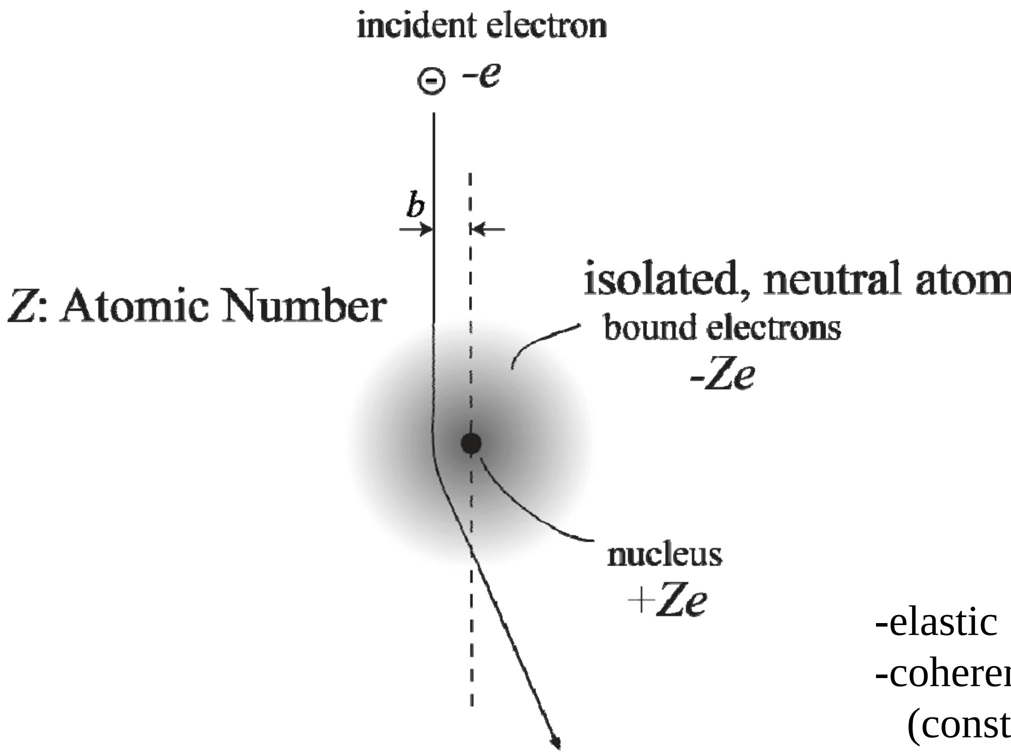
Small-Angle, Elastic Scattering from Atoms



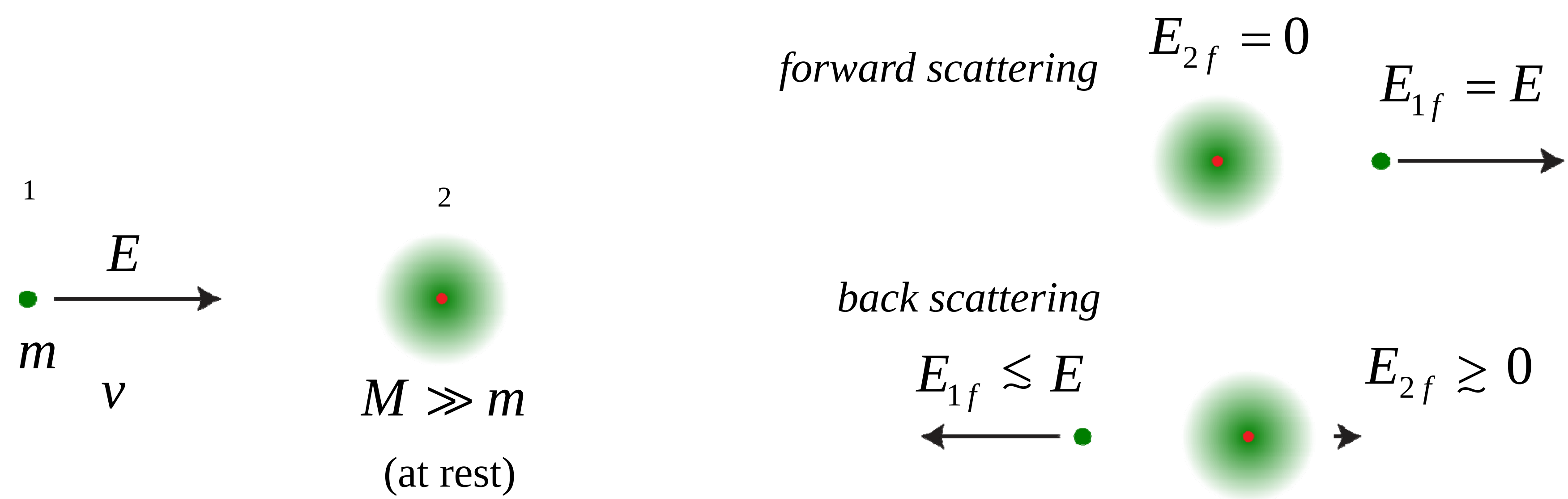
-elastic
-coherent
(constant phase shift)
(no significant energy loss)
-low-angle (forward)

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:



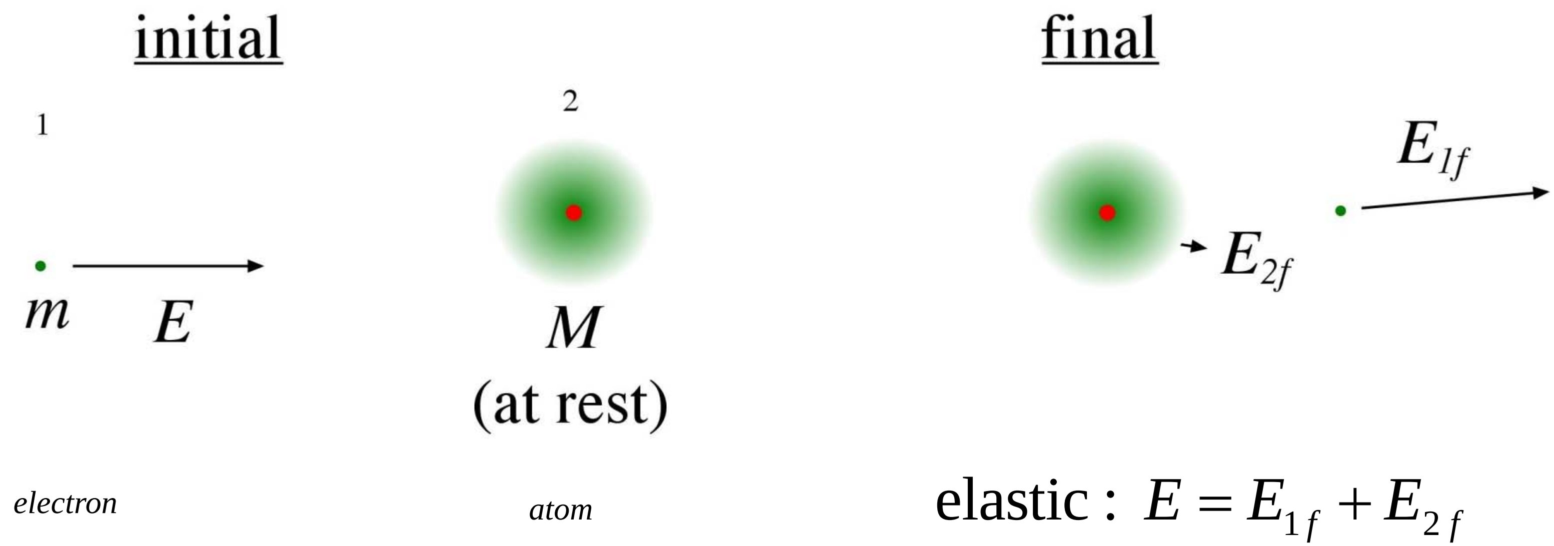
$$E = E_{1f} + E_{2f} \qquad \text{//elastic}$$

center-of-mass motion:

$$v_{COM} = \left(\frac{m}{m+M}\right) \cdot v$$

$$v_{1f} = v_{COM} \pm (v - v_{COM}) = \begin{cases} v & \textit{//forward} \\ -\left(\dfrac{M-m}{M+m}\right) \cdot v & \textit{//back} \end{cases}$$

Grazing-incidence elastic collision ⇒ forward scattering



$$\text{elastic}: \; E = E_{1f} + E_{2f}$$

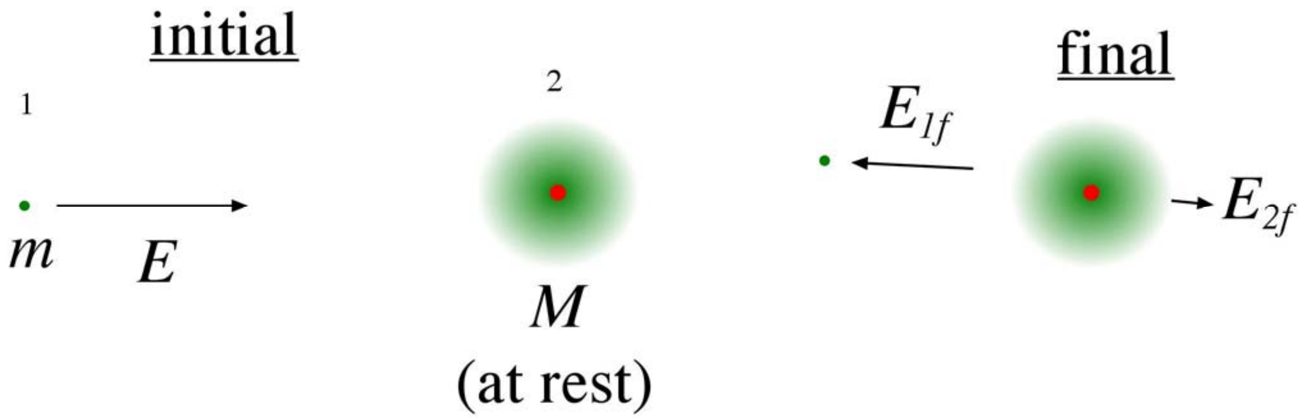
$$M > m: \; E_{1f} \lesssim E, \; E_{2f} \approx 0$$

-Less-massive electron forward scattered in grazing collision

-Almost no kinetic energy transferred to atom

-Electron energy essentially unchanged ⇒ coherent

Nearly head-on elastic collision ⇒ backscattering



electron

atom

$$\text{elastic}: \; E = E_{1f} + E_{2f}$$

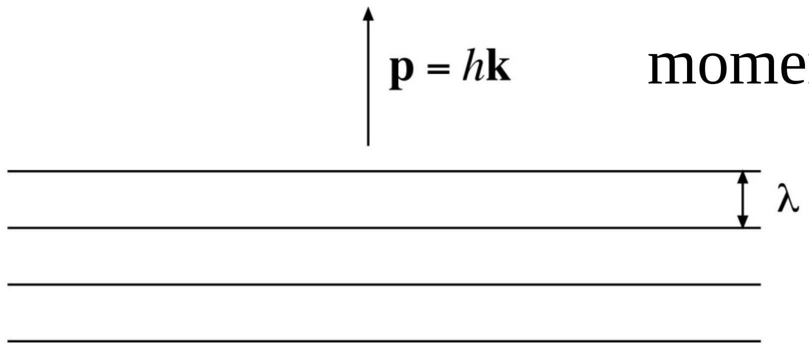
$$M > m: \; E_{1f} < E$$

-Less-massive electron backscattered in head-on collision

-Kinetic energy transferred to atom

-Electron loses energy ⇒ incoherent

Plane waves: sinusoidal form



momentum

A: amplitude

ϕ: phase

$\mathbf{k}$: wave vector

$\mathbf{v}_p$: phase velocity

f: frequency

t: time

We could write a plane wave as :

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

or

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

wavenumber: $k = |\mathbf{k}| = \dfrac{1}{\lambda}$

Plane waves: complex exponential form

$$\psi(\mathbf{r},t) = \psi_0 \cdot \mathrm{e}^{2\pi i(\mathbf{k}\cdot\mathbf{r} - f\cdot t)} \qquad \psi_0 = A\cdot \mathrm{e}^{i\phi}$$

Euler relation: $$\mathrm{e}^{i\theta} = \cos\theta + i\sin\theta$$

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

$$A = 1 \qquad \phi = 0 \qquad \psi_0 = 1$$

$$\Longrightarrow \psi(\mathbf{r},t) = \mathrm{e}^{2\pi i(\mathbf{k}\cdot\mathbf{r} - f\cdot t)}$$

Operators

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

$p = |\mathbf{p}| = \frac{h}{\lambda}$ $\mathbf{p} = h\mathbf{k}$ //de Broglie

$$\hat{\mathbf{p}} \cdot \psi(\mathbf{r},t) = (h\mathbf{k}) \cdot \psi(\mathbf{r},t) = -i\hbar\vec{\nabla}\psi(\mathbf{r},t)$$

$\vec{\nabla} = \frac{\partial}{\partial x}\hat{\mathbf{x}} + \frac{\partial}{\partial y}\hat{\mathbf{y}} + \frac{\partial}{\partial z}\hat{\mathbf{z}}$ //gradient

$\boxed{\hat{\mathbf{p}} = -i\hbar\vec{\nabla}}$ //momentum operator

$E = hf$ //from photoelectric effect

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

$\boxed{\hat{E} = i\hbar\frac{\partial}{\partial t}}$ //energy operator

Schrodinger equation

For a free, non-relativistic particle: $E = \frac{p^2}{2m_0}$

$$\hat{H} = \frac{\hat{p}^2}{2m_0} = \frac{-\hbar^2}{2m_0}\nabla^2$$ //Hamiltonian operator

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$ //Laplacian

$$\psi(\mathbf{r},t) = \psi_0 \cdot \mathrm{e}^{2\pi i(\mathbf{k}\cdot\mathbf{r} - f\cdot t)}$$ //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: $$\psi(\mathbf{r},t)=\psi_0\cdot e^{2\pi i(\mathbf{k}\cdot\mathbf{r}-f\cdot t)}=\psi(\mathbf{r})\cdot e^{-iE\cdot t/\hbar}$$

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

Time-independent Hamiltonian
-acts on **r** *only*:

Energy operator
-acts on *t* only:

$$\left[\hat{H}\psi(\mathbf{r})\right]\cdot \cancel{e^{-iE\cdot t/\hbar}}=E\cdot\psi(\mathbf{r})\cdot \cancel{e^{-iE\cdot t/\hbar}}$$

$$\hat{H}\psi(\mathbf{r})=E\cdot\psi(\mathbf{r})$$

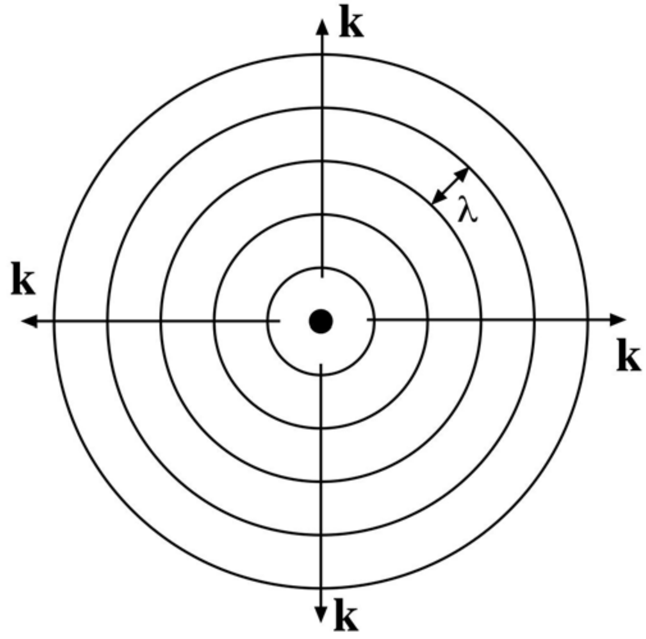
The time-independent part satisfies the *time-independent SE*:

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

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

Spherical waves

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



No unique direction of wavevector

$$\text{Intensity} = \frac{\text{Power}}{\text{Area}}$$

Intensity of wave function $\propto$ probability density

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

$$\psi \propto \frac{e^{2\pi i k r}}{r}$$

Atomic Scattering Factor

Spherical Scattered Wave

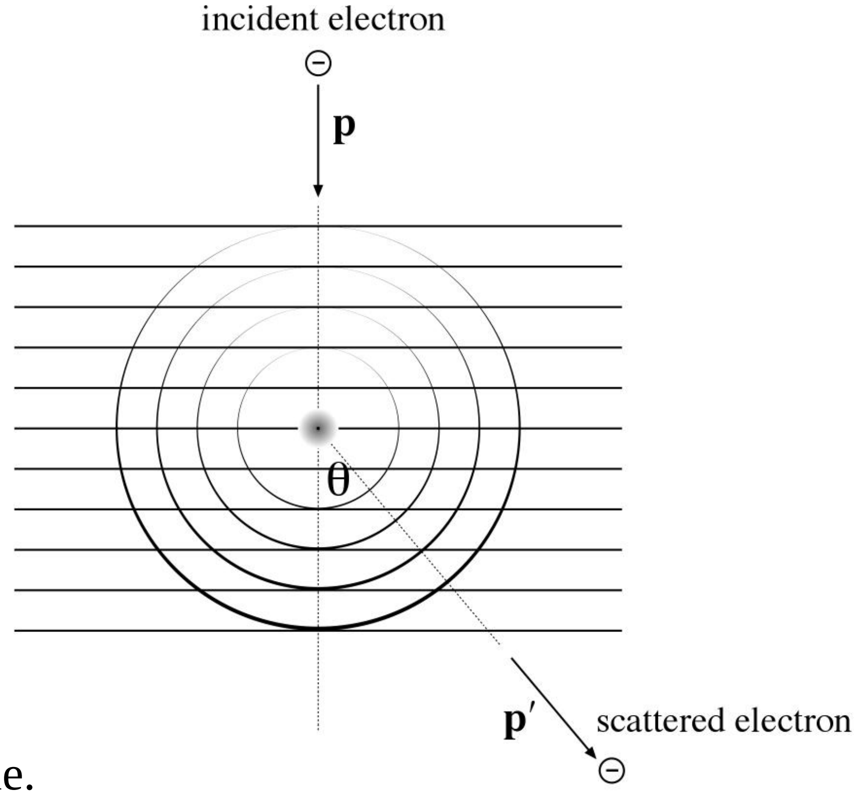
Elastic scattering: $|\mathbf{k}'| = |\mathbf{k}| = k$

Amplitude depends on scattering angle.

incident wave: scattered wave:

$$\psi_i(\mathbf{r}) = \mathrm{e}^{2\pi i \mathbf{k}\cdot\mathbf{r}} \qquad \psi_{sc}(\mathbf{r}) = f(\theta)\cdot\frac{\mathrm{e}^{2\pi ikr}}{r}$$

$f(\theta)$: 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:

small angle

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

final   initial   90° phase shift

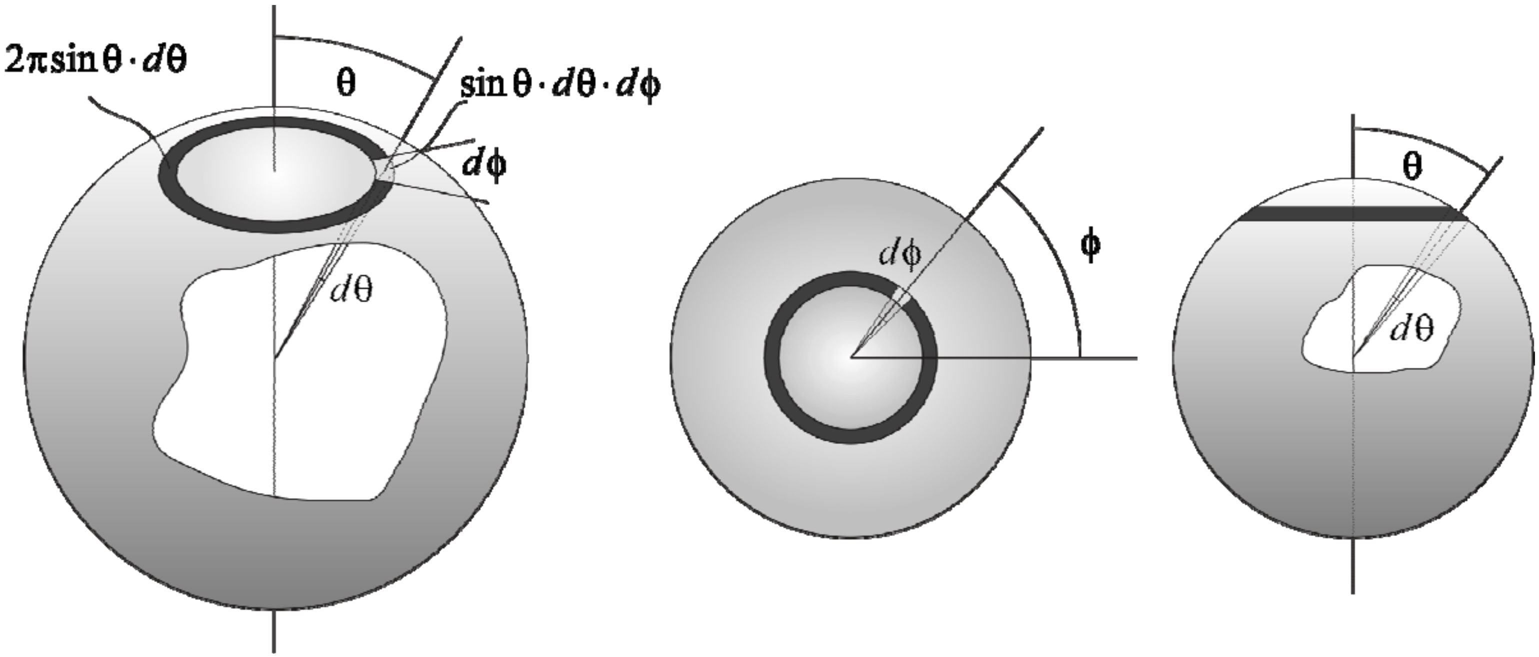
Weak-phase scattering by atoms:

$$\psi_f(\mathbf{r}) \approx \psi_i(\mathbf{r}) + i\psi_{sc}(\mathbf{r})$$

$$\psi_f(\mathbf{r}) = e^{2\pi i\mathbf{k}\cdot\mathbf{r}} + i\, f(\theta)\frac{e^{2\pi ikr}}{r}$$

//Scattered wave is spherical

Solid-angle projections



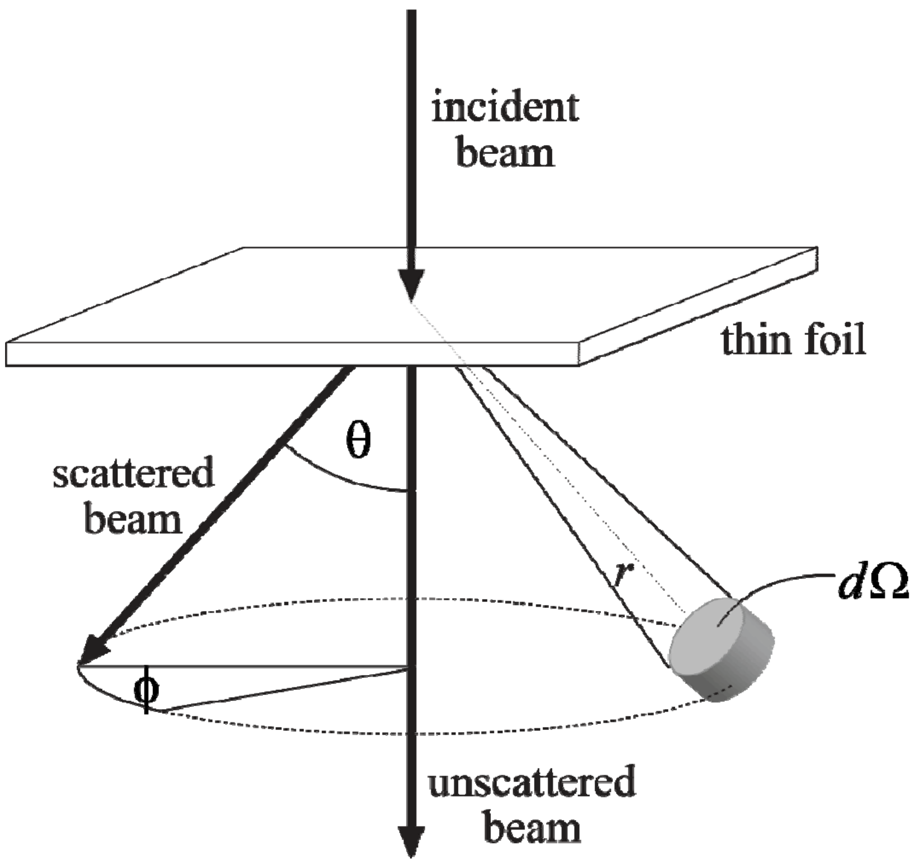
Differential solid angle:

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

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



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

$$\sigma_{tot} = \int_{\sigma} d\sigma$$

$$= \int_{\Omega} d\Omega \cdot \left(\frac{d\sigma}{d\Omega} \right)$$

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

Azimuthal symmetry:

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

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

Total scattering into angles less than θ:

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

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

Total scattering into angles greater than θ:

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

$$\sigma_>(\theta) = \int_{\theta'=\theta}^{\pi} d\theta' \cdot \left(\frac{d\sigma_\theta}{d\Omega} \right)$$

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:

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

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

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

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

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

Another Type of Problem:

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

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

Example:

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

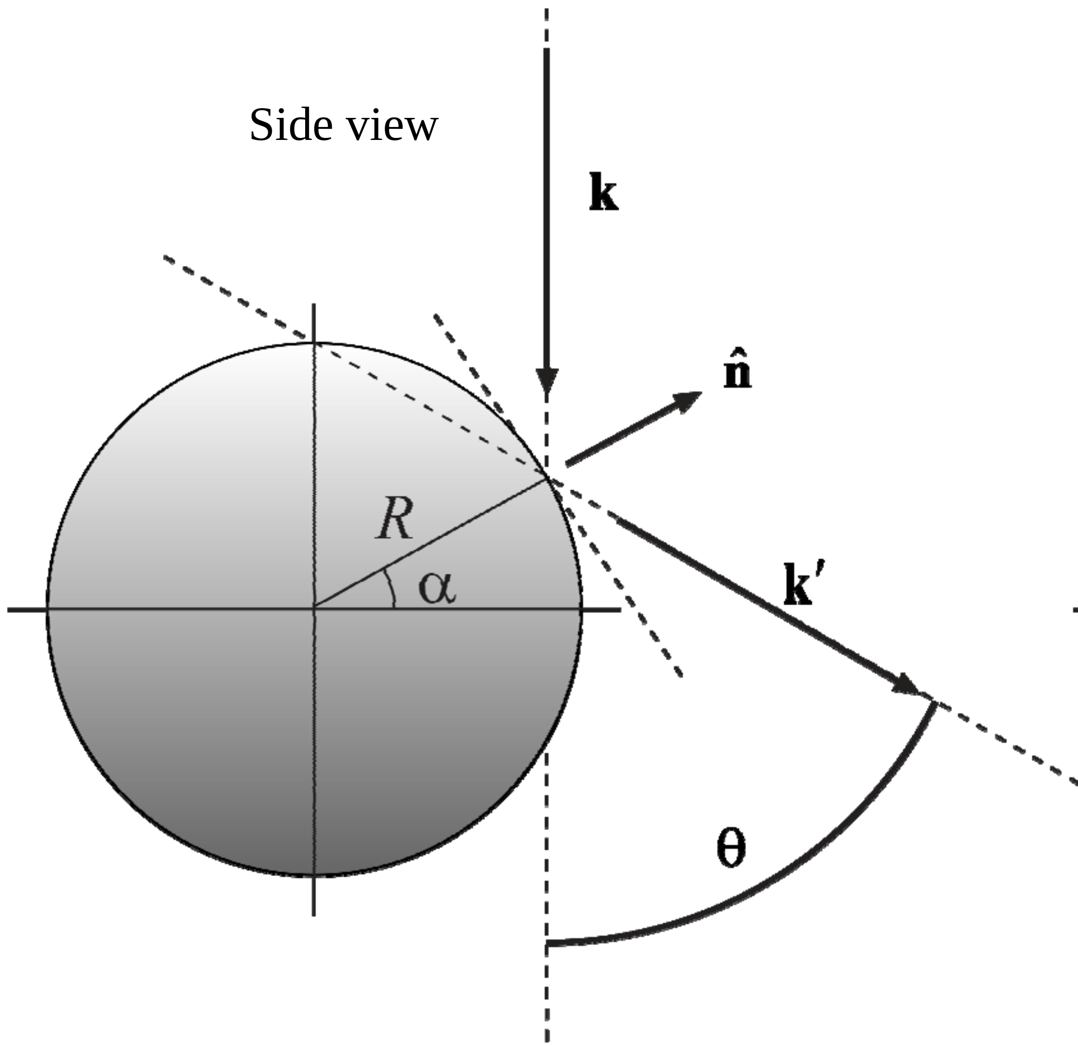
$$\frac{d\sigma}{d\Omega} = \frac{\sigma_{tot}}{2\pi \cdot \sin\theta} \frac{d}{d\theta}\left[\sin\left(\frac{\theta}{2}\right)\right]$$

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

$$\Rightarrow \quad \frac{d\sigma}{d\Omega} = \frac{\sigma_{tot}}{8\pi \cdot \sin\left(\frac{\theta}{2}\right)}$$

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

Interpreting differential cross-section



Uniform, hard sphere

Scattering cross-section: hard sphere (I)

Relate angles:

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

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 θ only:

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

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

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

$$\sigma_{tot} = \int_{\theta=0}^{\theta} \int_{\phi=0}^{2\pi} \frac{R^2}{4} \cdot \sin\theta \cdot d\theta \cdot d\phi = \boxed{\pi \cdot R^2}$$

Azimuthal (ϕ) sum (annulus):

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

Scattering into angles less than θ:

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

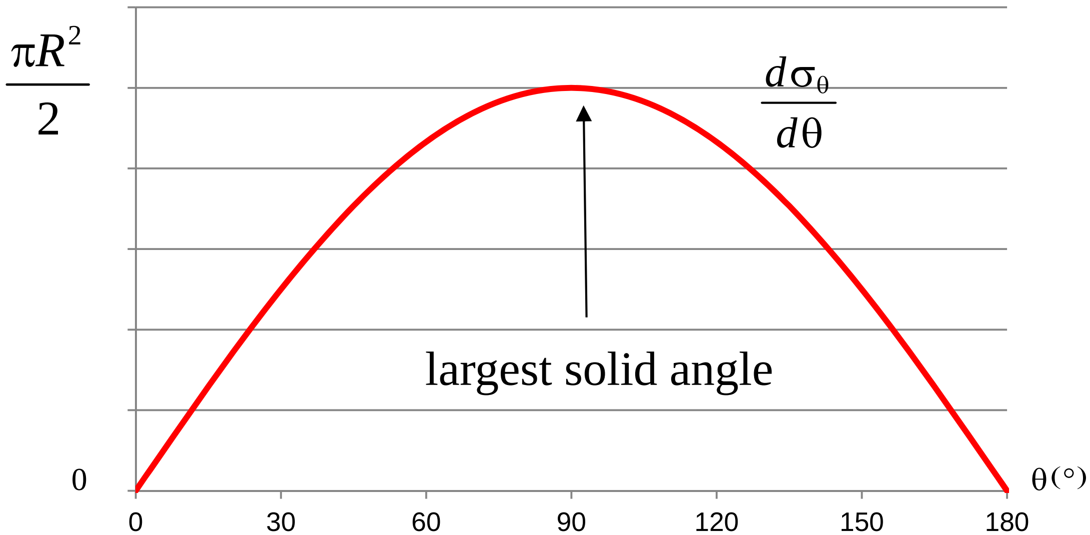
$$= \int_{\theta'=0}^{\theta} d\theta' \cdot \left(\frac{\pi R^2}{2} \cdot \sin\theta'\right)$$

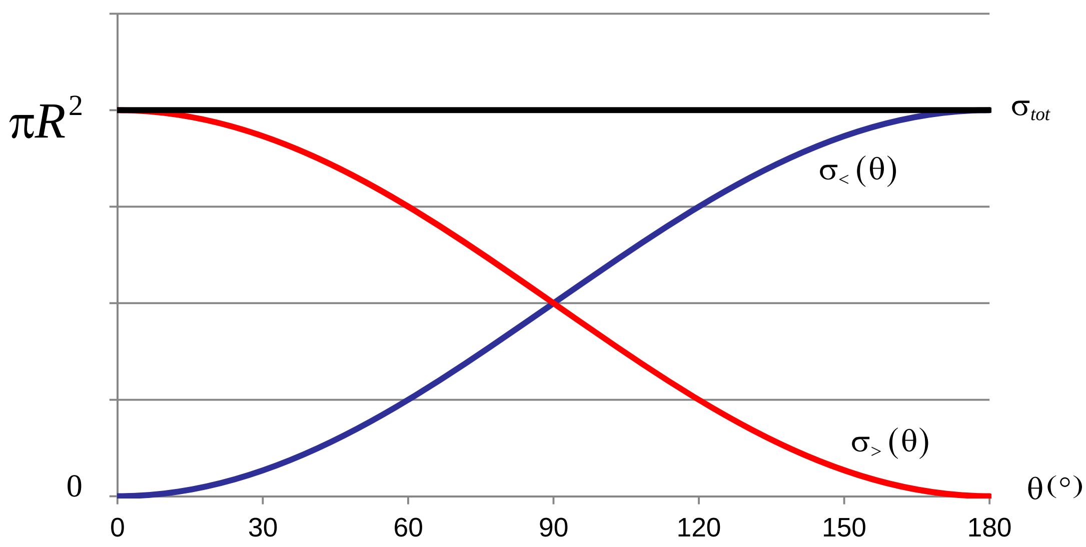
$$= -\frac{\pi R^2}{2} \cdot \cos\theta'\Big|_{\theta'=0}^{\theta} = \frac{\pi}{2} \cdot R^2 \cdot \cos\theta'\Big|_{\theta'=\theta}^{0}$$

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

$$\Rightarrow \sigma_{tot} = \sigma_<(\pi) = \pi \cdot R^2$$ as expected!

Scattering Cross-Section: Hard Sphere (II)





$$\sigma_<(\theta) + \sigma_>(\theta) = \sigma_{tot}$$

Electric current in scattered wave (I)

$$n_{sc}(\mathbf{r},t) = -e\cdot\left|\psi_{sc}(\mathbf{r},t)\right|^2 = -e\cdot\psi_{sc}^*\psi_{sc}$$ //electron "concentration"

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

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

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

$$= \nabla\cdot\left[\frac{ie\hbar}{2m}\cdot\left(\psi_{sc}^*\cdot\nabla\psi_{sc} - \nabla\psi_{sc}^*\cdot\psi_{sc}\right)\right]$$ //result

$$\frac{\partial}{\partial t}n_{sc}(x,t) = \nabla\cdot\vec{j}_{sc}$$ //continuity eqn.

$$\vec{j}_{sc} = \frac{ie\hbar}{2m}\cdot\left(\psi_{sc}\cdot\vec{\nabla}\psi_{sc}^* - \psi_{sc}^*\cdot\vec{\nabla}\psi_{sc}\right)$$ //current

Electric current in scattered wave (II)

$$\psi_i(\mathbf{r}) = \psi_0 \cdot \mathrm{e}^{2\pi i \mathbf{k}\cdot\mathbf{r}}$$ //incident plane wave

$$\psi_{sc}(\mathbf{r}) = \psi_0 \cdot f(\theta) \cdot \frac{\mathrm{e}^{2\pi i k r}}{r}$$ //scattered wave

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

$$j_0 = e \cdot v \cdot \left|\psi_0\right|^2$$ //incident current density

$$\vec{\nabla}\psi_{sc} = \psi_0 \cdot \left\{ i f(\theta) \left[2\pi i k - \frac{1}{r} \right] \cdot \hat{\mathbf{r}} + i \frac{df}{d\theta} \cdot \hat{\boldsymbol{\theta}} \right\} \cdot \frac{\mathrm{e}^{2\pi i k r}}{r}$$ //gradient

$$\vec{j}_{sc} = \frac{j_0}{r^2} \cdot \left| f(\theta) \right|^2 \cdot \hat{\mathbf{r}}$$ //scattered current density

$$dI_{sc} = j_0 \cdot d\sigma$$ //electric current in scattering cross-sectional area

$$\vec{j}_{sc} = \frac{dI_{sc}}{r^2 \cdot d\Omega} \cdot \hat{\mathbf{r}} = \frac{j_0}{r^2} \cdot \frac{d\sigma}{d\Omega} \cdot \hat{\mathbf{r}}$$ //scattered current density $\longrightarrow$ $$\frac{d\sigma}{d\Omega} = \left| f(\theta) \right|^2$$

Scattering Amplitude

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

Scattering amplitude:

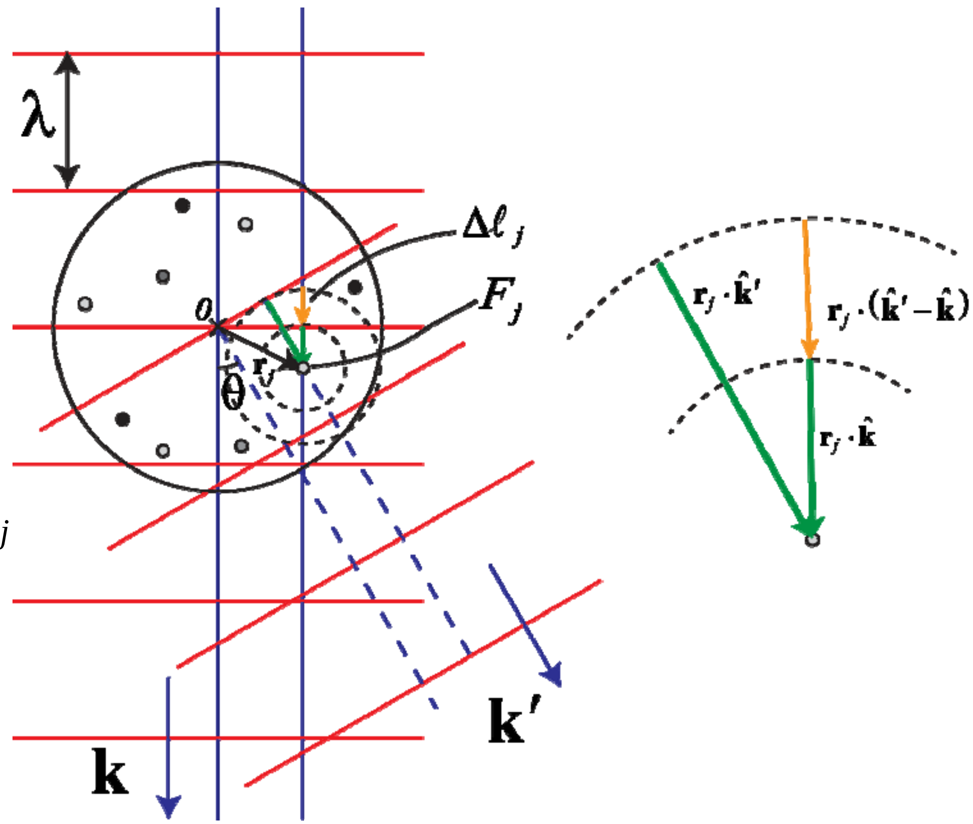
$$f(\mathbf{k}', \mathbf{k}) = \sum_{j=1}^{N} F_j e^{2\pi i \Delta\phi_j}$$

Path-length difference:

$$\Delta\ell_j = \left(\hat{\mathbf{k}}' - \hat{\mathbf{k}}\right) \cdot \mathbf{r}_j$$

Phase difference:

$$\Delta\phi_j = 2\pi \cdot \left(\frac{\Delta\ell_j}{\lambda}\right) = 2\pi \cdot (\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}_j$$



Rewrite:

$$f(\mathbf{k}' - \mathbf{k}) = \sum_{j=1}^{N} F_j e^{2\pi i (\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}_j}$$

Continuous medium:

$$f(\mathbf{k}' - \mathbf{k}) \to \int_{\mathbf{r}} F(\mathbf{r}) e^{2\pi i (\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}} \cdot d^3 r$$

The scattering amplitude is the Fourier transform of the target scattering strength.

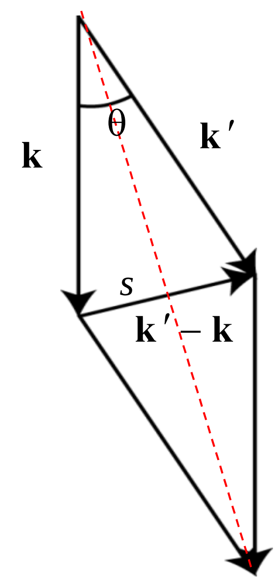
Scattering Amplitude (Atomic Form Factor)

$$f(\mathbf{k}'-\mathbf{k}) \equiv \int_{\mathbf{r}} F(\mathbf{r}) e^{2\pi i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}} \cdot d\mathbf{r}$$ //scattering amplitude

Atom at origin, spherically symmetric: $F(\mathbf{r}) \rightarrow F(r)$

Relate to scattering angle:

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



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

$$F(r) = \frac{2\pi me}{h^2}\varphi(r)$$ //scattering strength at radius *r*

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

nucleus ↘ electron density ↙

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

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

$$f_X(s) \equiv 4\pi\int_{r=0}^{\infty} r^2\rho(r)\frac{\sin(4\pi sr)}{(4\pi sr)}\cdot dr$$

The two are closely related: $$f_e(s) \propto \frac{\left[Z - f_X(s)\right]}{s^2}$$

Electrostatic Potential of a Neutral Atom

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

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

"Effective" Charge: $$Z_{eff}(r) = Z - Z_{enc}^{(e)}(r)$$

Enclosed Electron Charge:

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

Model of Screened Nuclear Potential: $$\varphi(r) \approx \frac{Ze}{4\pi\varepsilon_0 r}\mathrm{e}^{-r/r_0}$$

Rutherford (Thomas-Fermi) Model

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

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

// 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:

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

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

Rutherford Model (II)

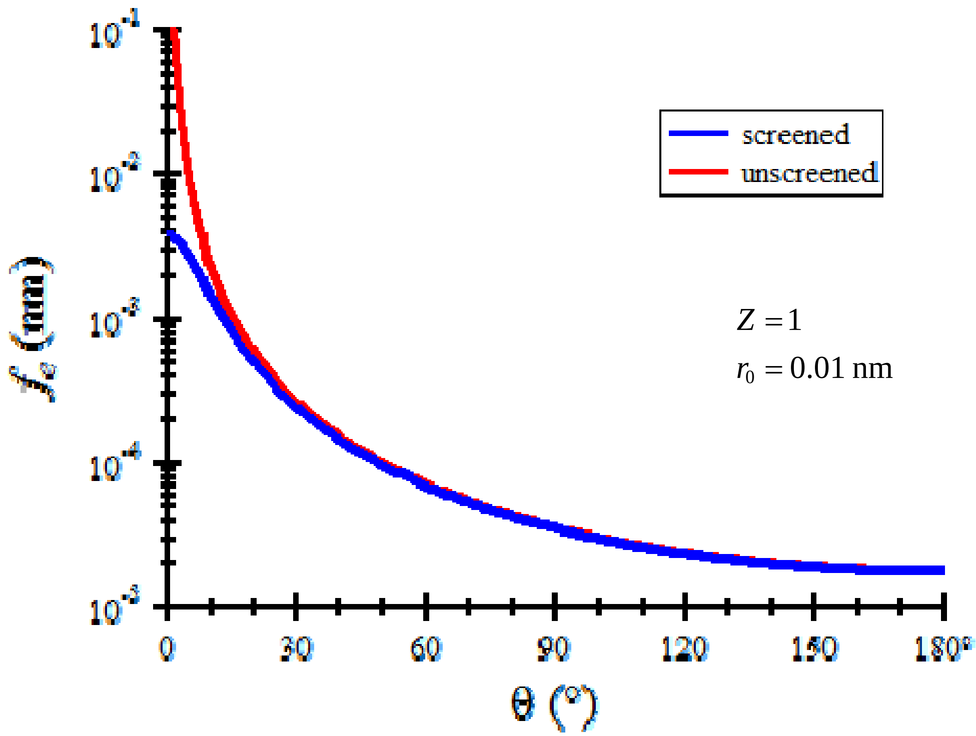
$$\frac{1}{R_c} = \frac{e^2 m}{8\pi h^2 \varepsilon_0} = \alpha \cdot \frac{mc^2}{4\pi hc} = \frac{1}{4.2\ \text{nm}}$$

$$\alpha = \frac{e^2}{2\varepsilon_0 hc} \approx \frac{1}{137}$$ //fine structure constant

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

Screening keeps form factor finite at origin:

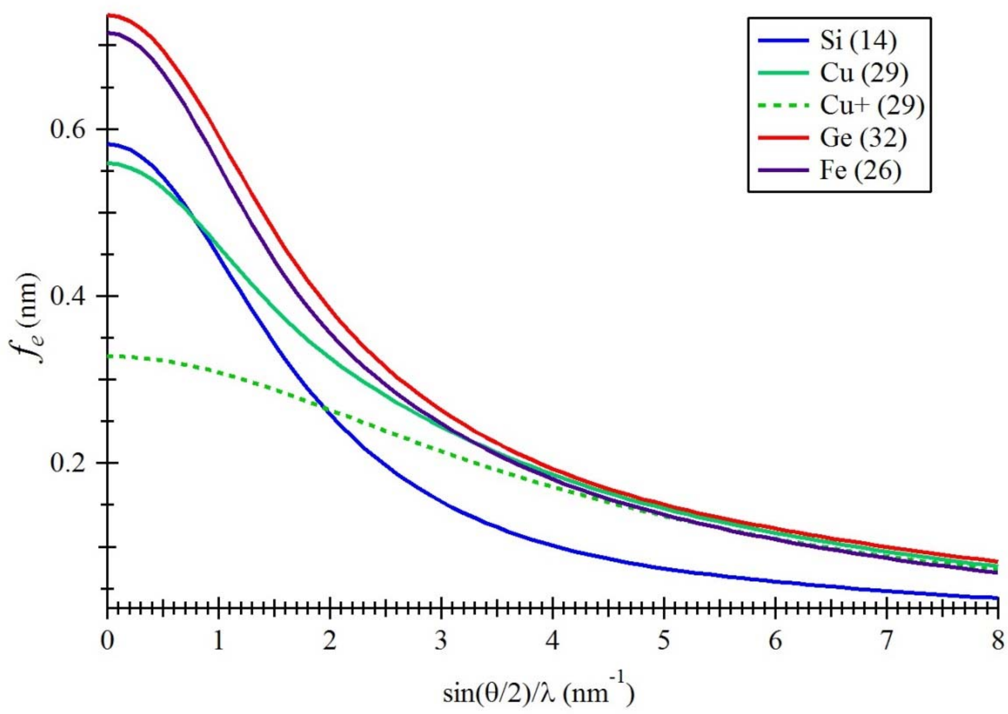
$$f_e(0) = \frac{\lambda^2 Z}{R_c \cdot \sin^2\left(\frac{\theta_0}{2}\right)}$$



Evaluating Form Factors

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

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



@E=0

Doyle & Turner, *Acta Cryst.* (1968) A **24**, 390

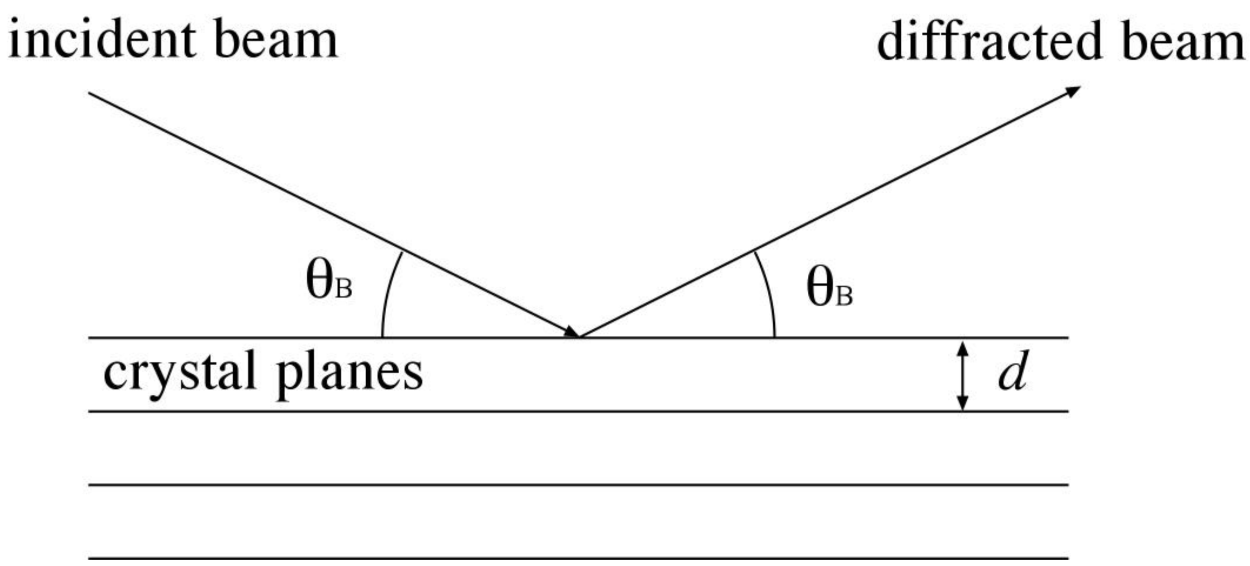
Note: point-charge correction added to ionic potential to eliminate infinities at origin

Bragg's Law

$$2d\sin\theta_B = n\lambda$$

The *n* is optional:

$$2d\sin\theta_B = \lambda$$

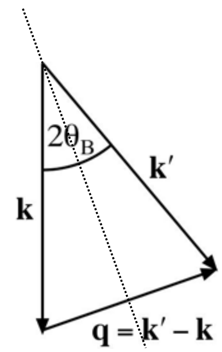


Crystal Structure Factor

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

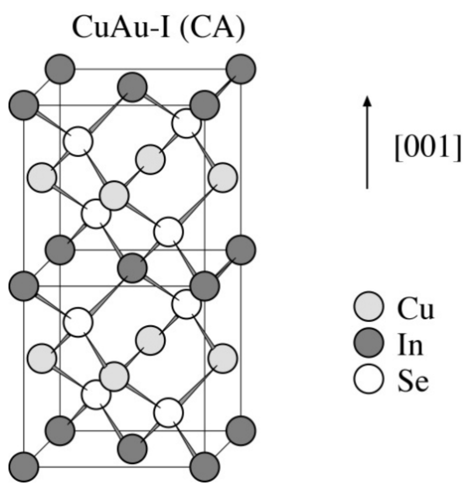
$$F(\mathbf{q}) = \sum_{m \text{ atoms}} f_m(q/2)\, e^{2\pi i \mathbf{q}\cdot\mathbf{d}^{(m)}}$$

$$\theta = 2\theta_B$$



$$\mathbf{q} \equiv \mathbf{k}' - \mathbf{k}$$

Example:



$$k = \frac{1}{\lambda} = |\mathbf{k}| = |\mathbf{k}'|$$

$$q = |\mathbf{q}| = 2\frac{\sin\theta_B}{\lambda} \qquad s = \frac{q}{2} = \frac{\sin\theta_B}{\lambda}$$