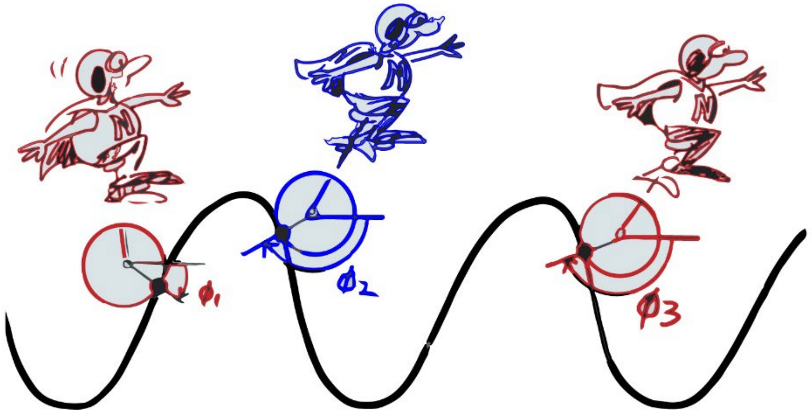
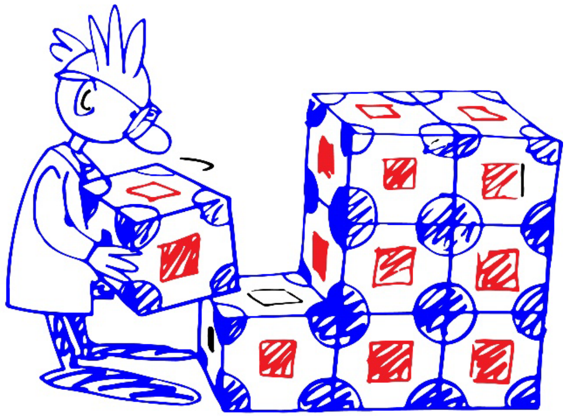
Outline: ~15 minute lectures for previewing

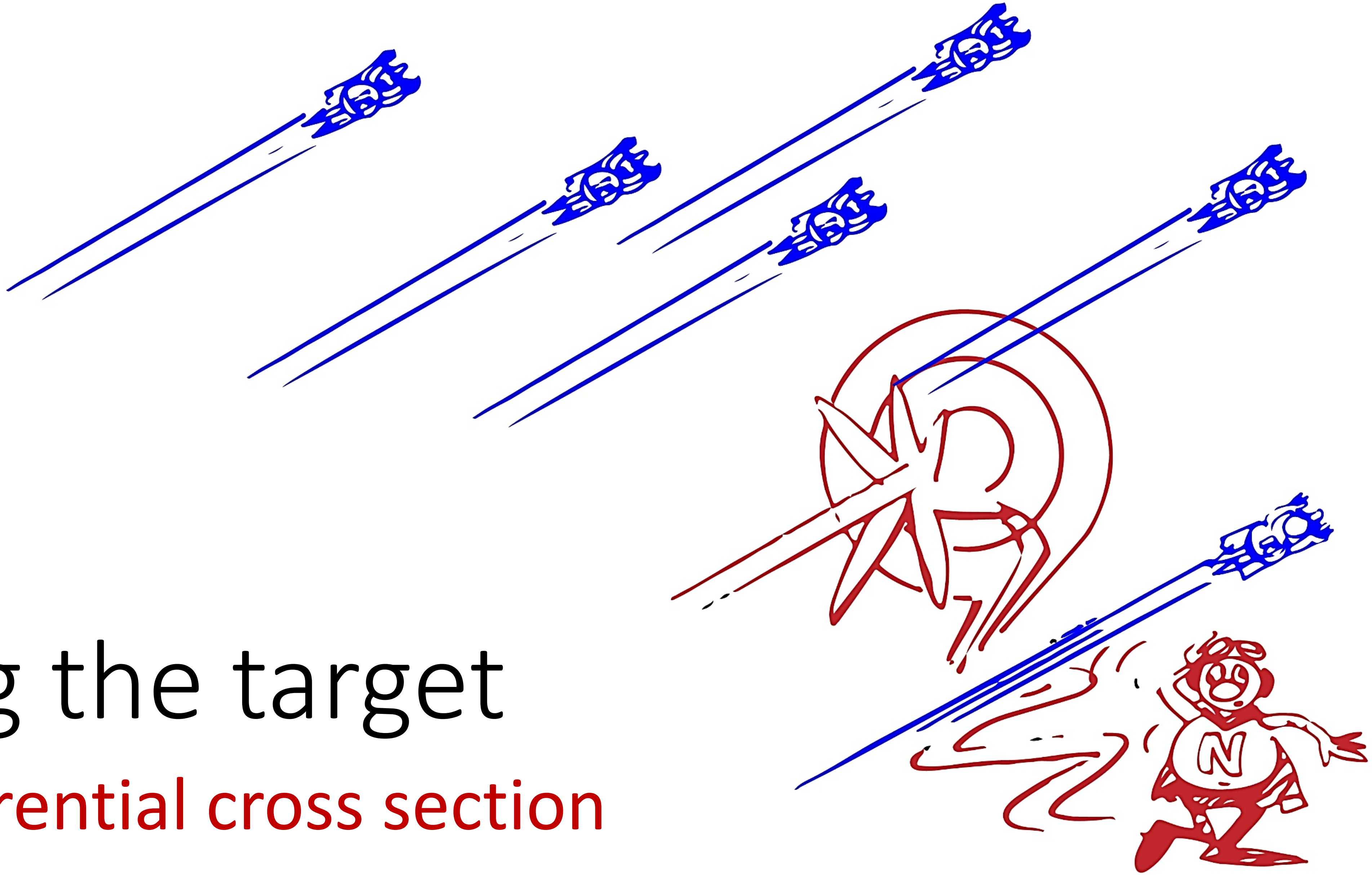
1. Going between real space and reciprocal space: Waves and Fourier transforms.



2. Hitting the target: The differential scattering cross section.

3. Crystals that glitter: Diffraction from materials with translational symmetry.





Hitting the target

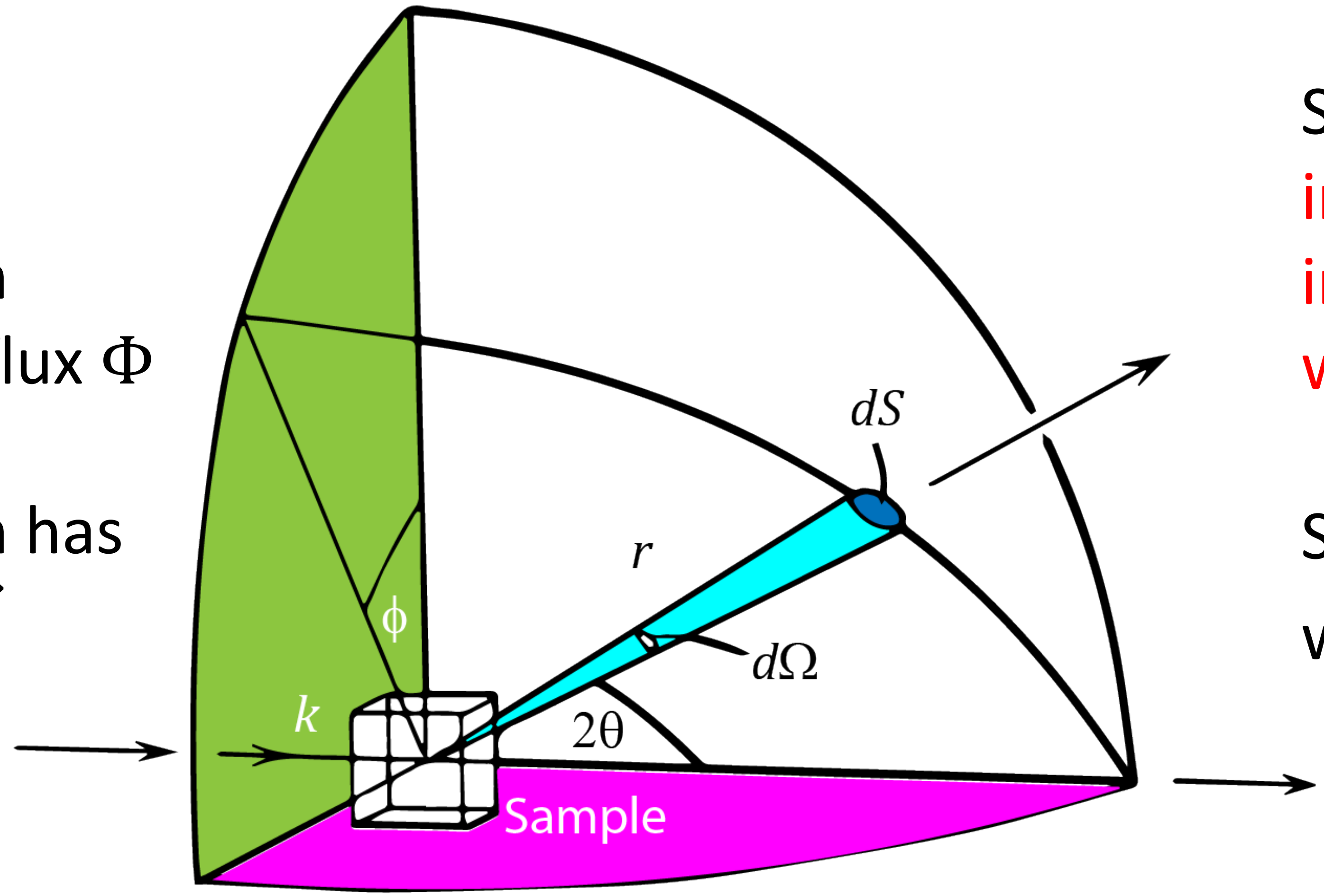
The differential cross section

Modified drawing of scattering system by Squires

Scattering geometry is in polar coordinates of r, ϕ, and 2θ

Incident beam described by flux Φ

Incident beam has wavevector $\overrightarrow{k_i}$



Scattered beam into solid angle dΩ in direction $\phi, 2\theta$ with energy $E' + dE'$

Scattered beam has wavevector $\overrightarrow{k_f}$

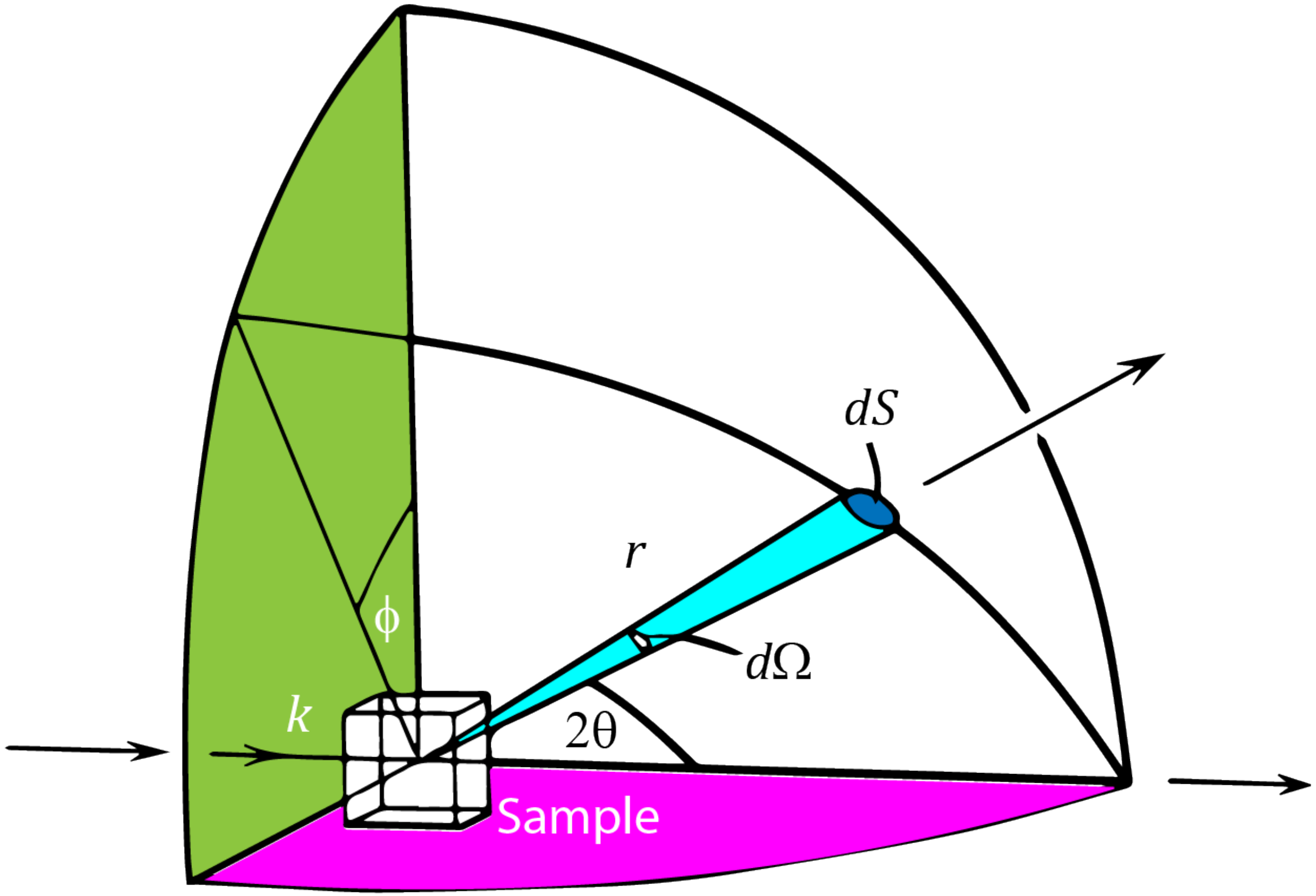
Flux of particles from beam and scattering at a solid angle

Φ = Flux of incoming particles

Φ has units of area^{-1} time^{-1}
(e.g. cm^{-2} s^{-1})

Scattering occurs
within the plane by angle 2θ
out of the plane by angle ϕ

We can define the
solid angle as $d\Omega$

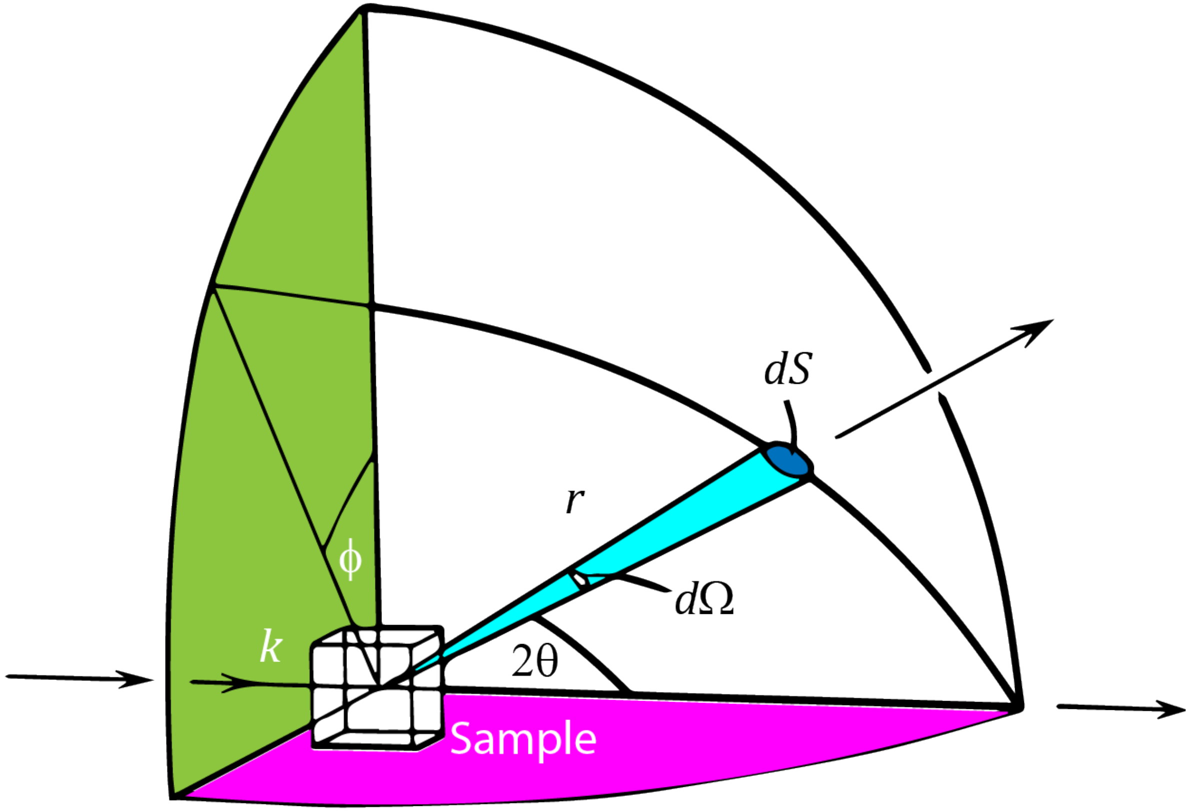


The partial differential cross-section

$$d\Omega = \frac{dS}{r^2}$$

We are after the **partial differential cross-section**

$$\boxed{\frac{d^2\sigma}{d\Omega dE'}}$$



Units

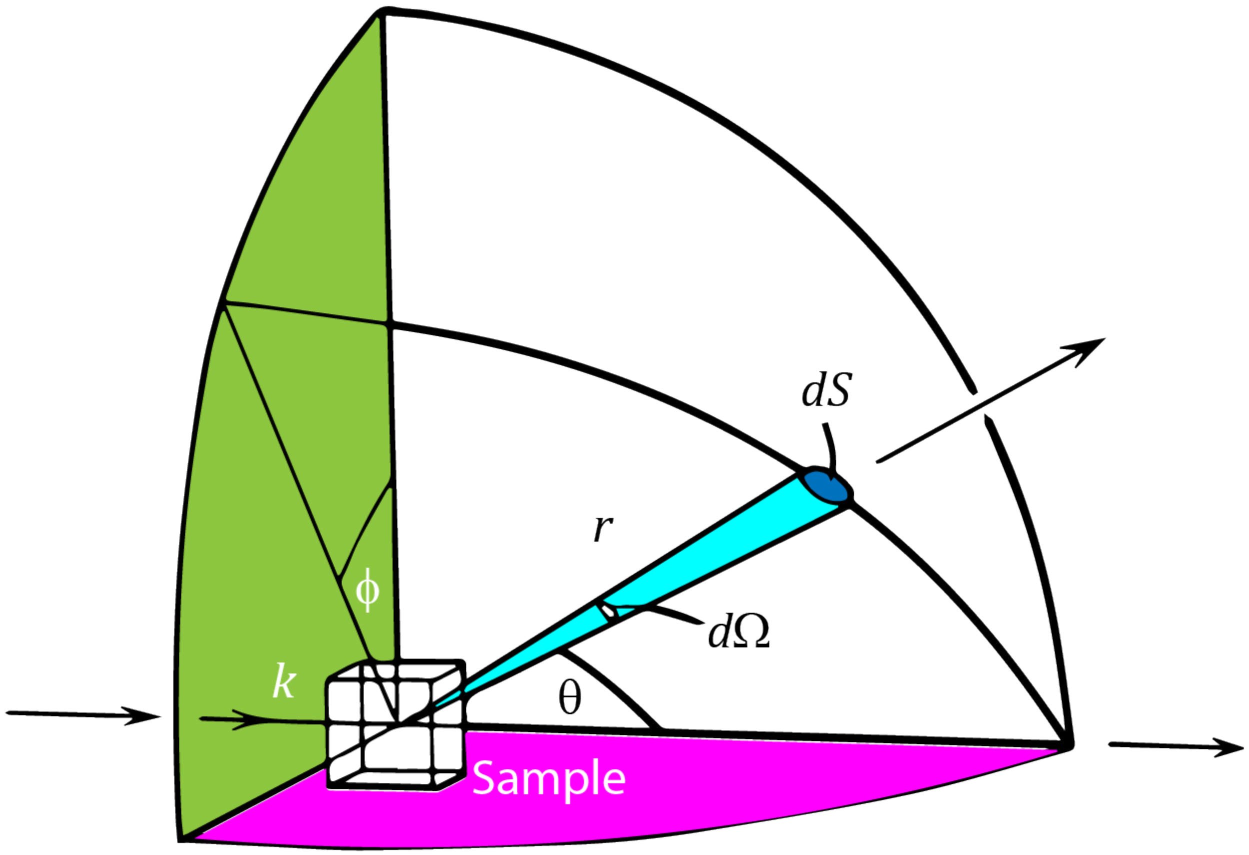
$$\frac{d^2\sigma}{d\Omega dE'} = \frac{\text{\# of particles scattered per second into } d\Omega dE'}{\Phi\ d\Omega dE'} \qquad \frac{\text{time}^{-1}}{\text{area}^{-1}\ \text{time}^{-1}} = \text{area}$$

The partial differential cross-section

$$\frac{d\sigma}{d\Omega} = \int_0^\infty \frac{d^2\sigma}{d\Omega dE'} dE'$$

The energy-integrated cross-section is the **differential cross-section**

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



$$\frac{d\sigma}{d\Omega} = \frac{\text{\# of particles scattered per second into } d\Omega}{\Phi \, d\Omega}$$

Units

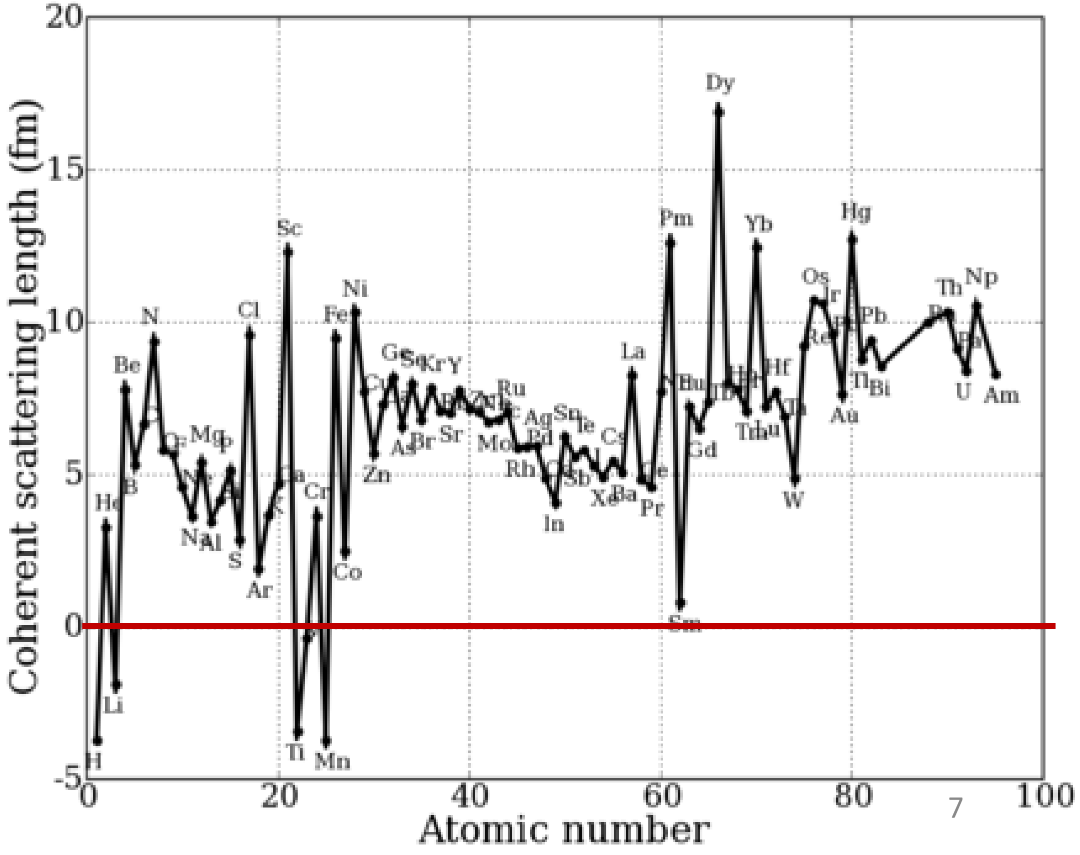
area

The neutron scattering length

- In neutron scattering, the nucleus is a point source.
- $f(\lambda,\theta)$ is therefore a constant
- $f(\lambda,\theta)$ = b where b is known as **the scattering length**

$$\psi_f = b\frac{e^{i\vec{k}\vec{r}}}{r}$$

- Note that $f(\lambda,\theta)$ and b must have units of length since it is divided by r
- Typical b are in fm or 10^{-15} m
- Can be positive or negative!



Neutron scattering length for hydrogen

- Neutron scattering length depends on nucleus and the spin state of the nucleus-neutron system.
- Units given in barns, where 1 barn = 10^{-28} m^2
- These are isotope specific and will depend on the orientation of nuclear spin with respect to the neutron
- **Example:** hydrogen vs. deuterium
- H proton plus neutron has either triplet or singlet state

$$b^+ = 1.085 \times 10^{-14} m$$

$$b^- = -4.750 \times 10^{-14} m$$

$$\langle b \rangle = \frac{3}{4} b^+ + \frac{1}{4} b^-$$

$$\Delta b = \sqrt{\langle b^2 \rangle - \langle b \rangle^2}$$

$$\langle b \rangle = -0.374 \times 10^{-14} m$$

$$\Delta b = 2.527 \times 10^{-14}\ m$$

$$\boxed{b = \langle b \rangle \pm \Delta b}$$

Neutron scattering length for deuterium

- Deuterium has a quartet and doublet that can form with neutron from proton and neutron in its nucleus→ six states
- 2/3 of states are quartet, 1/3 are doublet

$$\langle b \rangle = \frac{2}{3} b^{+} + \frac{1}{3} b^{-}$$

$$\langle b \rangle = 0.668 \times 10^{-14} m$$

$$\Delta b = 0.403 \times 10^{-14} m^2$$

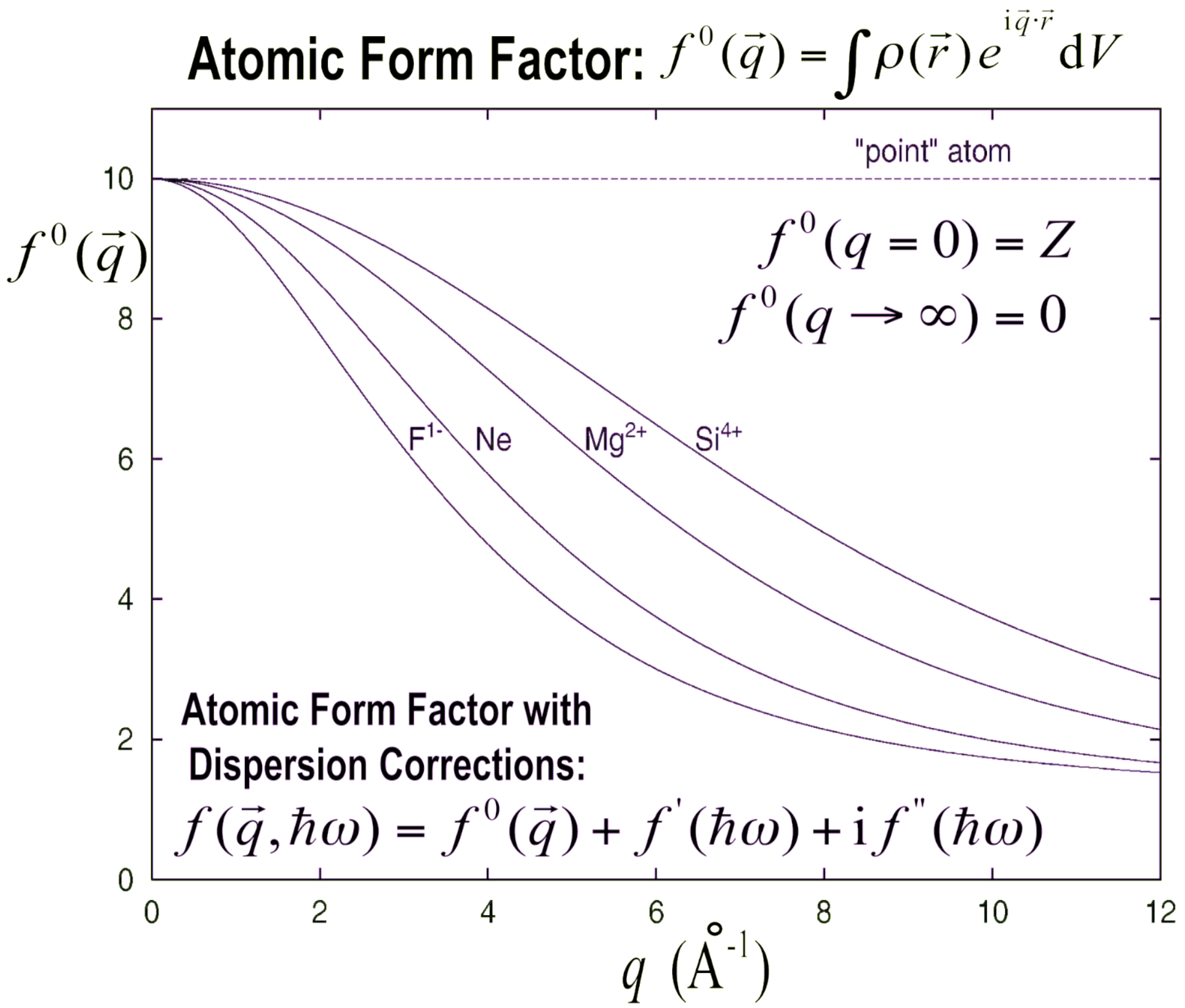
$$\boxed{\sigma = 4\pi |b|^2}$$

$$\langle b^2 \rangle = \langle b \rangle^2 + (\Delta b)^2$$

$$\langle \sigma \rangle = \sigma_{coh} + \sigma_{inc}$$

(in units of barns)	$\sigma_{coh} = 4\pi \langle b \rangle^2$	$\sigma_{incoh} = 4\pi (\Delta b)^2$
Hydrogen	1.76	80.27
Deuterium	5.59	2.05

The atomic form factor for x-rays



Summary of the differential cross sections

For x-ray and neutron scattering, we are dealing with the scattering of plane waves by atoms and nuclei.

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-\mathrm{i}kx} \mathrm{d}x$$

neutrons

$$\frac{d\sigma}{d\Omega} = \sum_{i,j} b_i b_j e^{-i\boldsymbol{Q}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_j)}$$

x-rays

$$\frac{d\sigma}{d\Omega} = r_0^2 \sum_{i,j} |f(Q)|^2 e^{-i\boldsymbol{Q}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_j)} P(2\theta)$$

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

Where $P(2\theta)$ is the polarization factor