Chapter 2

RADIATION AND SCATTERING
AT EUV AND SOFT
X-RAY WAVELENGTHS

\[
\frac{dP}{d\Omega} = \frac{e^2 |a|^2 \sin^2 \Theta}{16 \pi^2 \epsilon_0 c^3} \quad (2.34)
\]

\[
r_e = \frac{e^2}{4\pi \epsilon_0 mc^2} \quad (2.44)
\]

\[
\sigma_e = \frac{8\pi}{3} r_e^2 \quad (2.45)
\]

\[
\sigma = \frac{8\pi}{3} r_e^2 \frac{\omega^4}{(\omega^2 - \omega_s^2)^2 + (\gamma \omega)^2} \quad (2.51)
\]

\[
f(\Delta k, \omega) = \sum_{s=1}^{Z} \frac{\omega^2 e^{-i\Delta k \cdot \Delta r_s}}{\omega^2 - \omega_s^2 + i\gamma \omega} \quad (2.66)
\]

\[
f^0(\omega) = \sum_{s=1}^{Z} \frac{\omega^2}{\omega^2 - \omega_s^2 + i\gamma \omega} \quad (2.72)
\]
Maxwell’s Equations

Wave Equation

- Radiation by a single electron (“dipole radiation”)
- Scattering cross-sections
- Scattering by a free electron (“Thomson scattering”)
- Scattering by a single bound electron (“Rayleigh scattering”)
- Scattering by a multi-electron atom
- Atomic “scattering factors”, $f_0'$ and $f_0''$

- Refractive index with many atoms present
- Role of forward scattering
- Contributions to refractive index by bound electrons
- Refractive index for soft x-rays and EUV
  \[ n = 1 - \delta + i\beta \quad (\delta, \beta << 1) \]
  
  \[ f_0' \quad f_0'' \]
- Determining $f_0'$ and $f_0''$; measurements and Kramers-Kronig
- Total external reflection
- Reflectivity vs. angle

Chapter 3

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Scattering, Refraction, and Reflection

Single scatterer, electron or atom, in vacuum.  (Chapter 2)

Many atoms, each with many electrons, constituting a “material”.  (Chapter 3)

- How are scattering, refraction, and reflection related?
- How do these differ for amorphous and ordered (crystalline) materials?
- What is the role of forward scattering?
Maxwell’s equations:

\[ \nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} \quad \text{(Ampere’s law)} \quad (2.1) \]

\[ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \quad \text{(Faraday’s law)} \quad (2.2) \]

\[ \nabla \cdot \mathbf{B} = 0 \quad \text{(2.3)} \]

\[ \nabla \cdot \mathbf{D} = \rho \quad \text{(Coulomb’s law)} \quad (2.4) \]

\[ \mathbf{D} = \epsilon_0 \mathbf{E} \quad (2.5) \]

\[ \mathbf{B} = \mu_0 \mathbf{H} \quad (2.6) \]

The wave equation:

\[ \left( \frac{\partial^2}{\partial t^2} - c^2 \nabla^2 \right) \mathbf{E}_T(\mathbf{r}, t) = -\frac{1}{\epsilon_0} \frac{\partial \mathbf{J}_T(\mathbf{r}, t)}{\partial t} \quad (3.1) \]
From Maxwell’s Equations, take the curl of equation 2.2

\[ \nabla \times \nabla \times E = -\frac{\partial B}{\partial t} \]  

(2.2)

and use the vector identity from Appendix D.1, pg. 440,

\[ \nabla \times (\nabla \times A) = \nabla (\nabla \cdot A) - \nabla^2 A \]  

(D.7)

to form the Wave Equation

\[
\left( \frac{\partial^2}{\partial t^2} - c^2 \nabla^2 \right) E(r, t) = -\frac{1}{\varepsilon_0} \left[ \frac{\partial J(r, t)}{\partial t} + c^2 \nabla \rho(r, t) \right] 
\]  

(2.7)

where

\[ c \equiv \frac{1}{\sqrt{\varepsilon_0 \mu_0}} \]  

(2.8)

where \( J(r,t) \) is the current density in vacuum and \( \rho \) is the charge density:

\[ J(r,t) = qn(r,t)v(r,t) \]  

(2.10)

For transverse waves the Wave Equation reduces to

\[
\left( \frac{\partial^2}{\partial t^2} - c^2 \nabla^2 \right) E_T(r, t) = -\frac{1}{\varepsilon_0} \frac{\partial J_T(r, t)}{\partial t} 
\]  

(3.1)
Conservation of Charge

\[ \nabla \cdot \nabla \times \mathbf{H} = \frac{\partial}{\partial t} \left( \nabla \cdot \mathbf{D} + \nabla \cdot \mathbf{J} \right) \]

Vector identity: \[ \nabla \cdot (\nabla \times \mathbf{H}) \equiv 0 \] \hspace{1cm} (D.9)

\[ \nabla \cdot \mathbf{J} + \frac{\partial \rho}{\partial t} = 0 \] \hspace{1cm} (2.9)

where the current density is

\[ \mathbf{J}(\mathbf{r}, t) = q n(\mathbf{r}, t) v(\mathbf{r}, t) \] \hspace{1cm} (2.10)
To obtain Poynting’s Theorem, begin with Maxwell’s Equations and form the difference

\[ \mathbf{H} \cdot [\text{Eq. (2.2)}] - \mathbf{E} \cdot [\text{Eq. (2.1)}] \]

To obtain

\[ \mathbf{H} \cdot (\nabla \times \mathbf{E}) - \mathbf{E} \cdot (\nabla \times \mathbf{H}) = -\mathbf{H} \cdot \frac{\partial \mathbf{B}}{\partial t} - \mathbf{E} \cdot \frac{\partial \mathbf{D}}{\partial t} - \mathbf{E} \cdot \mathbf{J} \]

Use \( \mathbf{B} = \mu_0 \mathbf{H} \) and \( \mathbf{D} = \epsilon_0 \mathbf{E} \), and the vector identity

\[ \nabla \cdot (\mathbf{A} \times \mathbf{B}) = \mathbf{B} \cdot (\nabla \times \mathbf{A}) - \mathbf{A} \cdot (\nabla \times \mathbf{B}) \), Eq. (D.5), to obtain Poynting’s Theorem:

\[ \nabla \cdot \left( \frac{\mathbf{E} \times \mathbf{H}}{S} \right) = -\frac{\partial}{\partial t} \left( \frac{\mu_0 \mathbf{H}^2}{2} \right) - \frac{\partial}{\partial t} \left( \frac{\epsilon_0 \mathbf{E}^2}{2} \right) - \mathbf{E} \cdot \mathbf{J} \quad \text{(2.27)} \]

Integrating over a volume of interest and using Gauss’ Divergence Theorem one obtains the integral form of Poynting’s Theorem

\[ \iiint_{\text{vol.}} \left( \frac{\mathbf{E} \times \mathbf{H}}{S} \right) \cdot d\mathbf{A} = -\frac{\partial}{\partial t} \iiint_{\text{vol.}} \left( \frac{\mu_0 \mathbf{H}^2}{2} + \frac{\epsilon_0 \mathbf{E}^2}{2} \right) dV - \iiint_{\text{vol.}} (\mathbf{E} \cdot \mathbf{J}) \ dV \quad \text{(2.28)} \]
Among \( E \) and \( H \), take \( \nabla \times E(r, t) = -\frac{\partial B(r, t)}{\partial t} \), with \( B = \mu_0 H \) in vacuum to obtain

\[
\nabla \times E = -\mu_0 \frac{\partial H}{\partial t}
\]

Write \( E \) and \( H \), in terms of Fourier representations

\[
E(r, t) = \int \int E_{k\omega} e^{-i(\omega t - k \cdot r)} \frac{d\omega dk}{(2\pi)^4} \quad \text{and} \quad H(r, t) = \int \int H_{k\omega} e^{-i(\omega t - k \cdot r)} \frac{d\omega dk}{(2\pi)^4}
\]

The \( \nabla \) and \( \partial/\partial t \) operates on the fields become algebraic multipliers on the Fourier-Laplace coefficients \( E_{k\omega} \) and \( H_{k\omega} \)

\[
i k \times E_{k\omega} = +i \omega \mu_0 H_{k\omega}
\]

\[
H_{k\omega} = \sqrt{\frac{\varepsilon_0}{\mu_0}} k_0 \times E_{k\omega}
\]

using the inverse transforms

\[
H(r, t) = \sqrt{\frac{\varepsilon_0}{\mu_0}} k_0 \times E(r, t) \quad (2.29)
\]

and

\[
S(r, t) = \sqrt{\frac{\varepsilon_0}{\mu_0}} |E|^2 k_0 \quad (2.31)
\]

with time average (one cycle)

\[
\bar{S} = \frac{1}{2} \sqrt{\frac{\varepsilon_0}{\mu_0}} |E|^2 k_0 \quad (2.37 \& 2.39)
\]
Radiated Fields Due to a Current $J$

To calculate the radiated fields we want to solve the wave equation for $E$ in terms of $J$. We introduce Fourier-Laplace transform methods, to algebrize the $\nabla$ and $\partial/\partial t$ operators, then integrate in $k$, $\omega$-space.

We start with the transverse wave equation:

$$\left[ \frac{\partial^2}{\partial t^2} - c^2 \nabla^2 \right] E(r, t) = -\frac{1}{\epsilon_0} \frac{\partial}{\partial t} J_T(r, t)$$

In a plane wave representation

$$E(r, t) = \int\int_{k\omega} E_{k\omega} e^{-i(\omega t - k \cdot r)} \frac{d\omega dk}{(2\pi)^4}$$

(2.12a)

where the amplitudes are

$$E_{k\omega} = \int\int_{r,t} E(r, t) e^{i(\omega t - k \cdot r)} dr \, dt$$

(2.12b)

so that

$$\partial/\partial t \rightarrow -i \omega \quad \text{and} \quad \nabla \rightarrow i k$$

In $k$, $\omega$-space, the algebrized form of the wave equation becomes

$$(\omega^2 - k^2 c^2) E_{k\omega} = \frac{-i \omega}{\epsilon_0} \cdot J_{T_{k\omega}}$$
Natural Modes of Oscillation

\[(\omega^2 - k^2 c^2) \mathbf{E}_{k\omega} = \frac{-i\omega}{\epsilon_0} \cdot \mathbf{J}_{T_{k\omega}}\]

The electromagnetic waves that naturally propagate in this medium (vacuum) correspond to finite fields \(\mathbf{E}_{k\omega}\) in the absence of a source, i.e., when \(\mathbf{J}_{T_{k\omega}} = 0\). In this case

\[
(\omega^2 - k^2 c^2) \mathbf{E}_{k\omega} = 0
\]

\[
= 0
\]

with solutions \(\omega = \pm kc\), or \(f\lambda = c\) (where \(k = 2\pi/\lambda\) and \(\omega = 2\pi f\))

Returning now to the case of interest with a finite source

\[
\mathbf{E}_{k\omega} = \frac{-i\omega}{\epsilon_0} \cdot \frac{\mathbf{J}_{T_{k\omega}}}{\omega^2 - k^2 c^2}
\]

which has an inverse transform

\[
\mathbf{E}(\mathbf{r}, t) = \int_{k} \int_{\omega} \left( -\frac{i\omega}{\epsilon_0} \right) \frac{\mathbf{J}_{T_{k\omega}} e^{-i(\omega t - k \cdot \mathbf{r})}}{(\omega^2 - k^2 c^2)} \frac{d\omega d\mathbf{k}}{(2\pi)^4}
\]

a Green’s function-like solution for \(\mathbf{E}\) in the presence of a source term \(\mathbf{J}\) in a frequency-wavenumber (energy-momentum) space. To perform the integrations we need a specific source function \(\mathbf{J}_{T_{k\omega}}\).
Current Density J Associated with an Accelerated Electron

For an oscillating point charge (size $<< \lambda$), e.g., a single electron

$$J(r, t) = -en(r, t)v(r, t) \quad \{ \begin{align*}
\delta(r) & \equiv \delta(x) \ \delta(y) \ \delta(z) \\
\delta(x) & = \begin{cases} 0 & \text{for } x \neq 0 \\ \infty & \text{for } x = 0 \\ \int_{-\infty}^{\infty} \delta(x) \, dx & = 1 
\end{cases}
\end{align*} \right.$$ (2.20)

To calculate the radiated field, as in eq.(2.19), we need an expression for $J_{k\omega}$.

Using the same Fourier-Laplace representation for the point source

$$J_{k\omega} = \int_r \int_t J(r, t)e^{i(\omega t - k \cdot r)} \, dr \, dt \quad (2.13b)$$

for the point source

$$J_{k\omega} = \int_r \int_t [-e\delta(r)v(t)]e^{i(\omega t - k \cdot r)} \, dr \, dt$$

$$J_{k\omega} = -e \int_t v(t)e^{i\omega t} \, dt \underbrace{v(\omega)}_{v(\omega)}$$

with transverse component

$$J_{k\omega} = -ev(\omega) \quad (2.21)$$

where $V_T$ is the component of $V$ perpendicular to the wave’s propagation direction $k_0$ (a unit vector).
Previously we determined that

\[ E(r, t) = \int_k \int_\omega \left( -\frac{i \omega}{\epsilon_0} \right) J_{Tk\omega} e^{-i(\omega t - k \cdot r)} \frac{d\omega \, dk}{(\omega^2 - k^2 c^2)} \frac{1}{(2\pi)^4} \quad (2.19) \]

Where now for an accelerated electron

\[ J_{Tk\omega} = -e \nu_T(\omega) \quad (2.21) \]

Then

\[ E(r, t) = \frac{i e}{\epsilon_0} \int_k \int_\omega \frac{\omega \nu_T(\omega)e^{-i(\omega t - k \cdot r)}}{\omega^2 - k^2 c^2} \frac{d\omega \, dk}{(2\pi)^4} \quad (2.22) \]

The k-integration can be performed in the complex k-plane using the Cauchy integral formula. The integrand is seen to have two poles, at \( k = \pm \omega/c \), representing incoming and outgoing waves. The integration path can be closed in the upper half plane with a semi-circle of infinite radius, which makes no contribution to the integral. The closed path then encloses a single pole, slightly displaced from the real axis, and the k-integral is readily evaluated. Details of the integration are given in Appendix E. The result of the k-integration is

\[ E(r, t) = \frac{e}{4\pi \epsilon_0 c^2 r} \int_{-\infty}^{\infty} (-i \omega)\nu_T(\omega)e^{-i\omega(t-r/c)} \frac{d\omega}{2\pi} \quad (2.24) \]

or

\[ E(r, t) = \frac{e}{4\pi \epsilon_0 c^2 r} \frac{d\nu_T(t-r/c)}{dt} \quad (2.25) \]
Combining \( \mathbf{E}(r, t) = \frac{e \mathbf{a}_T (t - r/c)}{4\pi \epsilon_0 c^2 r} \) (2.25) and \( \mathbf{S}(r, t) = \sqrt{\frac{\epsilon_0}{\mu_0}} |\mathbf{E}|^2 \mathbf{k}_0 \) (2.31)

one obtains the instantaneous power per unit area radiated by an accelerated electron

\[
\mathbf{S}(r, t) = \frac{e^2 |\mathbf{a}_T|^2}{16\pi^2 \epsilon_0 c^3 r^2} \mathbf{k}_0 \quad (2.32)
\]

\[\begin{cases}
\mathbf{k}_0, \text{ propagation direction} \\
|\mathbf{a}_T| = |\mathbf{a}| \sin \Theta
\end{cases}\]

For an angle \( \Theta \) between the direction of acceleration, \( \mathbf{a} \), and the observation direction, \( \mathbf{k}_0 \), the instantaneous power per unit area is

\[
\mathbf{S}(r, t) = \frac{e^2 |\mathbf{a}|^2 \sin^2 \Theta}{16\pi^2 \epsilon_0 c^3 r^2} \mathbf{k}_0 \quad (2.33)
\]

Noting that \( \mathbf{S} = (dP/dA)\mathbf{k}_0 \) and \( dA = r^2 \, d\Omega \), one obtains the power per unit solid angle

\[
\frac{dP}{d\Omega} = \frac{e^2 |\mathbf{a}|^2 \sin^2 \Theta}{16\pi^2 \epsilon_0 c^3} \quad (2.34)
\]

the well known “donut-shaped” radiation pattern characteristic of a radiator whose size is much smaller than the wavelength (“dipole radiation”).
The total power radiated, \( P \), is determined by integrating \( S \) over the area of a distant sphere:

\[
P = \iiint \mathbf{S} \cdot d\mathbf{A} = \iiint \mathbf{S} \cdot (r^2 \, d\Omega \, \mathbf{k}_0)
\]  

(2.35)

where for \( 0 \leq \Theta \leq \pi \) and \( 0 \leq \phi \leq 2\pi \) we have \( d\Omega = \sin \Theta \, d\Theta \, d\phi \), thus

\[
P = \iiint \left[ \frac{e^2 |\mathbf{a}|^2 \sin^2 \Theta}{16\pi^2 \varepsilon_0 c^3 r^2} \mathbf{k}_0 \right] \cdot r^2 \sin \Theta \, d\Theta \, d\phi \, \mathbf{k}_0
\]

\[
P = \frac{e^2 |\mathbf{a}|^2}{16\pi^2 \varepsilon_0 c^3} \int_0^{2\pi} \int_0^\pi \sin^3 \Theta \, d\Theta \, d\phi
\]

\[
\int_0^\pi (1 - \cos^2 \Theta) \sin \Theta \, d\Theta = \frac{4}{3}
\]

Thus the \textit{instantaneous power radiated} to all angles by an oscillating electron of acceleration \( \mathbf{a} \) is

\[
P = \frac{8\pi}{3} \left( \frac{e^2 |\mathbf{a}|^2}{16\pi^2 \varepsilon_0 c^3} \right)
\]  

(2.36)

For \textit{sinusoidal motion}, averaging over a full cycle, \( \sin^2 \omega t \) or \( \cos^2 \omega t \), introduces a factor of 1/2

\[
\bar{P} = \frac{1}{2} \cdot \frac{8\pi}{3} \left( \frac{e^2 |\mathbf{a}|^2}{16\pi^2 \varepsilon_0 c^3} \right)
\]

The same factor 1/2 appears in the expressions for \( S \) (eq. 2.33) and \( dP/d\Omega \) (eq.2.34) for sinusoidal motion averaged over one or many cycles.
Scattering Cross-Sections

Measures the ability of an object to remove particles or photons from a directed beam and send them into new directions.

\[ \sigma = \frac{\bar{P}_{\text{scattered}}}{|\bar{S}|} \]

Diminished by both scattering and absorption.

- Isotropic or anisotropic?
- Energy or wavelength dependent?
Define the cross-section as the average power radiated to all angles, divided by the average incident power per unit area

\[ \sigma \equiv \frac{\overline{P_{\text{scatt.}}}}{|\overline{S}_i|} \]  

(2.38)

For an incident electromagnetic wave of electric field \( \mathbf{E}_i(r,t) \)

\[ \overline{S} = \frac{1}{2} \sqrt{\frac{\epsilon_0}{\mu_0}} |\mathbf{E}_i|^2 \mathbf{k}_0 \]  

(2.39)

For a free electron the incident field causes an oscillatory motion described by Newton’s second equation of motion, \( \mathbf{F} = m\mathbf{a} \), where \( \mathbf{F} \) is the Lorentz force on the electron

\[ m\mathbf{a} = -e[\mathbf{E}_i + \mathbf{v} \times \mathbf{B}_i] \]  

(2.40)

Thus the instantaneous acceleration is

\[ \mathbf{a}(\mathbf{r}, t) = -\frac{e}{m} \mathbf{E}_i(\mathbf{r}, t) \]  

(2.42)
Scattering by a Free Electron (continued)

The average power scattered by an oscillating electron is

\[
\bar{P}_{\text{scatt.}} = \frac{1}{2} \frac{8\pi}{3} \frac{e^2}{m^2} \frac{|E_i|^2}{16\pi^2 \epsilon_0 c^3}
\]

The scattering cross-section is

\[
\sigma = \frac{\bar{P}_{\text{scatt.}}}{|\mathbf{S}|} = \frac{4\pi}{3} \left( \frac{e^4 |E_i|^2}{16\pi^2 \epsilon_0 m^2 c^3} \right) \frac{1}{\frac{1}{2} \sqrt{\frac{\epsilon_0}{\mu_0}} |E_i|^2}
\]

Introducing the “classical electron radius”

\[
\rho_e = \frac{e^2}{4\pi \epsilon_0 mc^2}
\]  
\hspace{1cm} (2.44)

One obtains the scattering cross-section for a single free electron

\[
\sigma_e = \frac{8\pi}{3} \rho_e^2
\]  
\hspace{1cm} (2.45)

which we observe is independent of wavelength. This is referred to as the Thomson cross-section (for a free electron), after J.J. Thomson. Numerically \( \rho_e = 2.82 \times 10^{-13} \text{ cm} \) and \( \sigma_e = 6.65 \times 10^{-25} \text{ cm}^2 \). The differential Thomson scattering cross-section is

\[
\frac{d\sigma_e}{d\Omega} \equiv \frac{1}{|\mathbf{S}_i|} \frac{d\bar{P}}{d\Omega} = \rho_e^2 \sin^2 \Theta
\]  
\hspace{1cm} (2.47)
Scattering by a Bound Electron

For an electromagnetic wave incident upon a bound electron of resonant frequency $\omega_s$, the force equation can be written semi-classically as

$$m \frac{d^2x}{dt^2} + m \gamma \frac{dx}{dt} + m \omega_s^2 x = -e (E_i + v \times B_i)$$  \hspace{1cm} (2.48)

with an acceleration term ($ma$), a damping term, a restoring force term, and the Lorentz force exerted by the fields. For an incident electric field $E = E_i e^{-i\omega t}$

the harmonic motion will be driven at the same frequency, $\omega$, so that

$$x = \frac{1}{\omega^2 - \omega_s^2 + i \gamma \omega} \frac{e E_i}{m}$$  \hspace{1cm} (2.49)

$$a = \frac{-\omega^2}{\omega^2 - \omega_s^2 + i \gamma \omega} \frac{e E_i}{m}$$  \hspace{1cm} (2.50)

Following the same procedures used earlier, one obtains the scattering cross-section for a bound electron of resonant frequency, $\omega_s$

$$\sigma = \frac{8\pi}{3} r_e^2 \frac{\omega^4}{(\omega^2 - \omega_s^2)^2 + (\gamma \omega)^2}$$  \hspace{1cm} (2.51)
Semi-Classical Scattering Cross-Section for a Bound Electron

\[ \sigma = \frac{8\pi r_e^2}{3} \frac{\omega^4}{(\omega^2 - \omega_s^2)^2 + (\gamma \omega)^2} \]  

(2.51)

Note that below the resonance, for \( \omega^2 << \omega_s^2 \)

\[ \sigma_R = \frac{8\pi}{3} r_e^2 \left( \frac{\omega}{\omega_s} \right)^4 = \frac{8\pi}{3} r_e^2 \left( \frac{\lambda_s}{\lambda} \right)^4 \]  

(2.52)

This is the Rayleigh scattering cross-section (1899) for a bound electron, with \( \omega/\omega_s << 1 \), which displays a very strong \( \lambda^{-4} \) wavelength dependence.
The sky appears blue because of the strong wave length dependence of scattering by bound electrons.

\[ \sigma_R \approx \sigma_T \left( \frac{\lambda_S}{\lambda} \right)^4 \]

- UV resonances in O$_2$ and N$_2$, at 8.6 and 8.2 eV
- Red (1.8 eV, 700 nm), green (2.3 eV, 530 nm), and blue light (3.3 eV, 380 nm)
- Density fluctuations essential
- Long path at sunset, color of clouds
- Photon energy and wavelength effects. Volcanic eruptions
Scattering by a Multi-Electron Atom

Semi-classical model of an atom with \( Z \) electrons and nucleus of charge \(+Ze\) at \( r = 0\).

\[
n(r, t) = \sum_{s=1}^{Z} \delta[r - \Delta r_s(t)] \quad (2.53)
\]

For each electron

\[
m \frac{d^2 \mathbf{x}_s}{dt^2} + m \gamma \frac{d \mathbf{x}_s}{dt} + m \omega_s^2 \mathbf{x}_s = -e (\mathbf{E}_i + \mathbf{v}_s \times \mathbf{B}) \quad (2.58)
\]

The acceleration has an additional phase term due to the position, \( \Delta r_s \), within the atom:

\[
\mathbf{a}_s(t) = \frac{-\omega^2}{\omega^2 - \omega_s^2 + i \gamma \omega} \frac{e}{m} \mathbf{E}_i e^{-i(\omega t - \mathbf{k}_i \cdot \Delta r_s)} \quad (2.61)
\]

The scattered electric field at a distance \( r \) summed for all \( Z \) electrons, is

\[
E(r, t) = -\frac{e^2}{4\pi \varepsilon_0 mc^2} \sum_{s=1}^{Z} \frac{\omega^2 E_i \sin \Theta}{\omega^2 - \omega_s^2 + i \gamma \omega} \frac{1}{r_s} e^{-i[\omega(t - r_s/c) - \mathbf{k}_i \cdot \Delta r_s]} \quad (2.62)
\]

where \( r_s \equiv r - \Delta r_s \) and \( r_s = |r_s| \). For \( r >> \Delta r_s \), \( r_s \approx r - k_0 \cdot \Delta r_s \).
where the quantity \( f(\Delta k, \omega) \) is the complex atomic scattering factor, which tells us the scattered electric field due to a multi-electron atom, relative to that of a single free electron (eq. 2.43). Note the dependence on frequency \( \omega \) (photon energy \( \hbar \omega \)), the various resonant frequencies \( \omega_s \) (resonant energies \( \hbar \omega_s \)), and the phase terms due to the various positions of electrons within the atom, \( \Delta k \cdot \Delta r_s \).
A General Scattering Diagram

\[ \mathbf{J}(r,t) = -e^{n(r,t)} \mathbf{v}(r,t) \quad (2.10) \]

\[ \mathbf{J}_{\text{scat}} e^{-i(\omega_s t - \mathbf{k}_s \cdot \mathbf{r})} = -ef^0(\omega_i)n_d e^{-i(\omega_d t - \mathbf{k}_d \cdot \mathbf{r})} \frac{-eE_i}{-i\omega_im} e^{-i(\omega_i t - \mathbf{k}_i \cdot \mathbf{r})} \]

matching exponents

\[ \omega_s = \omega_i + \omega_d \]

\[ \mathbf{k}_s = \mathbf{k}_i + \mathbf{k}_d \]

\[ |\mathbf{k}_d| = 2\pi/d \text{ represents a spatial non-uniformity in the medium, such as atoms of periodicity } d, \text{ a grating, or a density distribution due to a wave motion.} \]

If the density distribution is stationary

\[ |\mathbf{k}_i| = \frac{\omega}{c} = \frac{2\pi}{\lambda} \]

\[ |\mathbf{k}_s| = \frac{\omega}{c} = \frac{2\pi}{\lambda} \]

\[ \therefore \text{ the scattering diagram is isosceles} \]

\[ \mathbf{k}_i + \mathbf{k}_d = \mathbf{k}_s \]

\[ \sin\theta = \frac{k_d/2}{k_i} \]

\[ \lambda = 2d \sin\theta \quad (2.62) \]

(Bragg’s Law, 1913)

(Reference: See chapter 4, eqs. 4.1 to 4.6)
The Atomic Scattering Factor

\[ f(\Delta k, \omega) = \sum_{s=1}^{Z} \frac{\omega^2 e^{-i\Delta k \cdot \Delta r_s}}{\omega^2 - \omega_s^2 + i\gamma \omega} \]  \hspace{1cm} (2.66)

In general the \( \Delta k \cdot \Delta r_s \) phase terms do not simplify, but in two cases they do. Noting that \(|\Delta k| = 2k_1 \sin \theta = 4\pi/\lambda \sin \theta\), and that the radius of the atom is of order the Bohr radius, \( a_0 \), the phase factor is then bounded by

\[ |\Delta k \cdot \Delta r_s| \leq \frac{4\pi a_0}{\lambda} \sin \theta \] \hspace{1cm} (2.70)

The atomic scattering factor \( f(\Delta k, \omega) \) simplifies significantly when

\[ |\Delta k \cdot \Delta r_s| \to 0 \quad \text{for} \quad a_0/\lambda \ll 1 \quad \text{(long wavelength limit)} \] \hspace{1cm} (2.71a)

\[ |\Delta k \cdot \Delta r_s| \to 0 \quad \text{for} \quad \theta \ll 1 \quad \text{(forward scattering)} \] \hspace{1cm} (2.71b)

In each of these two cases the atomic scattering factor \( f(\Delta k, \omega) \) reduces to

\[ f^0(\omega) = \sum_{s=1}^{Z} \frac{\omega^2}{\omega^2 - \omega_s^2 + i\gamma \omega} \] \hspace{1cm} (2.72)

where we denote these special cases by the superscript zero.
Comparing the scattered electric field for a multi-electron atom (2.65) with that for the free electron (2.43), the atomic scattering cross-sections are readily determined by the earlier procedures to be

\[
\frac{d\sigma(\omega)}{d\Omega} = r_e^2 |f^0(\omega)|^2 \sin^2 \Theta
\]  

(2.75)

\[
\sigma(\omega) = \frac{8\pi}{3} r_e^2 |f^0(\omega)|^2
\]  

(2.76)

where

\[
f^0(\omega) = \sum_s \frac{g_s \omega^2}{\omega^2 - \omega_s^2 + i\gamma \omega}
\]  

(2.77)

and where the super-script zero refers to the special circumstances of long wavelength (\(\lambda >> a_0\)) or forward scattering (\(\theta << 1\)). With the Bohr radius \(a_0 = 0.529\ \text{Å}\), the long wavelength condition is easily satisfied for soft x-rays and EUV. Note too that we have introduced the concept of oscillator strengths, \(g_s\), associated with each resonance, normalized by the condition

\[
\sum_s g_s = Z
\]  

(2.73)
Example: Complex Atomic Scattering Factor for Carbon

\[ f^0(\omega) = f_1^0(\omega) - i f_2^0(\omega) \]  \hspace{1cm} (2.79)

Note that for \( \hbar \omega \gg \hbar \omega_s \), \( f_1^0 \rightarrow Z \). This works here for carbon \( f_1^0 \rightarrow 6 \), but note that in general this conflicts with the condition \( \lambda \gg a_0 \). For the case of carbon at 4 Å wavelength (\( \lambda \gg a_0 \)), and thus \( \hbar \omega = 3 \text{ keV} \) (\( \gg \hbar \omega_s \approx 274 \text{ eV} \)), the atomic scattering cross-section (2.76) becomes

\[ \sigma(\omega) \simeq \frac{8\pi}{3} r_e^2 Z^2 = Z^2 \sigma_e \]  \hspace{1cm} (2.78c)

that is, all \( Z \) electrons are scattering cooperatively (in-phase) - the so-called \( N^2 \) effect.
Atomic Scattering Factors for Carbon (Z = 6)

\[ \sigma_a \text{(barns/atom)} = \mu \text{(cm}^2/\text{g}) \times 19.95 \]
\[ E(\text{keV}) \mu \text{(cm}^2/\text{g}) = f_2^0 \times 3503.31 \]

<table>
<thead>
<tr>
<th>Energy (eV)</th>
<th>( f_1^0 )</th>
<th>( f_2^0 )</th>
<th>( \mu \text{ (cm}^2/\text{g}) )</th>
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<tbody>
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Edge Energies: K 284.2 eV

(Henke and Gullikson; www-cxro.LBL.gov)
Atomic Scattering Factors for Silicon (Z = 14)

\[ \sigma_a(\text{barns/atom}) = \mu(\text{cm}^2/\text{g}) \times 46.64 \]

\[ E(\text{keV})\mu(\text{cm}^2/\text{g}) = f_2^0 \times 1498.22 \]

<table>
<thead>
<tr>
<th>Energy (eV)</th>
<th>( f_1^0 )</th>
<th>( f_2^0 )</th>
<th>( \mu(\text{cm}^2/\text{g}) )</th>
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Silicon (Si)

\[ Z = 14 \]

Atomic weight = 28.086

\( f_1^0 \) vs. \( E \) (eV)

\( f_2^0 \) vs. \( E \) (eV)

\( \mu \) (cm²/g) vs. \( E \) (eV)

Edge Energies: K 1838.9 eV L₁ 149.7 eV L₂ 99.8 eV L₃ 99.2 eV

(Henke and Gullikson; www-cxro.LBL.gov)
### Atomic Scattering Factors for Molybdenum (Z = 42)

\[ \sigma_0(\text{barns/atom}) = \mu(\text{cm}^2/\text{g}) \times 159.31 \]

\[ E(\text{keV}) \mu(\text{cm}^2/\text{g}) = f_2^0 \times 438.59 \]

<table>
<thead>
<tr>
<th>Energy (eV)</th>
<th>( f_1^0 )</th>
<th>( f_2^0 )</th>
<th>( \mu ) (cm(^2)/g)</th>
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<td>2.292E+04</td>
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</table>

Edge Energies:

- **K**: 19999.5 eV
- **L\(_1\)**: 2865.5 eV
- **L\(_2\)**: 2625.1 eV
- **L\(_3\)**: 2520.2 eV
- **M\(_1\)**: 506.3 eV
- **M\(_2\)**: 411.6 eV
- **M\(_3\)**: 394.0 eV
- **M\(_4\)**: 231.1 eV
- **M\(_5\)**: 227.9 eV
- **N\(_1\)**: 63.2 eV
- **N\(_2\)**: 37.6 eV
- **N\(_3\)**: 35.5 eV

(Henke and Gullikson; www-cxro.LBL.gov)