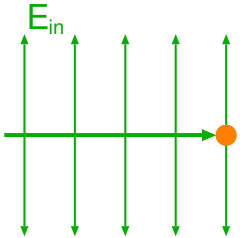

Thomson scattering

Assumptions:

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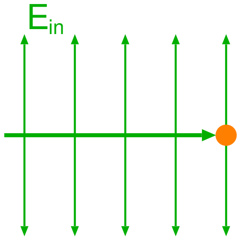

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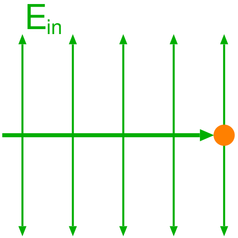

The electron is exposed to the incident electric field $E_{in}(t')$ and is accelerated

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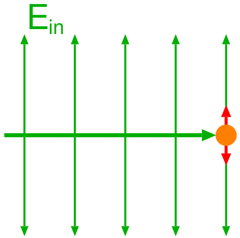

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The acceleration of the electron, $a_x(t')$, results in the radiation of a spherical wave with the same frequency

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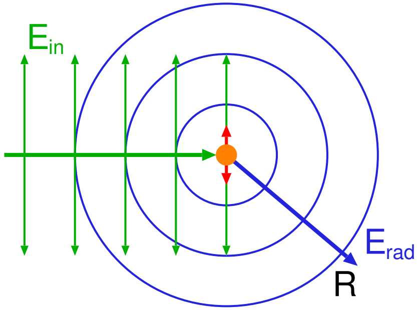

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The observer at R "sees" a scattered electric field $E_{rad}(R, t)$ at a later time $t = t' + R/c$

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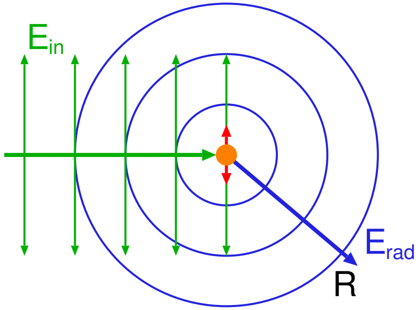

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Using this, calculate the elastic scattering cross-section

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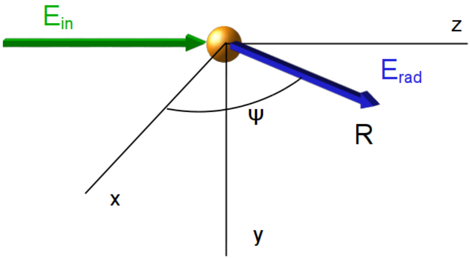

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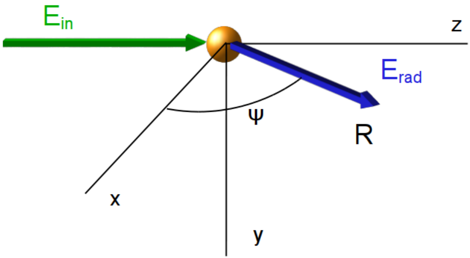

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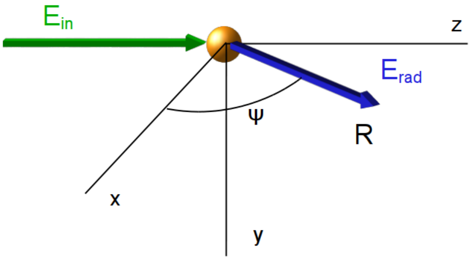
Thomson scattering



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

$$a_x(t') = -\frac{e}{m} E_{x0} e^{-i\omega t'}$$

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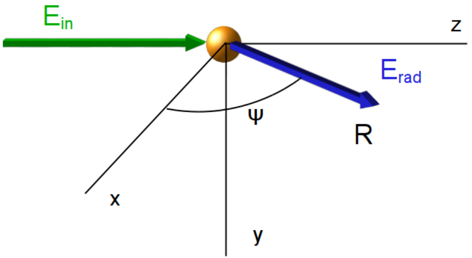

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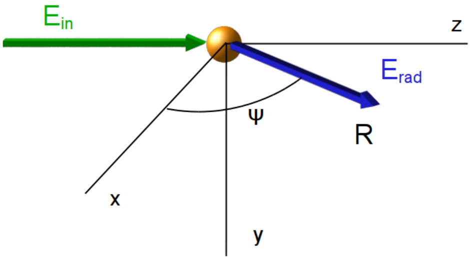

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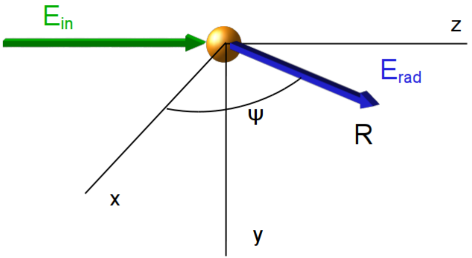

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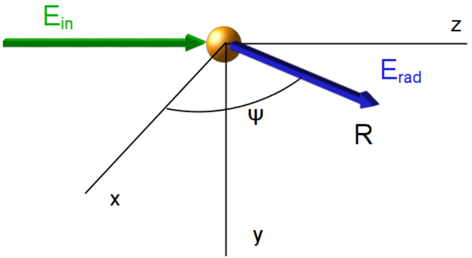

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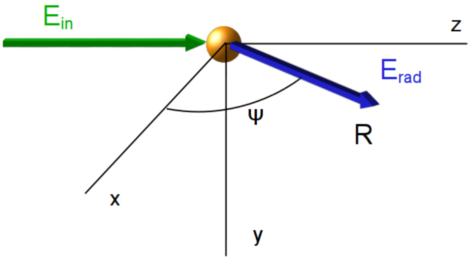

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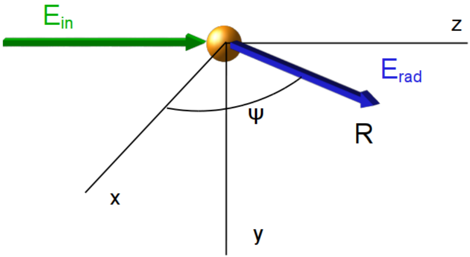
Thomson scattering length



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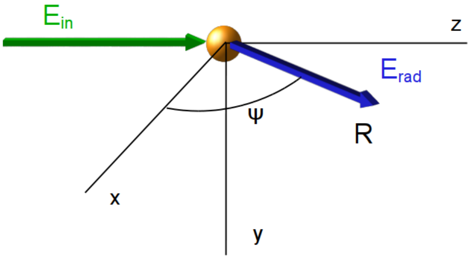

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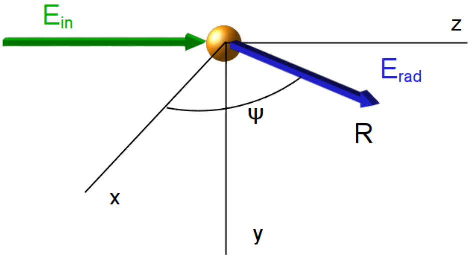

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r_0 is called the Thomson scattering length or the “classical” radius of the electron

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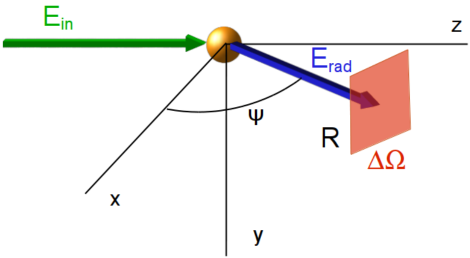

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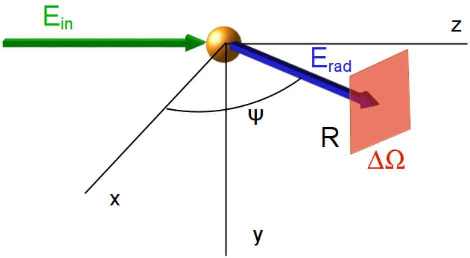
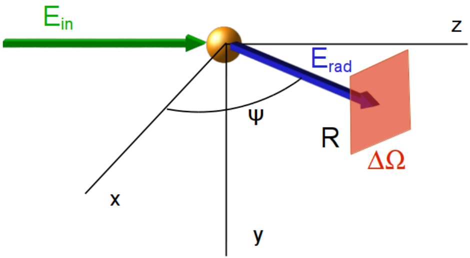


detector of solid angle $\Delta\Omega$ located a distance R from electron

Scattering cross-section



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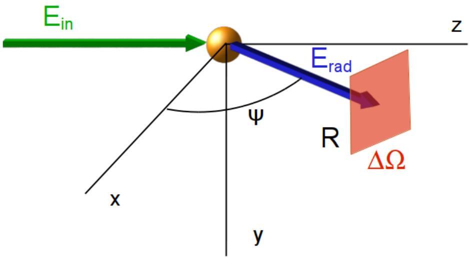

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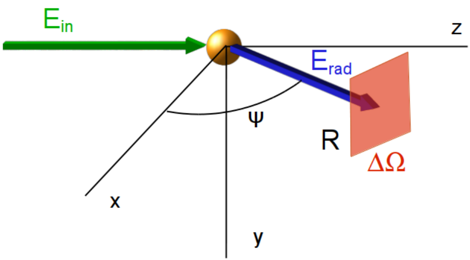

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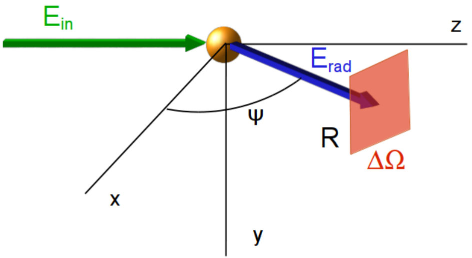

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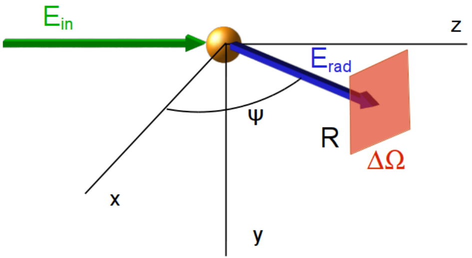

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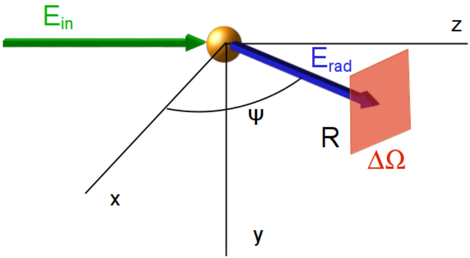

Differential cross-section is obtained by normalizing

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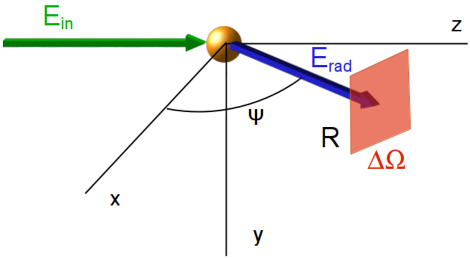

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$$\frac{d\sigma}{d\Omega}$$

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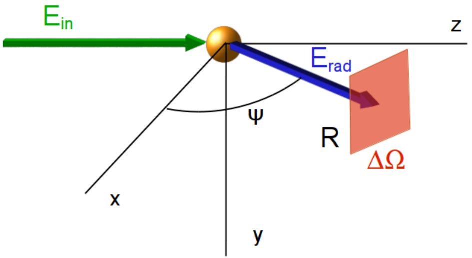

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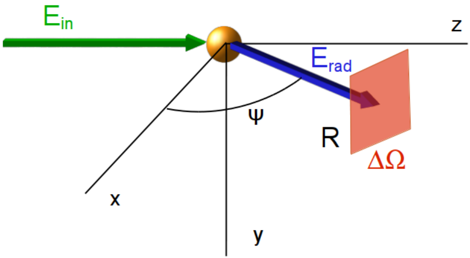

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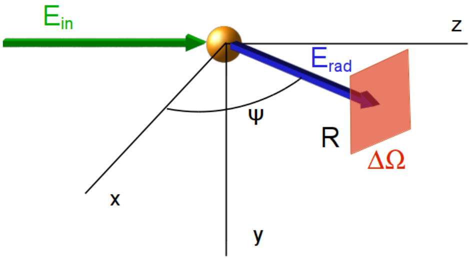

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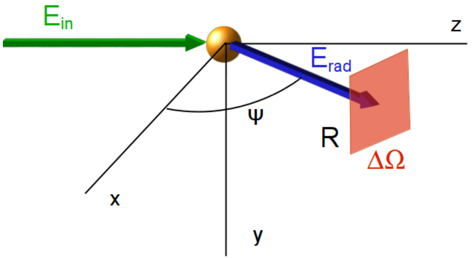

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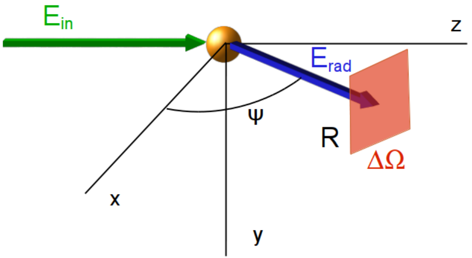

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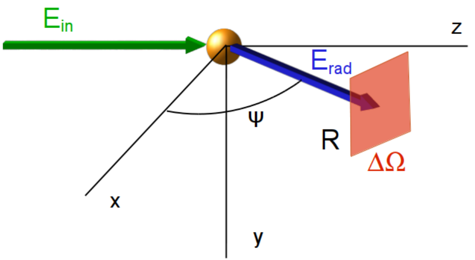

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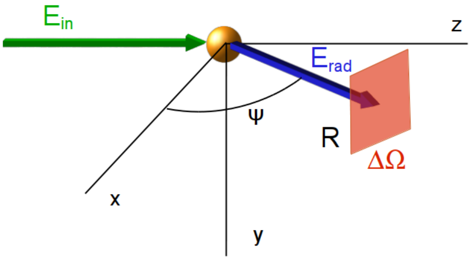

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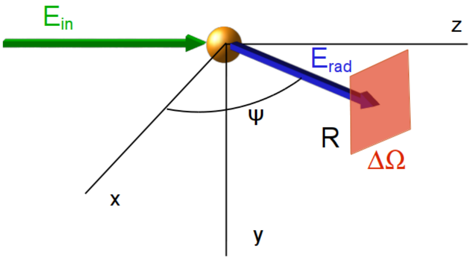

Integrate to obtain the total Thomson scattering cross-section from an electron.

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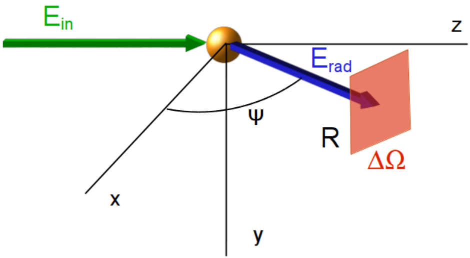

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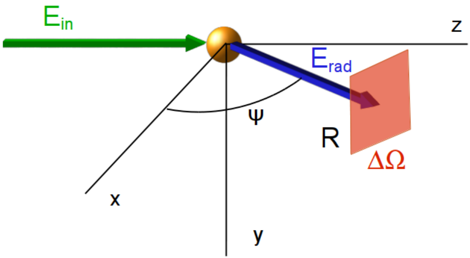

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$$\begin{aligned}\sigma &= \frac{8\pi}{3} r_0^2 \\ &= 0.665 \times 10^{-24}\ cm^2 \\ &= 0.665\ barn\end{aligned}$$

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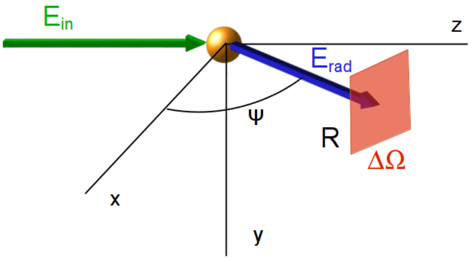

Integrate to obtain the total Thomson scattering cross-section from an electron. If displacement is in vertical direction, $\sin\Psi$ term is replaced by unity and if the source is unpolarized, it is a combination.

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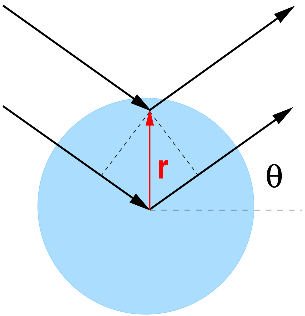
$$\text{Polarization factor} = \begin{cases} 1 \\ \sin^2\Psi \\ \frac{1}{2}\left(1+\sin^2\Psi\right) \end{cases}$$

Atomic scattering

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



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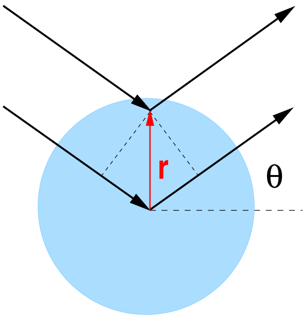
A phase shift arises because of scattering from different portions of extended electron distribution



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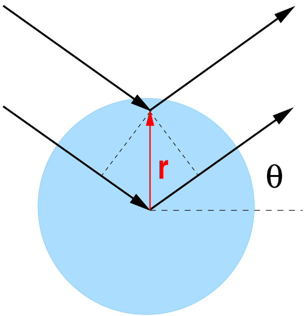

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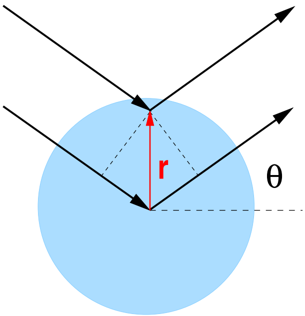

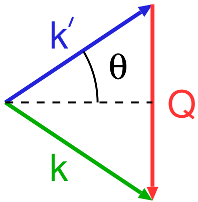

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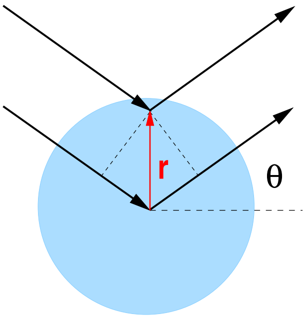

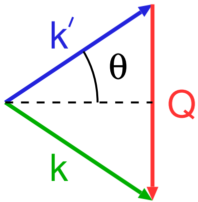

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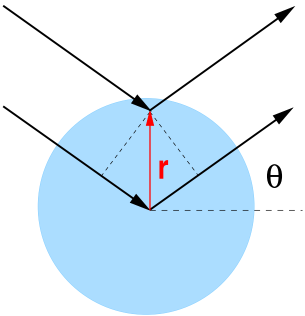

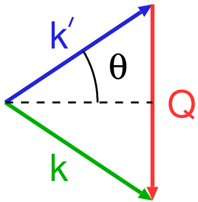

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$$|\mathbf{Q}| = 2\,|\mathbf{k}|\,sin\theta = \frac{4\pi}{\lambda} sin\theta$$

Atomic form factor

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

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The volume element at $\mathbf{r}$ contributes $-r_0\rho(\mathbf{r})d^3r$ with phase factor $e^{i\mathbf{Q}\cdot\mathbf{r}}$ for an entire atom, integrate to get the atomic form factor $f^0(\mathbf{Q})$:

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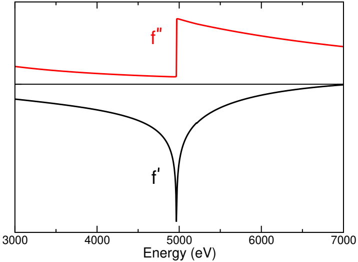

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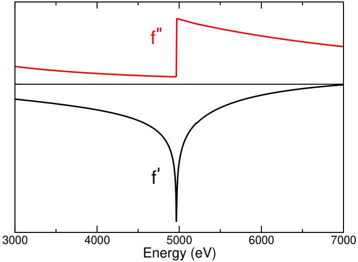


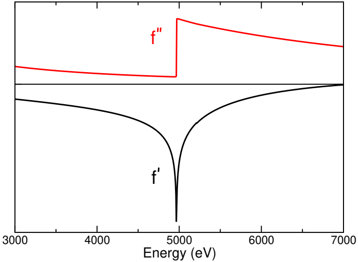
the total atomic scattering factor is

Atomic form factor

The volume element at $\mathbf{r}$ contributes $-r_0\rho(\mathbf{r})d^3r$ with phase factor $e^{i\mathbf{Q}\cdot\mathbf{r}}$ for an entire atom, integrate to get the atomic form factor $f^0(\mathbf{Q})$:

$$-r_0 f^0(\mathbf{Q}) = -r_0 \int \rho(\mathbf{r}) e^{i\mathbf{Q}\cdot\mathbf{r}} d^3r$$

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

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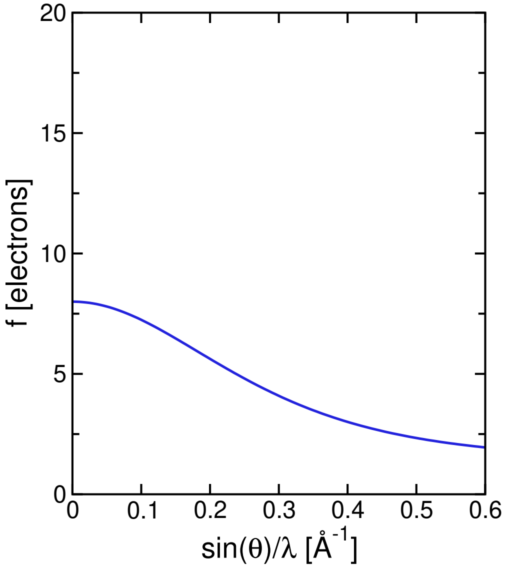

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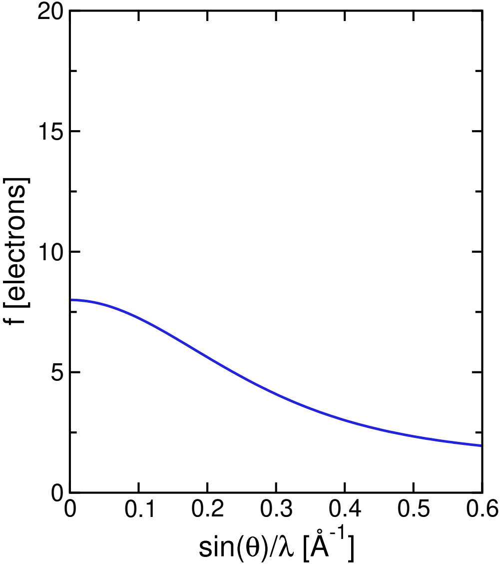

The atomic form factor has an angular dependence

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

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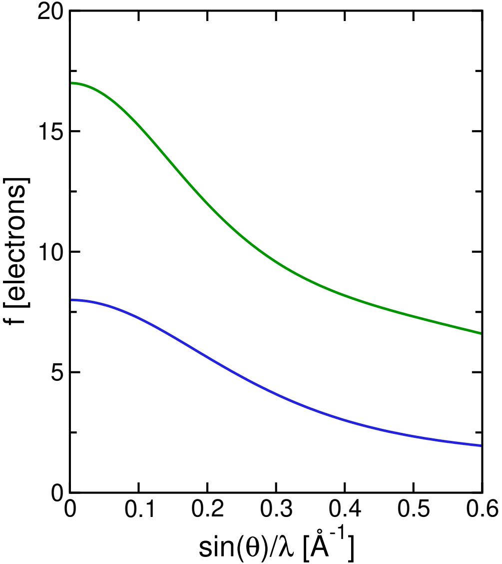

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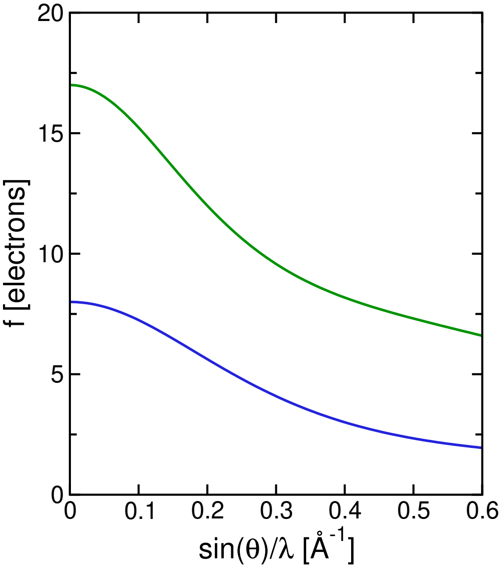

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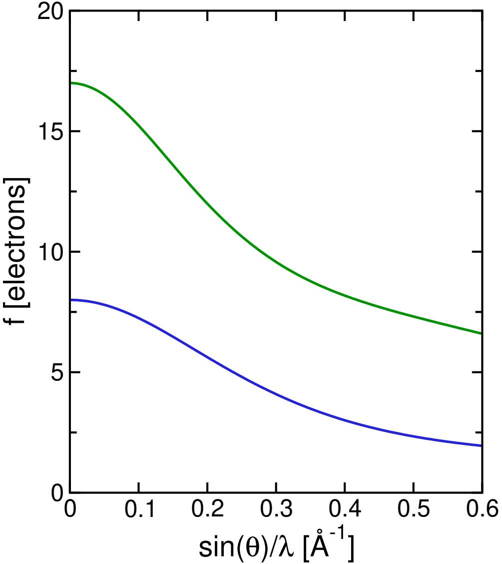

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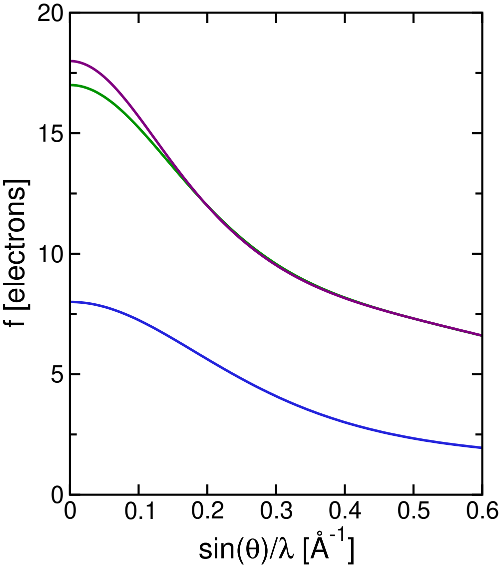

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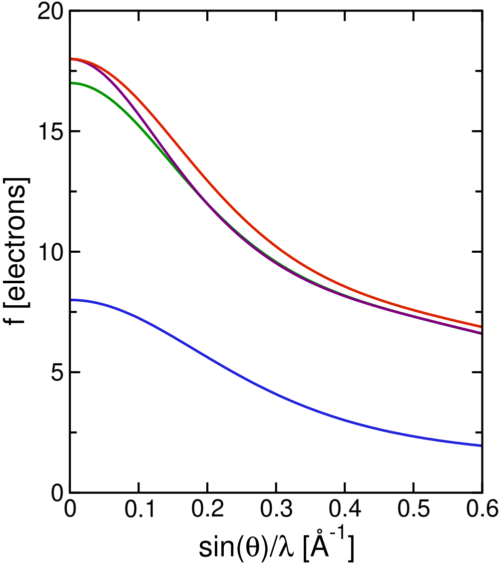

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polarization factor $$P = \begin{cases} 1 \\ \sin^2\Psi \\ \frac{1}{2}(1+\sin^2\Psi) \end{cases}$$

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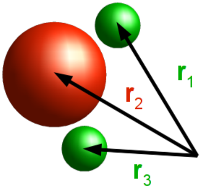

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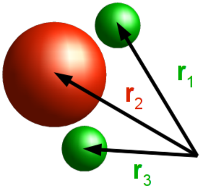

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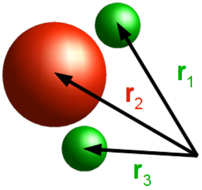

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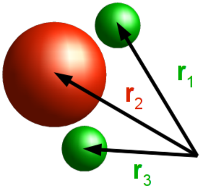

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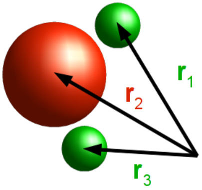

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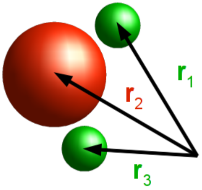

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and similarly, to a crystal lattice ...

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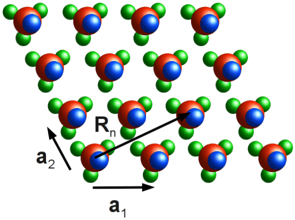

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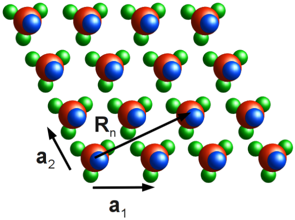

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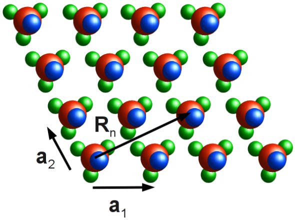

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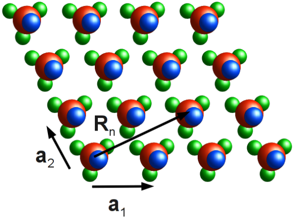

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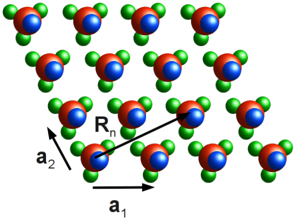

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The lattice term, $\sum e^{i\mathbf{Q}\cdot\mathbf{R}_n}$, is a sum over a large number so it is always small unless $\mathbf{Q}\cdot\mathbf{R}_n = 2\pi m$ where $\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$ is a real space lattice vector and m is an integer.