Elastic scattering

Lecture 2

Part 1

Particle vs. wave

Particle:

- Scattering cross section & differential scattering cross section
- Scatter to particular angles
- Columbic interaction with the nucleus
- Used as primary description when considering spectroscopies

Wave:

- Consider the wave to be diffracted by atoms or scattering centers
- Strength of scatter depends on ‘atomic form factor’
- Used as primary description when considering diffraction & imaging

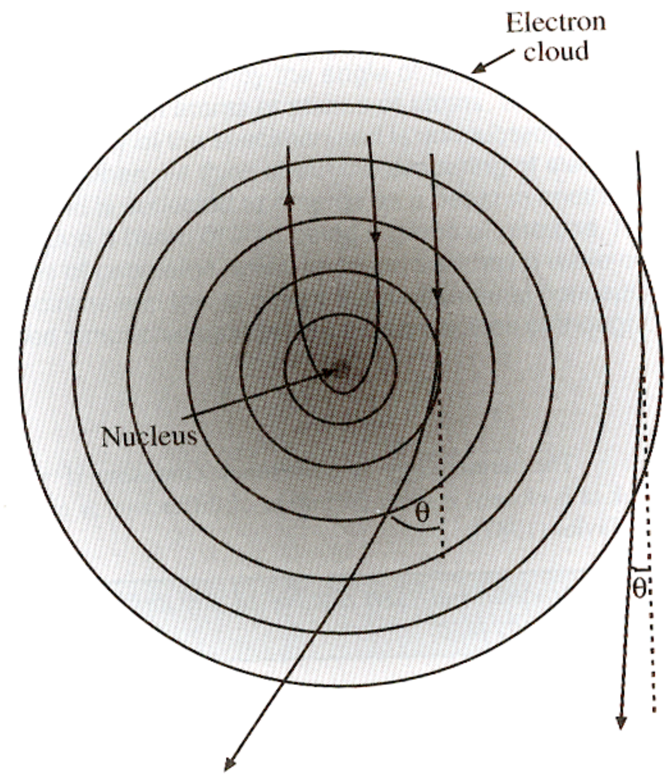
Brief review of particle model …

Elastic scattering

single electron / isolated atom

Interaction between electron & atom is Coulombic

- Incident electron & electron cloud
- Incident electron & nucleus



In a prior lecture, we discussed

- Interaction cross section
- Mean free path
- Differential cross section

Elastic scattering

single electron / isolated atom

Interaction cross section expresses the probability of a given scattering event. Generally:

$$\sigma = \pi \mathbf{r}^2$$

Elastic scattering radius has the form:

$$r_{electron} = \frac{e}{V\theta} \quad ; \quad r_{nucleus} = \frac{Ze}{V\theta}$$

Z = atomic weight
e = charge of the electron
V = potential of the electron
θ = angle

Implications:

$V \Uparrow \quad \sigma \Downarrow$

$Z \Uparrow \quad \sigma \Uparrow$

$\theta \Uparrow \quad \sigma \Downarrow$

Elastic scattering

through specimen thickness

Consider instead specimen of N atoms / unit thickness.

Total cross section for scattering from specimen:

$$Q_T = N\sigma_T = \frac{N_o \sigma_T \rho}{A}$$

N = # atoms / unit volume
r = density
A = atomic weight

Scattering probability for a sample of thickness t:

$$Q_T t = \frac{N_o \sigma_T \rho t}{A}$$

ρt ⇒ *'mass-thickness'*

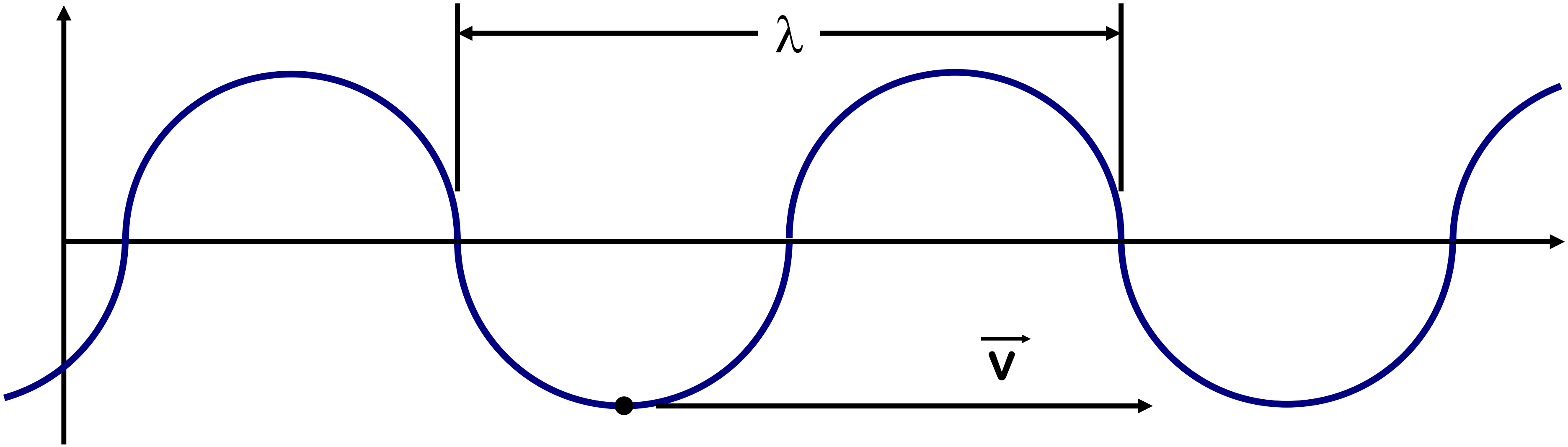
Can re-arrange to give another useful concept:

Mean free path: mfp or λ

$$mfp = \frac{1}{Q} = \frac{A}{N_o \sigma_T \rho}$$

On to the wave perspective …

What is a wave?



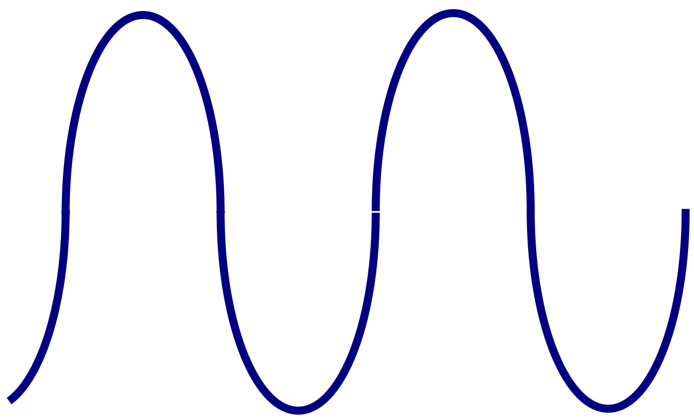
A wave: periodic disturbance in both space and time

Characteristics:

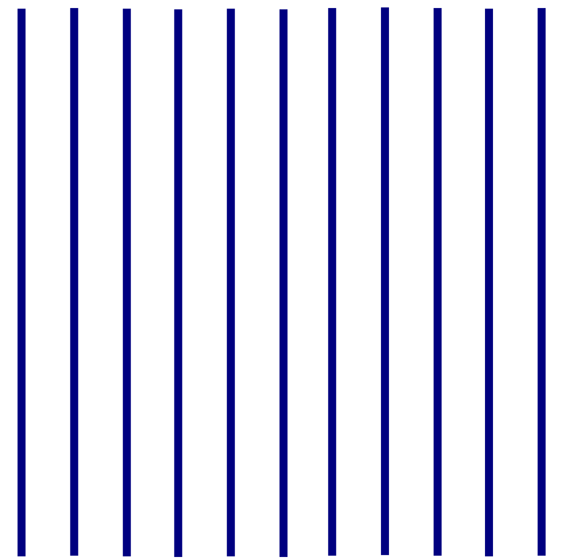
- **Wavelength (λ), velocity (v), frequency (f):** $v = f\,\lambda$
- **Wave number (k):** $k = 1/\lambda$ *
- **Angular frequency (ω):** $\omega = f\,k$

* Sometimes written as: $k = 2\pi/\lambda$

Ways that we'll depict waves

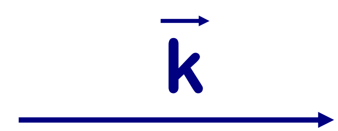


This is our plane wave …



Here we show it propagating, with the lines being the location of e.g. the peaks of the wave …

Wave number k can be expressed as a vector $\vec{k}$, which then captures both the direction of the wave and it's wavelength



This is thus an equivalent representation of the wave …

Mathematics of waves

A wave: periodic disturbance in both space and time, u(x,y,z,t):

$$v^2\left[\frac{d^2u}{dx^2}+\frac{d^2u}{dy^2}+\frac{d^2u}{dz^2}\right]=\frac{d^2u}{dt^2}$$

$$v^2\nabla^2 u=\frac{\partial^2 u}{\partial t^2}$$

Wave Eqn.

(2^{nd} order differential equation)

In one dimension, u(z,t), "plane wave":

$$\frac{\partial^2 u}{\partial z^2}=\frac{1}{v^2}\frac{\partial^2 u}{\partial t^2}$$

Solutions:

$$u(z,t)=\sin\left(kz+\omega t\right)$$

$$u(z,t)=\exp\left[-i\left(\omega t-kz\right)\right]$$

Preferred form → (exp form)

via Euler's Equations

Mathematics of vibrations

A vibration: time-dependent or space-dependent periodic disturbance

Space dependent periodicity, u(x):

$$a\frac{d^2u}{dx^2}+bu=0$$

A solution:

$$u=A\exp\left[i\alpha x\right]+B\exp\left[-i\alpha x\right]$$

$$\alpha=\sqrt{\frac{b}{a}}$$

Electron in free space

Electron moving:

- in absence of a potential field (V=0)
- independent of t

$$\frac{h^2}{2m}\frac{\partial^2\psi}{\partial z^2}+E\psi=0$$

Solution:

$$\psi = A\exp(ikx)+B\exp(-ikx)$$

with $k=\sqrt{\frac{2mE}{h^2}}$

Electron in free space

Time independent propagation only one arbitrary direction (+r):

Plane wave: $\psi = \psi_o \exp(ikr)$ **with** $k = \sqrt{\frac{2mE}{h^2}}$

Easy to add time dependence back in:

$$\Psi = \Psi_o \exp(ikr) \exp\left[-i\frac{E}{h}t\right]$$

Have a wave, with energy given by:

$$E = \frac{h^2 k^2}{2m}$$

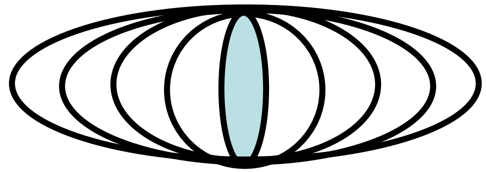
k $\Rightarrow$ fixed

p $\Rightarrow$ infinite (unknown)

Electron in free space

Spherical wave:

- Isotropic wave propagating outwards from a point



Wave Eqn:

$$\frac{\partial^2 (r\Psi)}{\partial t^2} = v^2 \frac{\partial^2 (r\Psi)}{\partial r^2}$$

Solution:

$$\Psi = \Psi_o \frac{\exp(ikr - \omega t)}{r}$$

Time independent

$$\psi = \psi_o \frac{\exp(ikr)}{r}$$

Coherence & Incoherence

Diffracted wave is either coherent or incoherent

Depends on the phase relationship:

$$\Psi(z,t) = \Psi_o \exp\left[-i\left(\underline{\underline{\omega t - kz}}\right)\right]$$

phase

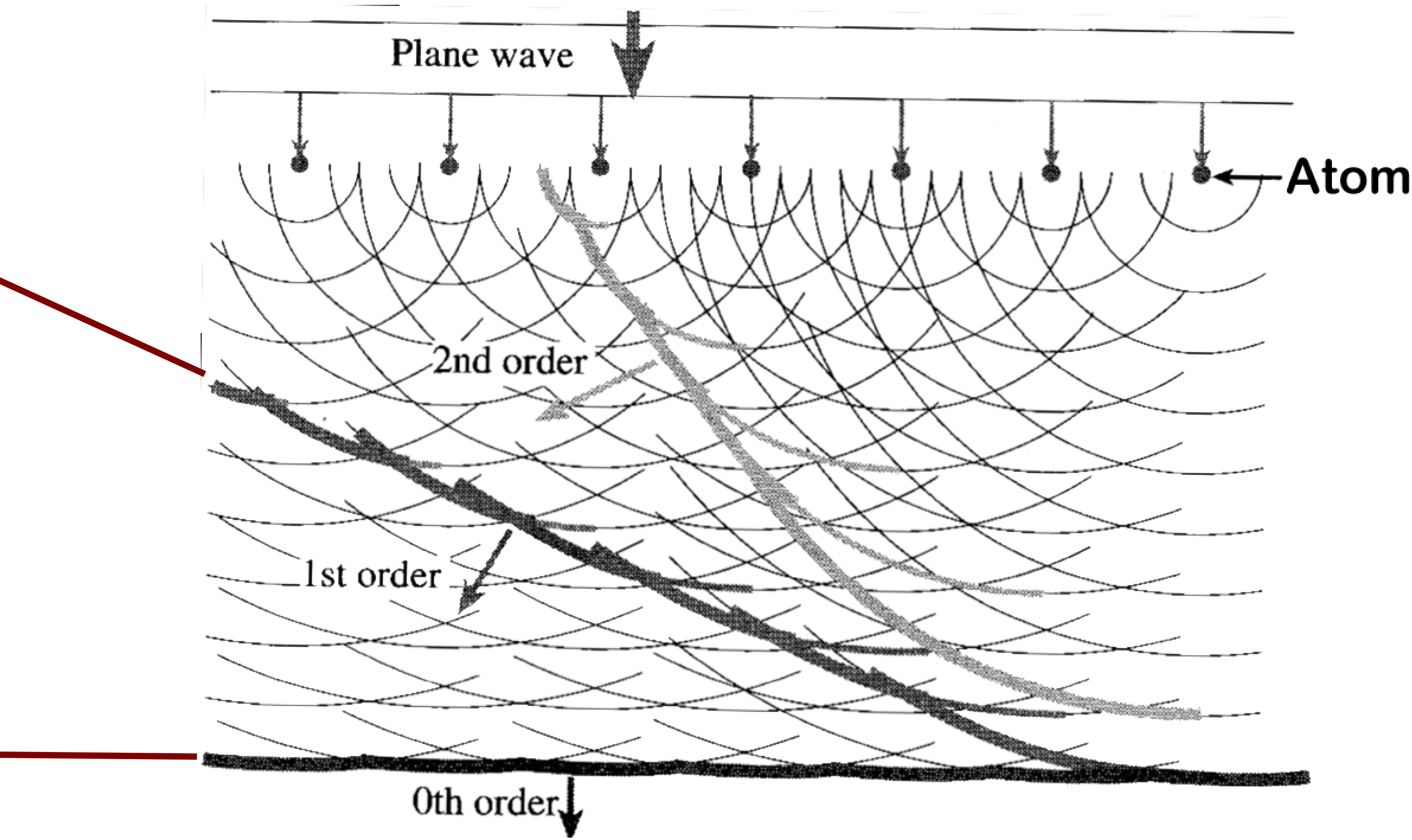
velocity

$$v_{phase} = \frac{\partial z}{\partial t} = \frac{\omega}{k}$$

Coherence: phase relationship preserved after scattering

Incoherence: phase relationship destroyed after scattering

Coherence & Incoherence



These waves have the same phase (are coherent) at these angles

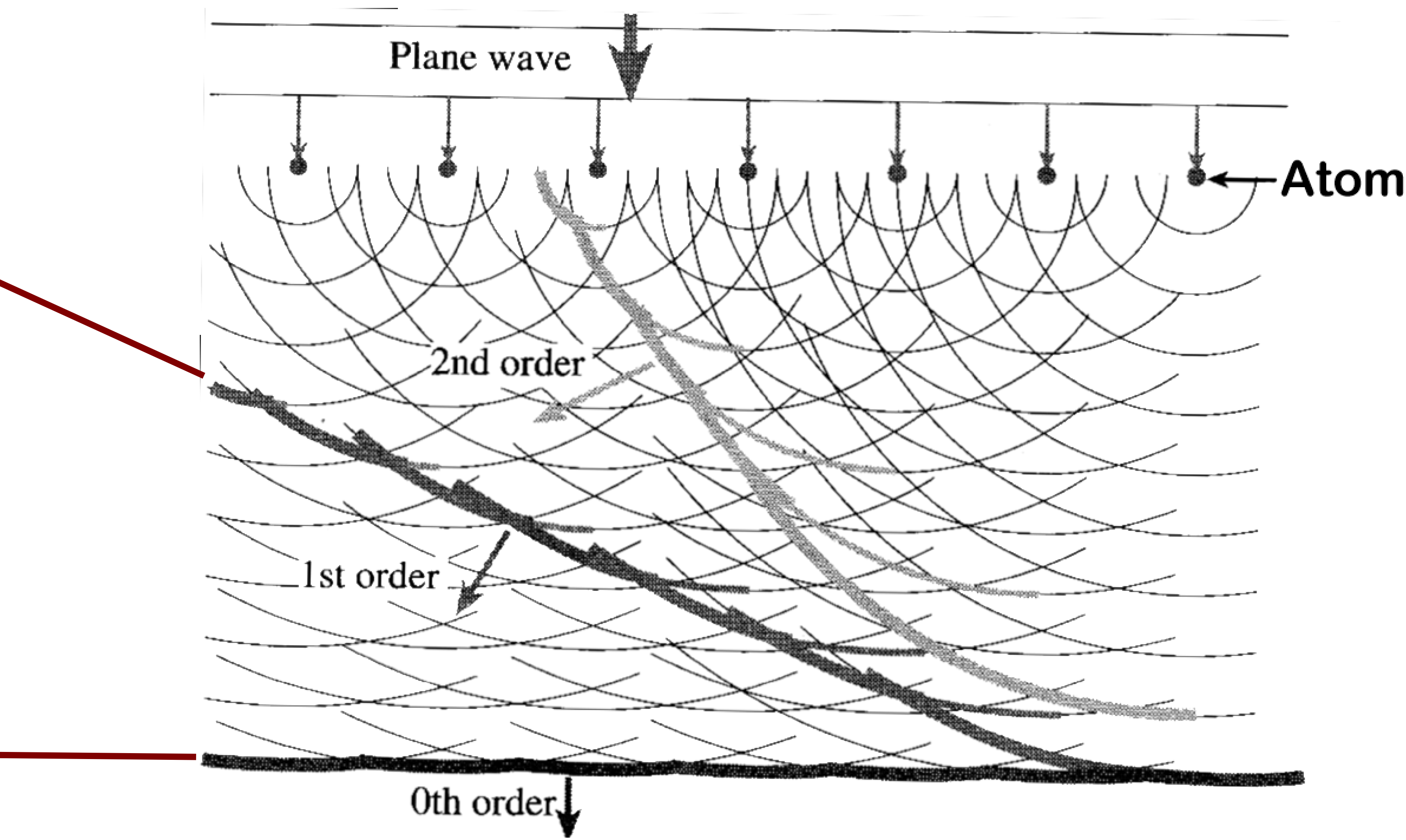
Coherence & Incoherence
Elastic & Inelastic

Note can have:

- Coherent elastic scattering
- Incoherent inelastic scattering
- Coherent inelastic scattering
- Incoherent inelastic scattering

For now, want to focus on <u>coherent</u> <u>elastic</u> scattering, as it is responsible for diffraction

Coherence & Incoherence

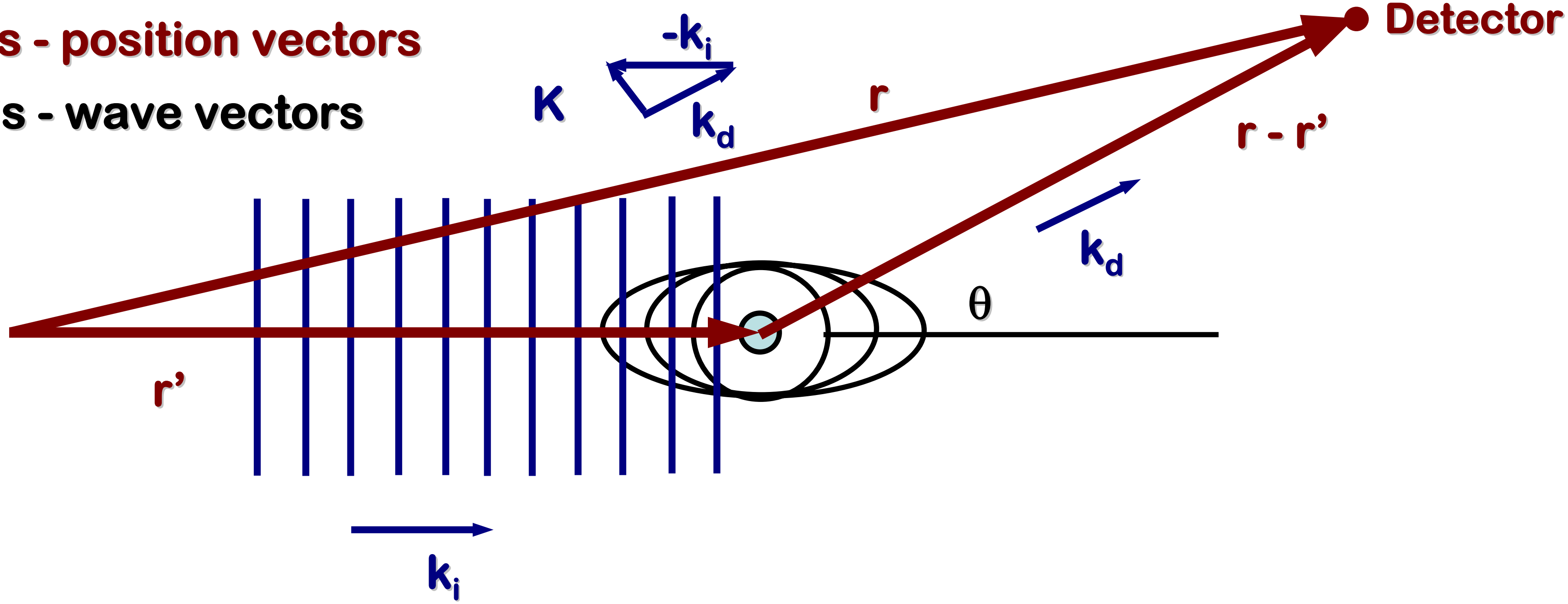


These waves have the same phase (are coherent) at these angles

Coherent elastic scattering

r's - position vectors

k's - wave vectors



Incident plane wave: $\Psi_{\text{incident}} = \exp\left[2\pi i(\vec{k}_i \cdot \vec{r}' - \omega t)\right] = \exp\left[2\pi i(\vec{k}_i \cdot \vec{r}')\right]$

Scattered wave:

$$\Psi_{\text{scattered}} = f\left(k_i, k_d\right)\frac{\exp\left[2\pi i\vec{k}_d \cdot \left(\vec{r} - \vec{r}'\right)\right]}{\left|\vec{r} - \vec{r}'\right|} = f\left(\theta\right)\frac{\exp\left[2\pi i\vec{k}_d \cdot \left(\vec{r} - \vec{r}'\right)\right]}{\left|\vec{r} - \vec{r}'\right|}$$

Atomic form factor $f(\theta)$

"scattering factor for electrons"

What is $f(\theta)$?

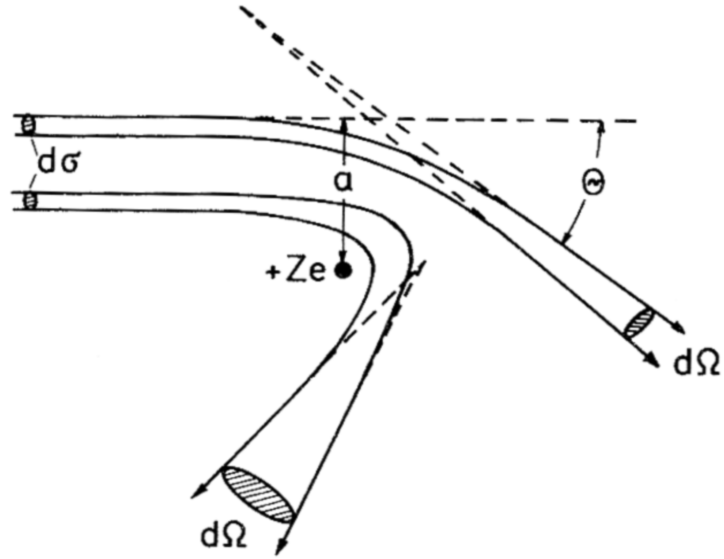
- Measures the strength of the scattering event

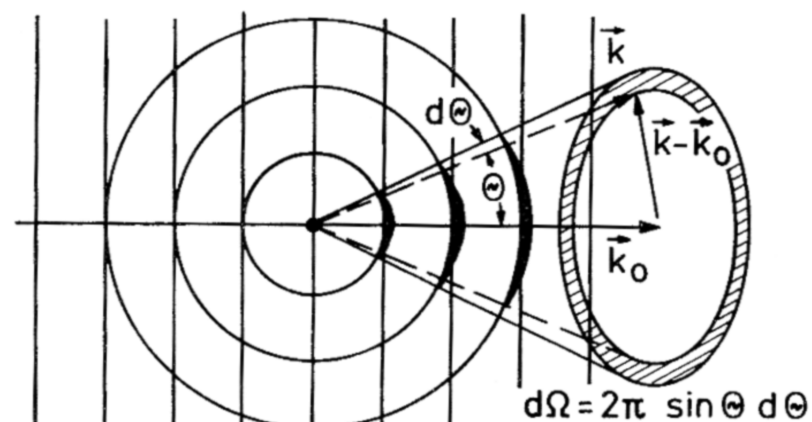
Elastic scatter has a strong angular dependence

Remember: "scattering cross section" used to describe strength of scatter earlier

See now that we are also concerned with the angular dependence

Called "differential cross section"





Atomic form factor $f(\theta)$
"scattering factor for electrons"

$f(\theta)$ is measure of amplitude of electron wave scattered from the atom

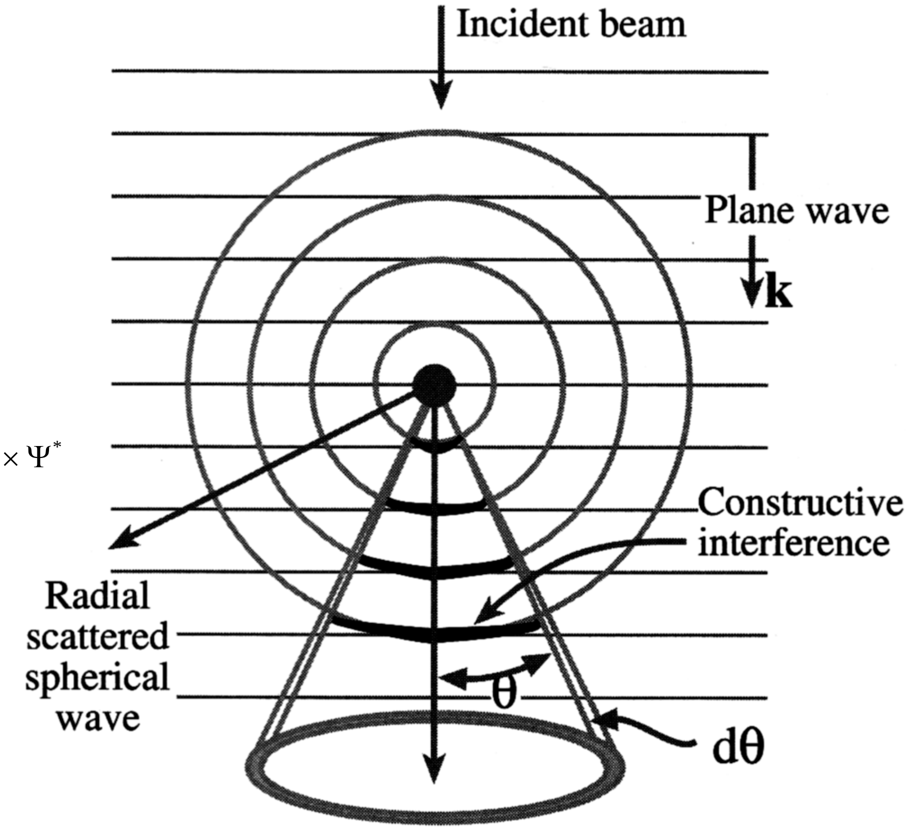
- Is thus the tendency of the scattered wave to interfere in a constructive manner with the incident wave (more on this later)

$I = \Psi \times \Psi^*$

$f^2(\theta)$ is proportional to the scattered intensity†

$$\left| f(\theta) \right|^2 = \frac{d\sigma(\theta)}{d\Omega}$$

"Differential cross section"



† $I = \Psi \times \Psi^*$

Differential cross sections

The area offered by the scatter (dσ) for scattering the incident electron into a particular increment of solid angle, dΩ

Differential cross sections can be found by solving Schrödinger Eqn inside the atom (!)

There are three primary models used to do this to find differential cross sections:

- "Screened Columbic"
- Thomas-Fermi / Rutherford
- Mott

Lots of heavier physics in this, which I'll ignore

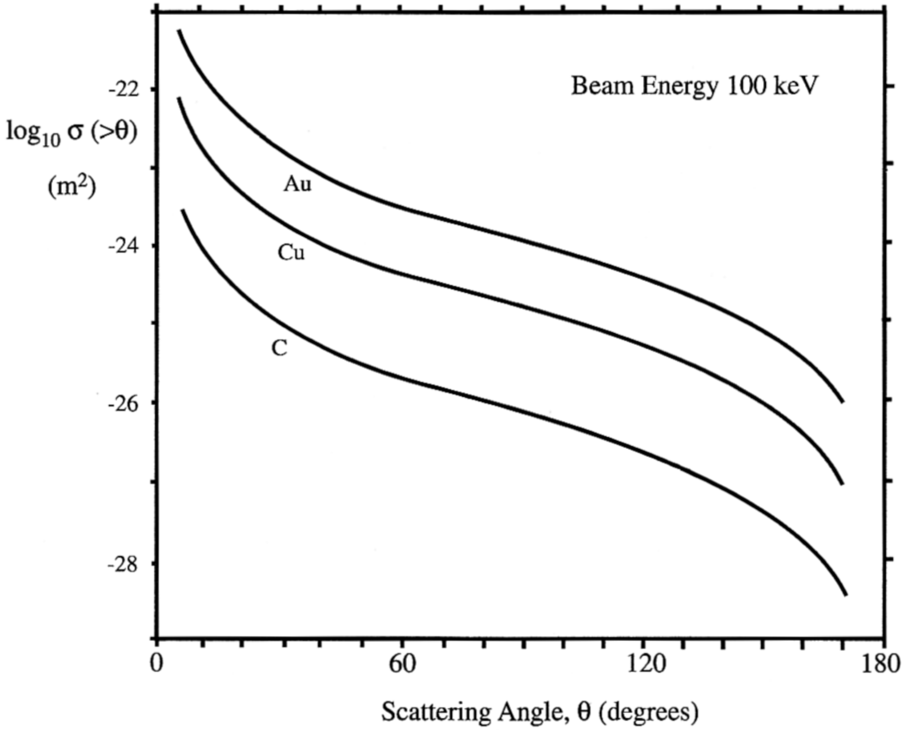
- See both Reimer and Fultz & Howe texts
- Ask me if you are interested, and we can discuss one on one

Differential cross section

Has general form shown to the right

For lower Z & lower V use the "Screened Relativistic Rutherford Cross Section"

$$\frac{d\sigma(\theta)}{d\Omega} = \frac{\lambda_R{}^4 Z^2}{64\pi^4 (a_o)^2 \left(\sin^2\frac{\theta}{2} + \left(\frac{\theta}{2}\right)^2 \right)^2}$$



Screened Relativistic Rutherford Cross Section vs. Angle

For heavier elements & larger voltages the "Mott Cross Section" is more accurate

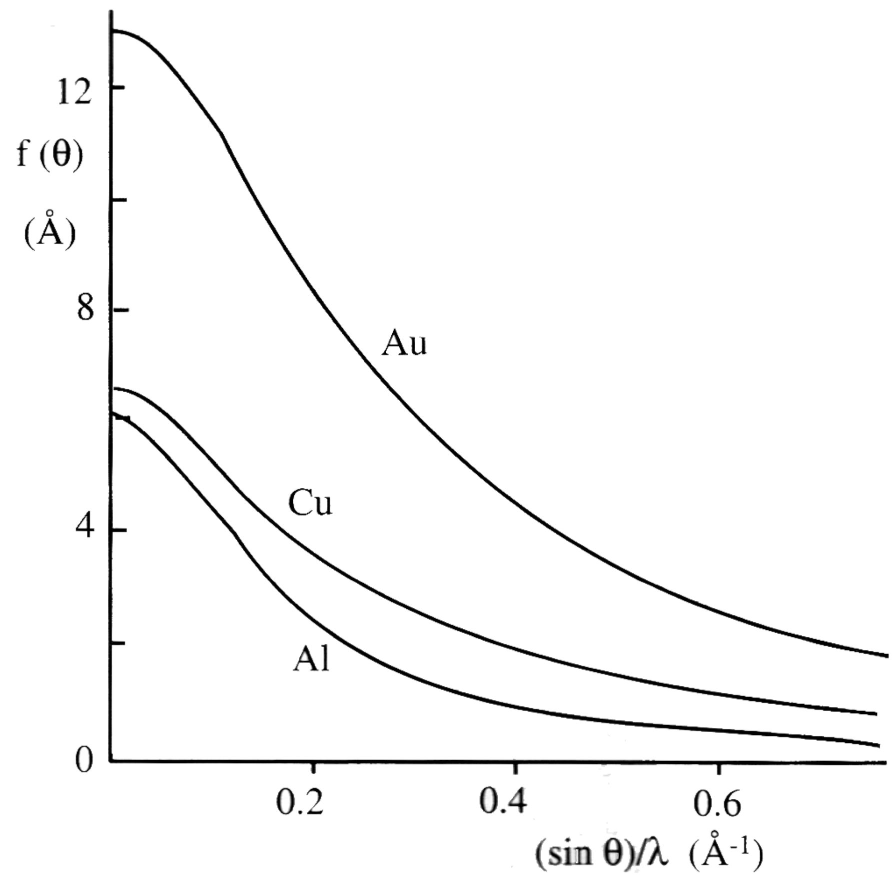
Atomic form factor $f(\theta)$

"scattering factor for electrons"

Now, with $d\sigma/d\Omega$ in hand can find $f(\theta)$:

$$\left| f(\theta) \right|^2 = \frac{d\sigma(\theta)}{d\Omega}$$

$$f(\theta) = \frac{1 + E/E_o}{8\pi^2 a} \left(\frac{\lambda}{\sin\frac{\theta}{2}} \right)^2 (Z - f_x)$$



Implications:

$\theta \Uparrow$ $\quad$ $f \Downarrow$

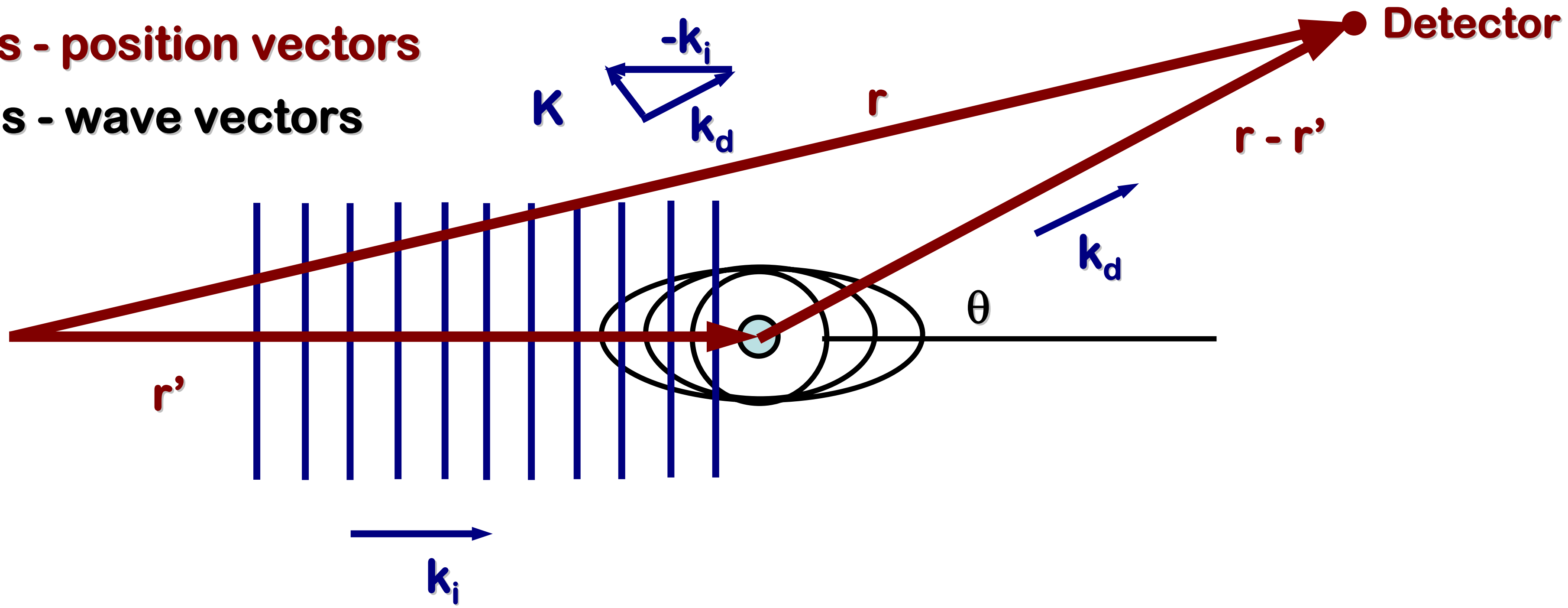
$\lambda \Uparrow$ $\quad$ $f \Downarrow$

$Z \Uparrow$ $\quad$ $f \Uparrow$

Coherent elastic scattering

r's - position vectors

k's - wave vectors



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