Small-Angle, Elastic Scattering from Atoms

Electrons scattered by the electrostatic potential of the nucleus, screened by the electron cloud

Most important for TEM imaging & diffraction!
Head-on elastic collision in 1-D

Two possible outcomes:

- **forward scattering**
  \[ E_{1f} = E \]
  \[ E_{2f} = 0 \]

- **back scattering**
  \[ E_{1f} \leq E \]
  \[ E_{2f} \geq 0 \]

Center-of-mass motion:

- \[ E = E_{1f} + E_{2f} \] //elastic

- \[ \nu_{\text{COM}} = \left( \frac{m}{m+M} \right) \cdot \nu \]

- \[ \nu_{1f} = \nu_{\text{COM}} \pm (\nu - \nu_{\text{COM}}) = \begin{cases} \nu & \text{forward} \\ -\left( \frac{M-m}{M+m} \right) \cdot \nu & \text{back} \end{cases} \]
Grazing-incidence elastic collision $\Rightarrow$ forward scattering

- Less-massive electron forward scattered in grazing collision
- Almost no kinetic energy transferred to atom
- Electron energy essentially unchanged $\Rightarrow$ coherent

\[ E = E_{1f} + E_{2f} \]
\[ M > m : E_{1f} \lesssim E, E_{2f} \approx 0 \]
Nearly head-on elastic collision $\Rightarrow$ backscattering

- Less-massive electron backscattered in head-on collision
- Kinetic energy transferred to atom
- Electron loses energy $\Rightarrow$ incoherent
Plane waves: sinusoidal form

We could write a plane wave as:

\[ \psi(\mathbf{r}, t) = A \cdot \cos \left[ 2\pi \mathbf{k} \cdot (\mathbf{r} - t \cdot \mathbf{v}_p) + \phi \right] \]

or

\[ \psi(\mathbf{r}, t) = A \cdot \cos \left[ 2\pi (\mathbf{k} \cdot \mathbf{r} - f \cdot t) + \phi \right] \]

wavenumber: \( k = |\mathbf{k}| = \frac{1}{\lambda} \)
Plane waves: complex exponential form

\[ \psi(r, t) = \psi_0 \cdot e^{2\pi i (k \cdot r - f \cdot t)} \]

\[ \psi_0 = A \cdot e^{i\phi} \]

Euler relation:

\[ e^{i\theta} = \cos \theta + i \sin \theta \]

For an incident plane wave, we often normalize and pick the phase:

\[ A = 1 \quad \phi = 0 \quad \psi_0 = 1 \]

\[ \Rightarrow \psi(r, t) = e^{2\pi i (k \cdot r - f \cdot t)} \]
Consider a plane wave: \[ \psi(r, t) = \psi_0 \cdot e^{2\pi i (k \cdot r - \omega t)} \]

\[ p = |\mathbf{p}| = \frac{h}{\lambda} \quad \text{p} = \hbar \mathbf{k} \quad \text{//de Broglie} \]

\[ \hat{p} \cdot \psi(r, t) = (\hbar \mathbf{k}) \cdot \psi(r, t) = -i\hbar \hat{\nabla} \psi(r, t) \]

\[ \nabla = \frac{\partial}{\partial x} \hat{x} + \frac{\partial}{\partial y} \hat{y} + \frac{\partial}{\partial z} \hat{z} \quad \text{//gradient} \]

\[ \hat{p} = -i\hbar \hat{\nabla} \quad \text{//momentum operator} \]

\[ E = hf \quad \text{//from photoelectric effect} \]

\[ \hat{E} \cdot \psi(r, t) = (hf) \cdot \psi(r, t) = i\hbar \frac{\partial}{\partial t} \psi(r, t) \]

\[ \hat{E} = i\hbar \frac{\partial}{\partial t} \quad \text{//energy operator} \]
Schrodinger equation

For a free, non-relativistic particle:

\[ \hat{H} = \frac{\hat{p}^2}{2m_0} = \frac{-\hbar^2}{2m_0} \nabla^2 \]

//Hamiltonian operator

\[ \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \]

//Laplacian

\[ \psi(\mathbf{r}, t) = \psi_0 \cdot e^{2\pi i (\mathbf{k} \cdot \mathbf{r} - \omega t)} \] //plane wave

Observe:

\[ \hat{H}\psi(\mathbf{r}, t) = E\psi(\mathbf{r}, t) \] //plane wave is an energy eigenfunction

\[ \hat{H}\psi(\mathbf{r}, t) = i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) \] //Schrodinger equation

In a potential:

\[ \hat{H} = \frac{\hat{p}^2}{2m_0} + U(\mathbf{r}) = \frac{-\hbar^2}{2m_0} \nabla^2 + U(\mathbf{r}) \]

The SE uses energy to relate the time and space dependences of the wave function.
Energy eigenstates

Plane wave: \[ \psi(r, t) = \psi_0 \cdot e^{2\pi i (k \cdot r - \omega t)} = \psi(r) \cdot e^{-iEt/\hbar} \]

Schrodinger Equation: \[ \hat{H} \psi(r, t) = i\hbar \frac{\partial}{\partial t} \psi(r, t) \]

Time-independent Hamiltonian - acts on \( r \) only: 
Energy operator - acts on \( t \) only:

\[ \left[ \hat{H} \psi(r) \right] \cdot e^{-iEt/\hbar} = E \cdot \psi(r) \cdot e^{-iEt/\hbar} \]

\[ \hat{H} \psi(r) = E \cdot \psi(r) \]

The time-independent part satisfies the time-independent SE:

These are energy eigenstates, i.e., states with constant energy.

So our plane wave is described completely as: \[ \psi(r) = \psi_0 \cdot e^{2\pi i k \cdot r} \]
Spherical waves

Surface area of a sphere: \( 4\pi r^2 \)

No unique direction of wavevector

Intensity = \( \frac{\text{Power}}{\text{Area}} \)

Intensity of wave function \( \propto \) probability density

\[
I = |\psi|^2 = \psi^* \psi \propto \frac{1}{r^2}
\]

\[
\psi \propto \frac{\mathrm{e}^{2\pi i kr}}{r}
\]
Atomic Scattering Factor

Spherical Scattered Wave

Elastic scattering: $|k'| = |k| = k$

Amplitude depends on scattering angle.

incident wave: scattered wave:

$$\psi_i (r) = e^{2\pi i k \cdot r} \quad \psi_{sc} (r) = f(\theta) \cdot \frac{e^{2\pi i kr}}{r}$$

$f(\theta)$: atomic scattering (form) factor

Smoothly varying functions of scattering angle.

Units of Length Increases with $Z$
Weak Phase-Object Approximation

Assume the only effect of scattering is a slight change in phase of the wave function:

\[ \psi_f = \psi_i \cdot e^{i\phi} = \psi_i \cdot (\cos \phi + i \sin \phi) \approx \psi_i \cdot (1 + i\phi) = \psi_i + i\psi_{sc} \]

Weak-phase scattering by atoms:

\[ \psi_f (r) \approx \psi_i (r) + i\psi_{sc} (r) \]

\[ \psi_f (r) = e^{2\pi i k \cdot r} + i f(\theta) e^{2\pi i kr} \]

//Scattered wave is spherical
Solid-angle projections

Differential solid angle:
\[ d\Omega = \sin \theta \cdot d\theta \cdot d\phi \]

Annular differential solid angle:
\[ d\Omega_\theta = \int_{\phi=0}^{2\pi} d\Omega = 2\pi \cdot \sin \theta \cdot d\theta \]
Differential Cross Section:

$$\frac{d\sigma}{d\Omega} = \frac{1}{\sin \theta} \cdot \frac{d\sigma}{d\theta \cdot d\phi}$$

scattering cross-section per unit solid angle

$$d\sigma_\theta = \sin \theta \cdot d\theta \cdot \int_{\phi=0}^{2\pi} d\phi \cdot \frac{d\sigma}{d\Omega}$$

Axial symmetry (atoms): $\frac{d\sigma}{d\Omega} = \frac{d\sigma}{d\Omega}(\theta)$

$$d\sigma_\theta = 2\pi \cdot \sin \theta \cdot d\theta \cdot \frac{d\sigma}{d\Omega}$$

Common Form: $\frac{d\sigma}{d\Omega} = \frac{1}{2\pi \cdot \sin \theta} \cdot \frac{d\sigma_\theta}{d\theta}$
Total cross-section forms

\[
\sigma_{\text{tot}} = \int d\sigma
\]

\[
= \int d\Omega \cdot \left(\frac{d\sigma}{d\Omega}\right)
\]

\[
\sigma_{\text{tot}} = \int_{\phi=0}^{2\pi} d\phi \cdot \int_{\theta=0}^{\pi} \sin \theta \cdot d\theta \cdot \left(\frac{d\sigma}{d\Omega}\right)
\]

Azimuthal symmetry:

\[
\sigma_{\text{tot}} = 2\pi \cdot \int_{\theta=0}^{\pi} \sin \theta \cdot d\theta \cdot \left(\frac{d\sigma}{d\Omega}\right)
\]

\[
\sigma_{\text{tot}} = \int_{\theta=0}^{\pi} d\theta \cdot \left(\frac{d\sigma_{\theta}}{d\theta}\right)
\]

Total scattering into angles less than \(\theta\):

\[
\sigma_{<}(\theta) = 2\pi \int_{\theta'=0}^{\theta} \sin \theta' d\theta' \cdot \left(\frac{d\sigma}{d\Omega}\right)
\]

\[
\sigma_{<}(\theta) = \int_{\theta'=0}^{\theta} d\theta' \cdot \left(\frac{d\sigma_{\theta}}{d\theta}\right)
\]

Total scattering into angles greater than \(\theta\):

\[
\sigma_{>}(\theta) = 2\pi \int_{\theta'=\theta}^{\pi} \sin \theta' d\theta' \cdot \left(\frac{d\sigma}{d\Omega}\right)
\]

\[
\sigma_{>}(\theta) = \int_{\theta'=\theta}^{\pi} d\theta' \cdot \left(\frac{d\sigma_{\theta}}{d\Omega}\right)
\]
Cross-section problems

One Type of Problem:

\[
\frac{d\sigma}{d\Omega}(\theta) \Rightarrow \sigma_<(\theta)
\]

\[
\sigma_<(\theta) = 2\pi \cdot \int_{\theta'=0}^{\theta} \left( \frac{d\sigma}{d\Omega} \right) \cdot \sin \theta' \cdot d\theta'
\]

Example:

\[
\frac{d\sigma}{d\Omega} = A \cdot \cos \left( \frac{\theta}{2} \right)
\]

\[
\sigma_<(\theta) = 2\pi \cdot A \cdot \int_{\theta'=0}^{\theta} \cos \left( \frac{\theta'}{2} \right) \cdot \sin \theta' \cdot d\theta'
\]

\[
= 4\pi \cdot A \cdot \int_{\theta'=0}^{\theta} \sin^2 \left( \frac{\theta'}{2} \right) \cdot \cos \left( \frac{\theta'}{2} \right) \cdot d\theta'
\]

\[
= \frac{4\pi}{3} \cdot A \cdot \sin^3 \left( \frac{\theta}{2} \right) \bigg|_{\theta'=0}^{\theta}
\]

\[
\Rightarrow \sigma_<(\theta) = \frac{4\pi}{3} \cdot A \cdot \sin^3 \left( \frac{\theta}{2} \right)
\]

Note: \( \sigma_{tot} = \sigma_<(\pi) \)

Another Type of Problem:

\[
\sigma_<(\theta) \Rightarrow \frac{d\sigma}{d\Omega}(\theta)
\]

\[
\frac{d\sigma}{d\Omega}(\theta) = \frac{1}{2\pi \cdot \sin \theta \cdot d\theta} [\sigma_<(\theta)]
\]

Example:

\[
\sigma_<(\theta) = \sigma_{tot} \cdot \sin \left( \frac{\theta}{2} \right)
\]

\[
\frac{d\sigma}{d\Omega} = \frac{\sigma_{tot}}{2\pi \cdot \sin \theta \cdot d\theta} [\sin \left( \frac{\theta}{2} \right)]
\]

\[
= \frac{\sigma_{tot}}{2\pi \cdot \sin \theta} \cdot \left[ \frac{1}{2} \cos \left( \frac{\theta}{2} \right) \right]
\]

\[
\Rightarrow \frac{d\sigma}{d\Omega} = \frac{\sigma_{tot}}{8\pi \cdot \sin \left( \frac{\theta}{2} \right)}
\]
Interpreting differential cross-section

Side view

Top view

Uniform, hard sphere
Scattering cross-section: hard sphere (I)

Relate angles:

$180^\circ - \theta = 2 \cdot (90^\circ - \alpha) \Rightarrow \theta = 2\alpha$

Differential elements:

$d\sigma = -db \cdot (b \cdot d\phi)$

$d\Omega = \sin \theta \cdot d\theta \cdot d\phi$

Differential cross-section:

$\frac{d\sigma}{d\Omega} = -\frac{b}{\sin \theta} \cdot \frac{db}{d\theta}$

In terms of $\theta$ only:

$b = R \cdot \cos \alpha = R \cdot \cos(\theta/2)$

$\frac{db}{d\theta} = -\frac{R}{2} \cdot \sin(\theta/2)$

$\frac{d\sigma}{d\Omega} = \frac{R \cdot \cos(\theta/2)}{\sin \theta} \cdot \frac{R \cdot \sin(\theta/2)}{2} = \frac{R^2}{4}$

$\sigma_{tot} = \int_0^{2\pi} \int_0^{\pi/2} \frac{R^2}{4} \sin \theta \cdot d\theta \cdot d\phi = \pi \cdot R^2$

Azimuthal ($\phi$) sum (annulus):

$\frac{d\sigma_\phi}{d\theta} = 2\pi \cdot \sin \theta \cdot \frac{d\sigma}{d\Omega} = \frac{\pi R^2}{2} \sin \theta$

Scattering into angles less than $\theta$:

$\sigma_<(\theta) = \int_0^\theta \int_0^{\pi/2} \left( \frac{d\sigma_\phi}{d\theta} \right) d\theta' \cdot \left( \frac{db}{d\theta} \right)$

$= \int_0^\theta \int_0^{\pi/2} \left( \frac{\pi R^2}{2} \cdot \sin \theta' \right) d\theta'$

$= -\frac{\pi R^2}{2} \cdot \cos \theta |_{\theta'=0}^{\theta'=0} = \frac{\pi}{2} \cdot R^2 \cdot \cos \theta |_{\theta'=0}^{\theta'=0}$

$\sigma_<(\theta) = \frac{\pi R^2}{2} \cdot (1 - \cos \theta)$

$\Rightarrow \sigma_{tot} = \sigma_<(\pi) = \pi \cdot R^2 \quad \text{as expected!}$
Scattering Cross-Section: Hard Sphere (II)

\[ \sigma_{\text{tot}} = \sigma_\text{\<}(\theta) + \sigma_\text{\>}(\theta) \]

\[ \frac{\pi R^2}{2} \]

\[ d\sigma_\theta \quad d\theta \]

largest solid angle

\[ \theta(\degree) \]

\[ \theta(\degree) \]
Electric current in scattered wave (l)

\[ n_{sc} (\mathbf{r}, t) = -e \cdot |\psi_{sc} (\mathbf{r}, t)|^2 = -e \cdot \psi^*_{sc} \psi_{sc} \quad \text{elect} \text{ron "concentration"} \]

\[ \frac{\partial}{\partial t} n_{sc} (\mathbf{r}, t) = -e \cdot \frac{\partial}{\partial t} \left( \psi^*_{sc} \psi_{sc} \right) = -e \cdot \left[ \left( \frac{\partial}{\partial t} \psi^*_{sc} \right) \cdot \psi_{sc} + \psi^*_{sc} \cdot \left( \frac{\partial}{\partial t} \psi_{sc} \right) \right] \quad \text{time rate of change} \]

\[ \frac{\partial}{\partial t} \psi = \frac{1}{i\hbar} \left( \frac{-\hbar^2}{2m} \nabla^2 \right) \psi = \frac{i\hbar}{2m} \cdot \nabla^2 \psi \quad \frac{\partial}{\partial t} \psi^* = \left( \frac{\partial}{\partial t} \psi \right)^* = \frac{-i\hbar}{2m} \cdot \nabla^2 \psi^* \quad \text{use Schodinger's eqn.} \]

\[ \frac{\partial}{\partial t} n_{sc} (x, t) = -e \cdot \left[ \left( \frac{-i\hbar}{2m} \cdot \nabla^2 \psi^*_{sc} \right) \cdot \psi_{sc} + \psi^*_{sc} \cdot \left( \nabla^2 \psi_{sc} \right) \right] \]

\[ = \nabla \cdot \left[ \frac{i\hbar}{2m} \cdot \left( \psi^*_{sc} \cdot \nabla \psi_{sc} - \nabla \psi^*_{sc} \cdot \psi_{sc} \right) \right] \quad \text{result} \]

\[ \frac{\partial}{\partial t} n_{sc} (x, t) = \nabla \cdot \mathbf{j}_{sc} \quad \text{continuity eqn.} \quad \mathbf{j}_{sc} = \frac{i\hbar}{2m} \cdot \left( \psi_{sc} \cdot \nabla \psi^*_{sc} - \psi^*_{sc} \cdot \nabla \psi_{sc} \right) \quad \text{current} \]
Electric current in scattered wave (II)

\[ \psi_i (\mathbf{r}) = \psi_0 \cdot e^{2\pi i k \cdot \mathbf{r}} \quad // \text{incident plane wave} \]

\[ \psi_{sc} (\mathbf{r}) = \psi_0 \cdot f(\theta) \cdot \frac{e^{2\pi i kr}}{r} \quad // \text{scattered wave} \]

\[ \left[ n_{sc} (\mathbf{r}) \right] = \left[ |\psi_0|^2 \right] = \frac{1}{\text{volume}} \quad // \text{units} \]

\[ j_0 = e \cdot v \cdot |\psi_0|^2 \quad // \text{incident current density} \]

\[ \nabla \psi_{sc} = \psi_0 \cdot \left\{ if(\theta) \left[ 2\pi k \frac{1}{r} \right] \cdot \hat{r} + i \frac{df}{d\theta} \cdot \hat{\theta} \right\} \cdot \frac{e^{2\pi i kr}}{r} \quad // \text{gradient} \]

\[ \mathbf{j}_{sc} = \frac{j_0}{r^2} \cdot |f(\theta)|^2 \cdot \hat{r} \quad // \text{scattered current density} \]

\[ dI_{sc} = j_0 \cdot d\sigma \quad // \text{electric current in scattering cross-sectional area} \]

\[ \mathbf{j}_{sc} = \frac{dI_{sc}}{r^2 \cdot d\Omega} \cdot \hat{r} = \frac{j_0}{r^2} \cdot \frac{d\sigma}{d\Omega} \cdot \hat{r} \quad // \text{scattered current density} \quad \rightarrow \quad \frac{d\sigma}{d\Omega} = |f(\theta)|^2 \]
Scattering Amplitude

Consider the interference between the incident wave and a scattered wave:

Scattering amplitude:
\[ f (k', k) = \sum_{j=1}^{N} F_j e^{2\pi i \Delta \phi_j} \]

Path-length difference:
\[ \Delta \ell_j = (\hat{k}' - \hat{k}) \cdot r_j \]

Phase difference:
\[ \Delta \phi_j = 2\pi \left( \frac{\Delta \ell_j}{\lambda} \right) = 2\pi \cdot (k' - k) \cdot r_j \]

Rewrite:
\[ f (k' - k) = \sum_{j=1}^{N} F_j e^{2\pi i (k' - k) \cdot r_j} \]

Continuous medium:
\[ f (k' - k) \rightarrow \int F(r) e^{2\pi i (k' - k) \cdot r} \cdot d^3r \]

The scattering amplitude is the Fourier transform of the target scattering strength.
Scattering Amplitude (Atomic Form Factor)

\[ f(k'-k) \equiv \int_{r} F(r) e^{2\pi i (k'-k) \cdot r} \cdot dr \] //scattering amplitude

Atom at origin, spherically symmetric: \( F(r) \rightarrow F(r) \)

Relate to scattering angle:

\[ |k'-k| = \frac{1}{\lambda} \sqrt{1 + 1 - 2 \cos \theta} = \frac{2 \sin(\theta/2)}{\lambda} \]

Define: \( s \equiv \frac{|k'-k|}{2} = \frac{\sin(\theta/2)}{\lambda} \) //scattering parameter

\[ f(s) \equiv 4\pi \int_{r=0}^{\infty} r^2 \cdot F(r) \cdot \frac{\sin(4\pi sr)}{(4\pi sr)} \cdot dr \]
Computing Atomic Scattering Factors

Electron scattering factor is proportional to the Fourier transform of the electrostatic potential of the atom:

\[ F(r) = \frac{2\pi me}{h^2} \phi(r) \]  //scattering strength at radius \( r \)

\[ f_e(s) = \frac{8\pi^2 me}{h^2} \int_{r=0}^{\infty} r^2 \phi(r) \frac{\sin(4\pi sr)}{(4\pi sr)} \cdot dr \]  //scattering amplitude at \( s \)

\[ \phi(r) = \frac{Ze}{4\pi\varepsilon_0 r} - \frac{e}{4\pi\varepsilon_0 r} \left[ 4\pi \int_{r'=0}^{r} \rho(r') \cdot r'^2 \cdot dr' \right] \]  //atomic potential

X-ray scattering factor is Fourier transform of electron density.

\[ f_x(s) = 4\pi \int_{r=0}^{\infty} r^2 \rho(r) \frac{\sin(4\pi sr)}{(4\pi sr)} \cdot dr \]

The two are closely related:

\[ f_e(s) \propto \left[ Z - f_x(s) \right] \]
Electrostatic Potential of a Neutral Atom

Bare Nuclear Potential: \[ \varphi(r) = \frac{Ze}{4\pi\varepsilon_0 r} \]

Screened Nuclear Potential: \[ \varphi(r) = \frac{Z_{\text{eff}}(r) \cdot e}{4\pi\varepsilon_0 r} \]

“Effective” Charge: \[ Z_{\text{eff}}(r) = Z - Z_{\text{enc}}^{(e)}(r) \]

Enclosed Electron Charge:

\[ Z_{\text{enc}}^{(e)}(r) = \int_{|r'|<r} \rho(r') d^3 r' = 4\pi \int_{r'=0}^{r} \rho(r') \cdot (r')^2 \cdot dr' \approx Z \left(1 - e^{-r/r_0}\right) \]

Model of Screened Nuclear Potential:

\[ \varphi(r) \approx \frac{Ze}{4\pi\varepsilon_0 r} e^{-r/r_0} \]
Rutherford (Thomas-Fermi) Model

Assume: \[ \varphi(r) = \frac{Ze}{4\pi\varepsilon_0 r} e^{-r/r_0} \]

\[ \Rightarrow f_e(s) = \frac{2\pi Z e^2 m}{h^2 \varepsilon_0} \left[ \frac{1}{(4\pi s)^2 + (1/r_0)^2} \right] \] // Form factor

\[ \lim_{r_0 \to \infty} f_e(s) = \frac{Z e^2 m}{8\pi h^2 \varepsilon_0 s^2} \] // Form factor for unscreened (bare) nucleus

In terms of scattering angle:

\[ s = \frac{\sin(\theta/2)}{\lambda} \]
\[ \frac{1}{r_0} = \frac{4\pi \sin(\theta_0/2)}{\lambda} \]

\[ \Rightarrow f_e(\theta) = \frac{\lambda^2 Z e^2 m}{8\pi h^2 \varepsilon_0} \left[ \frac{1}{\sin^2(\theta/2) + \sin^2(\theta_0/2)} \right] \]
Rutherford Model (II)

\[
\frac{1}{R_c} = \frac{e^2 m}{8\pi \hbar^2 \varepsilon_0} = \alpha \cdot \frac{mc^2}{4\pi \hbar c} = \frac{1}{4.2 \text{ nm}}
\]

\[
\alpha = \frac{e^2}{2\varepsilon_0 \hbar c} \approx \frac{1}{137}
\]

//fine structure constant

\[
f_c(\theta) = \frac{\lambda^2 Z}{R_c \cdot \sin^2 \left( \frac{\theta}{2} \right) + \sin^2 \left( \frac{\theta_0}{2} \right)}
\]

Screening keeps form factor finite at origin:

\[
f_c(0) = \frac{\lambda^2 Z}{R_c \cdot \sin^2 \left( \frac{\theta_0}{2} \right)}
\]

\[
Z = 1
\]
\[
r_0 = 0.01 \text{ nm}
\]
Evaluating Form Factors

Theoretically calculated potentials have been fit to functions of the form:

$$f_e(s) = \sum_{i=1}^{3 \text{ or } 4} a_i \exp(-b_i s^2) + c$$

Note: point-charge correction added to ionic potential to eliminate infinities at origin.

Bragg’s Law

\[ 2d \sin \theta_B = n\lambda \]

The \( n \) is optional:

\[ 2d \sin \theta_B = \lambda \]
Crystal Structure Factor

Sum of atomic form factors for constituent atoms with appropriate phase factors for lattice positions

\[ F(q) = \sum_{m \text{ atoms}} f_m(q/2) e^{2\pi i q \cdot d^{(m)}} \]

\[ \theta = 2\theta_B \]

\[ q \equiv k' - k \]

\[ k = \frac{1}{\lambda} = |k| = |k'| \]

\[ q = |q| = 2 \frac{\sin \theta_B}{\lambda} \quad s = \frac{q}{2} = \frac{\sin \theta_B}{\lambda} \]

Example:

CuAu-I (CA)