Elastic scattering

Lecture 2

Part 2

On to the wave perspective …

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:

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

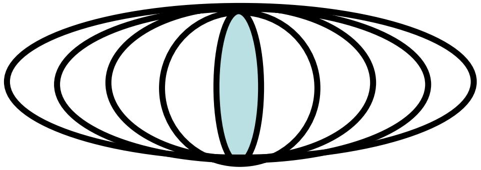
k → fixed

p → infinite (unknown)

Electron in free space

Spherical wave:

- Isotropic wave propagating outwards from a point



Wave Eqn:

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

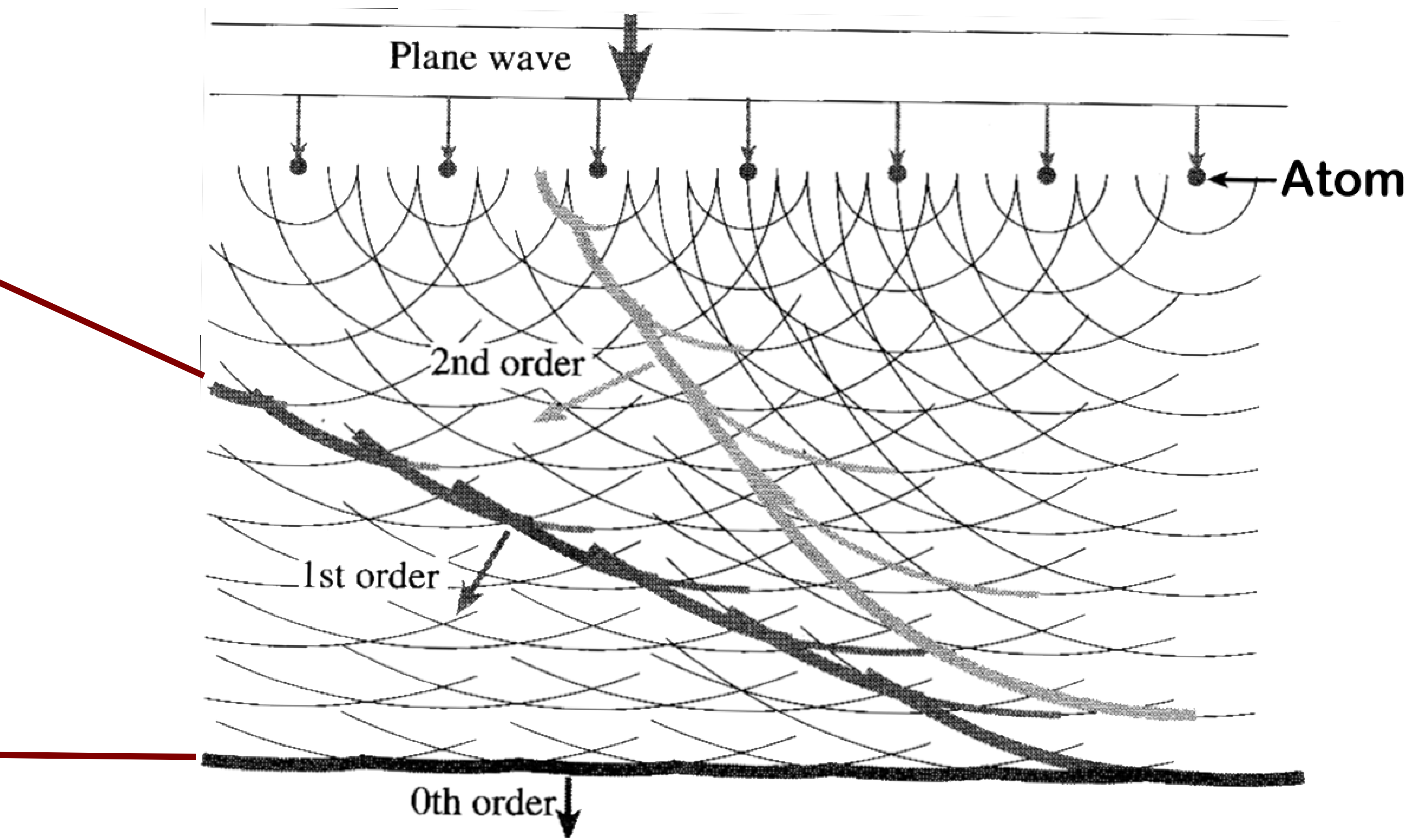
Solution:

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

Time independent

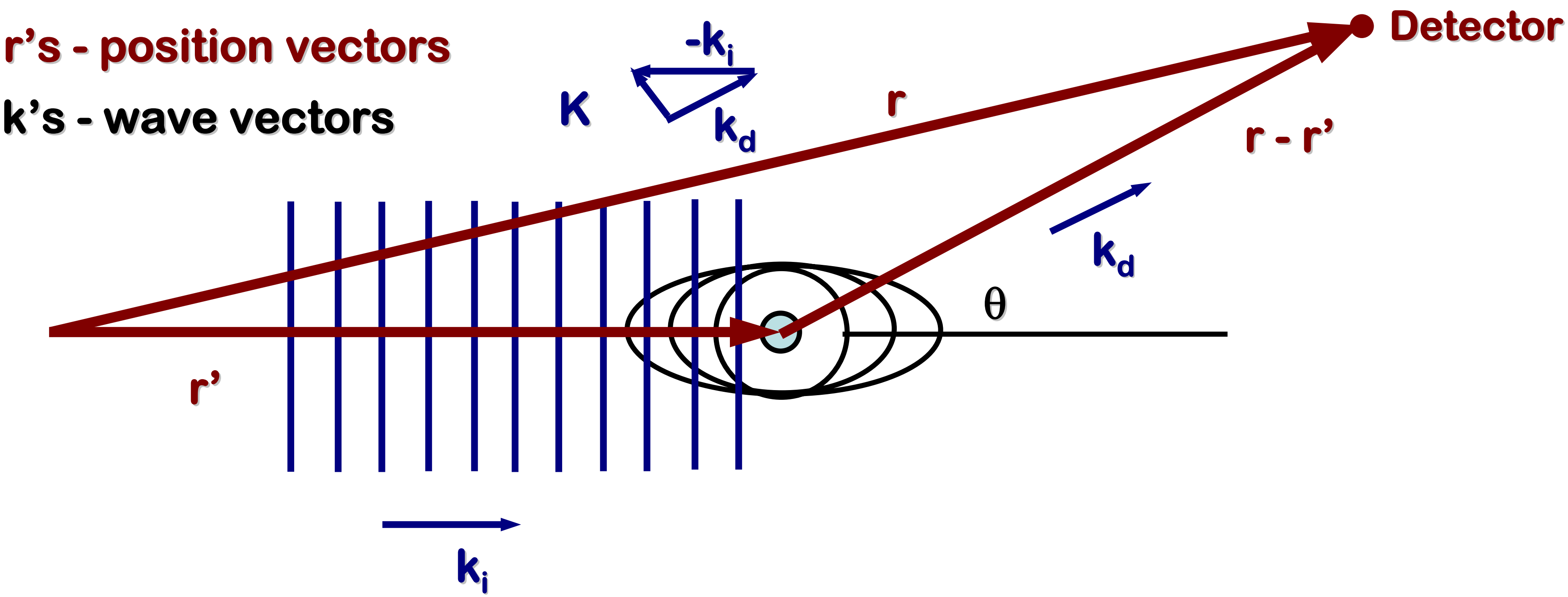
$$\psi = \psi_o \frac{\exp(ikr)}{r}$$

Coherence & Incoherence



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

Coherent elastic scattering



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:

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

Atomic form factor $f(\theta)$

"scattering factor for electrons"

What is $f(\theta)$?

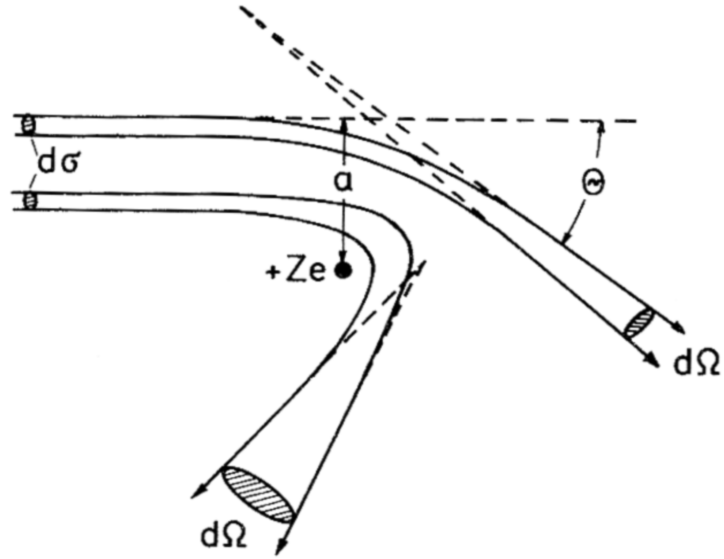
- Measures the strength of the scattering event

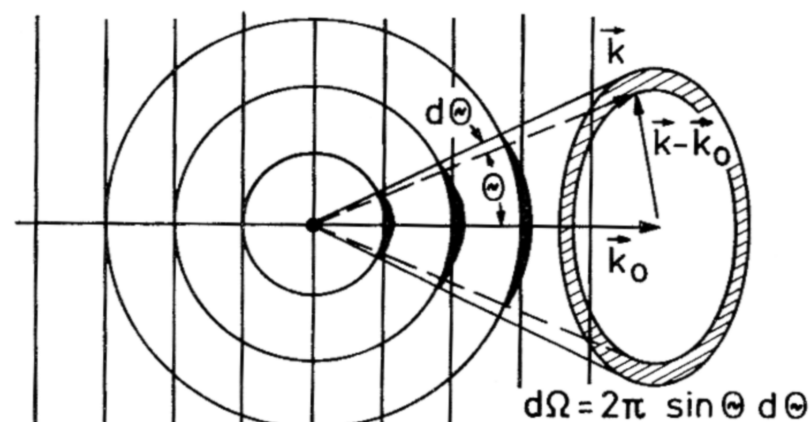
Elastic scatter has a strong angular dependence

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"

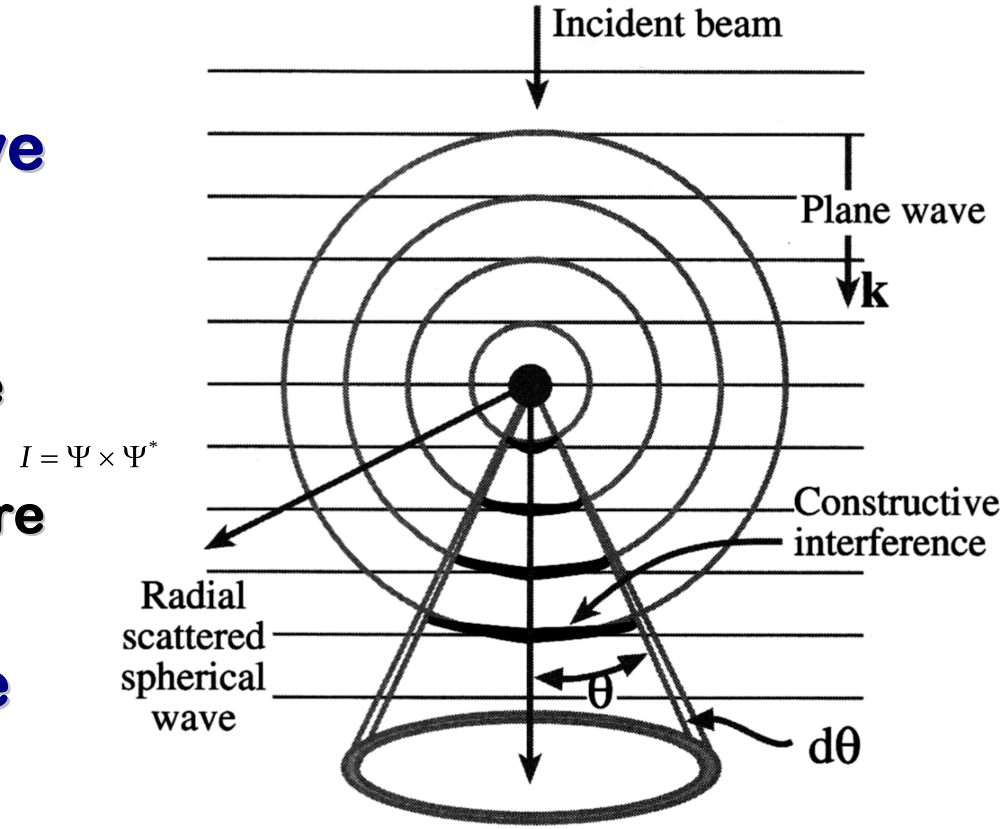
$f(\theta)$ is measure of amplitude of electron wave scattered from the atom

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

$f^2(\theta)$ 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

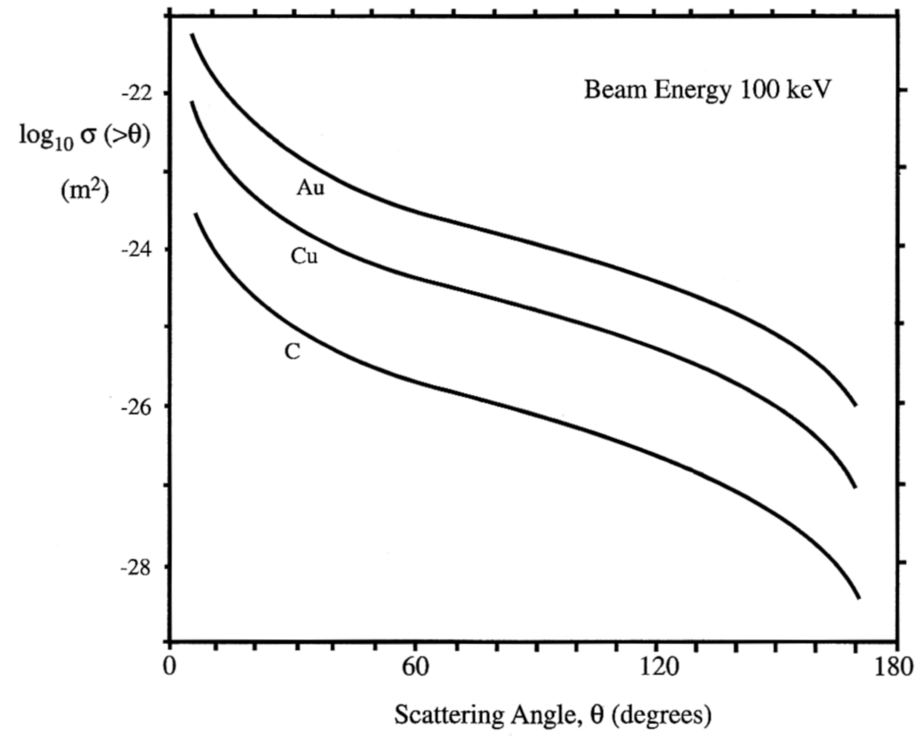
- The area offered by the scatter ($d\sigma$) for scattering the incident electron into a particular increment of solid angle, $d\Omega$
- Differential cross sections can be found by solving Schrödinger Eqn inside the atom (!)
- There are three primary <u>models</u> used to do this to find differential 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

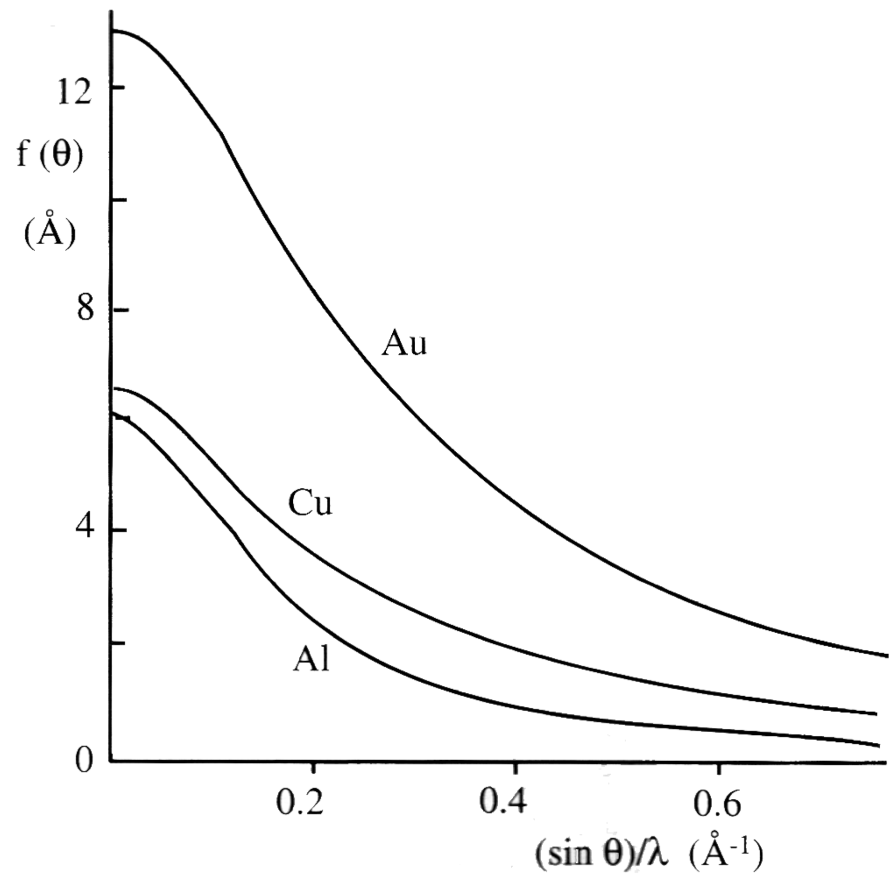
Atomic form factor $f(\theta)$

"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:

$\theta \Uparrow$ $f \Downarrow$

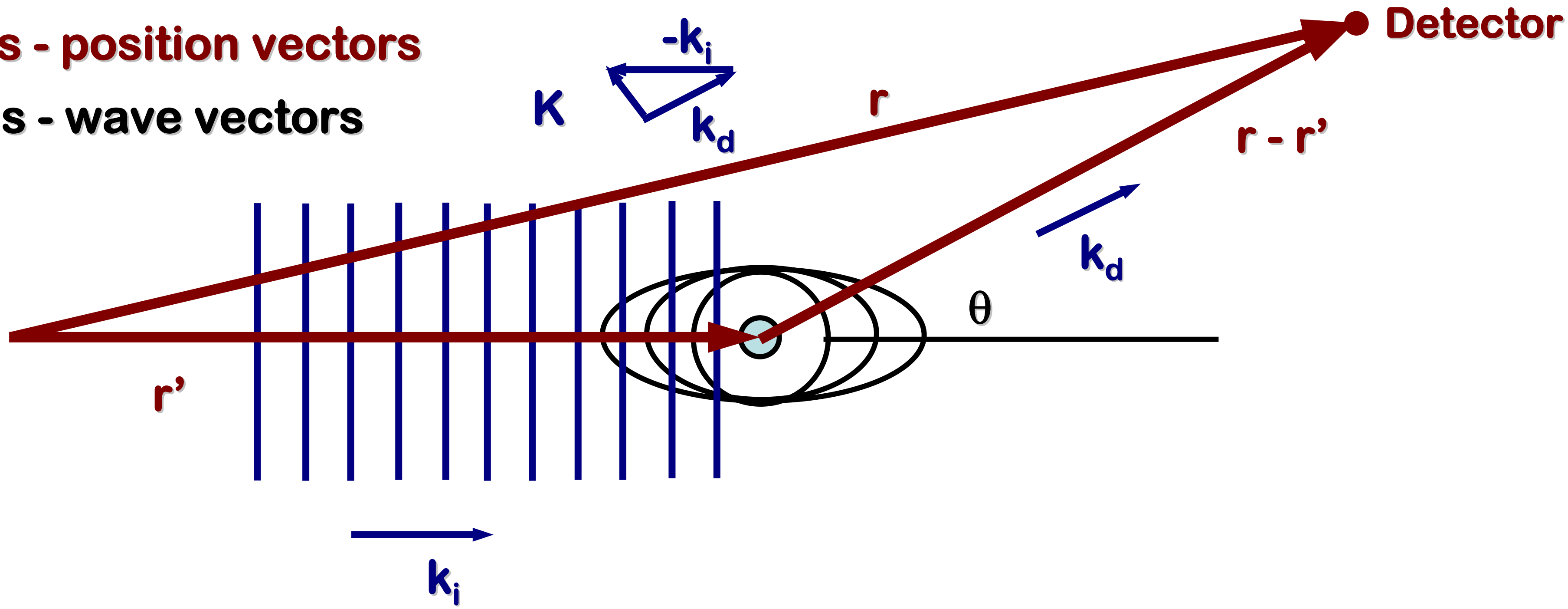
$\lambda \Uparrow$ $f \Downarrow$

$Z \Uparrow$ $f \Uparrow$

Coherent elastic scattering

r's - position vectors

k's - wave vectors



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Scattered wave:

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

Atomic form factor $f(\theta)$

"scattering factor for electrons"

Additionally, can use a Green's function approach to formally solve the Schrödinger Eqn. for the electron when it is under the influence of the atomic potential

$$\psi(\vec{r}) = \psi_{inc} + \psi_{scatt}$$

$$= \exp\left(2\pi i \vec{k}_i \cdot \vec{r}\right) + \frac{2m}{h^2}\int V(\vec{r}')\psi(\vec{r}')G(\vec{r},\vec{r}')d^3\vec{r}'$$

Atomic form factor $f(\theta)$

"scattering factor for electrons"

In the limit of weak scattering (called "first Born approximation" or "kinematical theory of diffraction"), this Green's function is:

$\vec{r} >> \vec{r}'$

$$G(\vec{r},\vec{r}') = \frac{-1}{4\pi}\frac{\exp\left[2\pi i \vec{k}_d \cdot (\vec{r}-\vec{r}')\right]}{|\vec{r}|}$$

Again: See Fultz & Howe or Reimer for details

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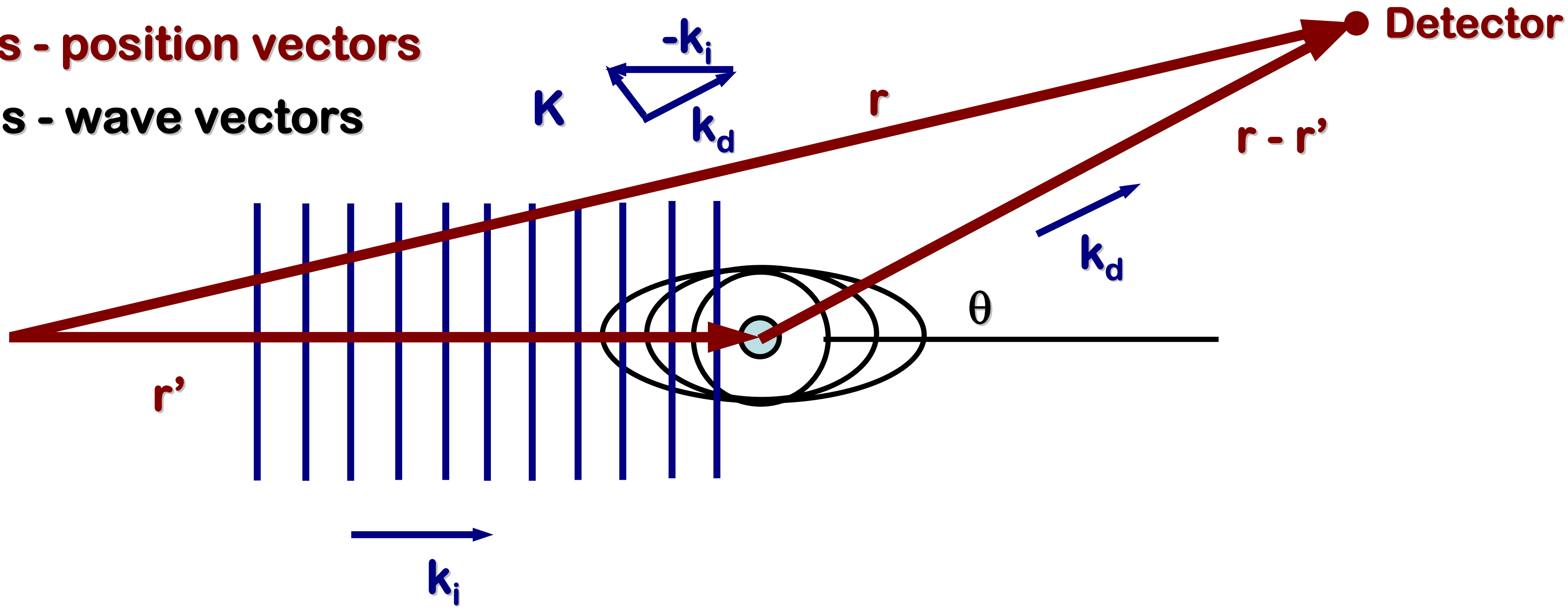

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Atomic form factor $f(\theta)$
"scattering factor for electrons"

$\vec{r} >> \vec{r}'$

Substitute:

$$\psi(\vec{r}) = \psi_{inc} + \psi_{scatt}$$

$$= \exp(2\pi i \vec{k}_i \cdot \vec{r}) - \frac{2m}{h^2}\int V(\vec{r}')\psi(\vec{r}')G(\vec{r},\vec{r}')d^3\vec{r}'$$

$$\exp(2\pi i \vec{k}_i \cdot \vec{r}') \qquad \frac{-1}{4\pi}\frac{\exp\left[2\pi i \vec{k}_d \cdot (\vec{r}-\vec{r}')\right]}{|\vec{r}|}$$

$$\psi(\vec{r}) =$$

$$\exp(2\pi i \vec{k}_i \cdot \vec{r}) - \frac{2m}{h^2}\frac{\exp(2\pi i \vec{k}_d \cdot \vec{r})}{|\vec{r}|}\int V(\vec{r}')\exp\left[2\pi i(\vec{k}_i - \vec{k}_d)\right]d^3\vec{r}'$$

Atomic form factor $f(\theta)$

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Additionally, can use a Green's function approach to formally solve the Schrödinger Eqn. for the electron when it is under the influence of the atomic potential

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Atomic form factor

So, with weak scattering, we have:

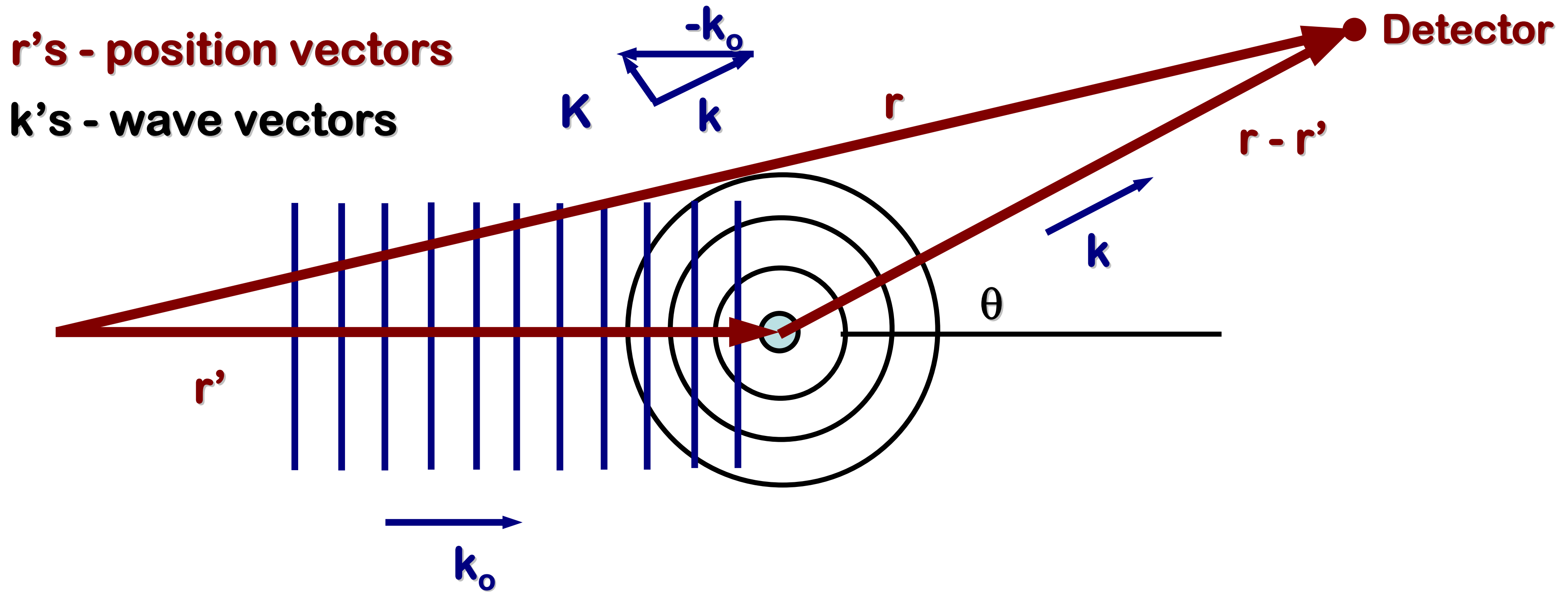
$$\psi_{scatt} = f_{el}(\vec{K}) \frac{\exp(2\pi i \vec{k}_d \cdot \vec{r})}{|\vec{r}|} \qquad \vec{K} = \vec{k}_i - \vec{k}_d$$

$$\text{w/ } f_{el}(\vec{K}) = \frac{-m}{2\pi h^2} \int V_{atom}(\vec{r}') \exp\left[-2\pi i (\vec{K} \cdot \vec{r}')\right] d^3\vec{r}'$$

Scattered wave is proportional to Fourier transform of scattering potential

$$\Psi_{scattered}(\vec{K},\vec{r}) = \frac{-m}{2\pi\hbar^2} \frac{\exp\left[2\pi i (\vec{k}_d \cdot \vec{r})\right]}{|\vec{r}|} \int V_{atom}(\vec{r}') \exp\left[-2\pi i (\vec{K} \cdot \vec{r}')\right] d^3\vec{r}'$$

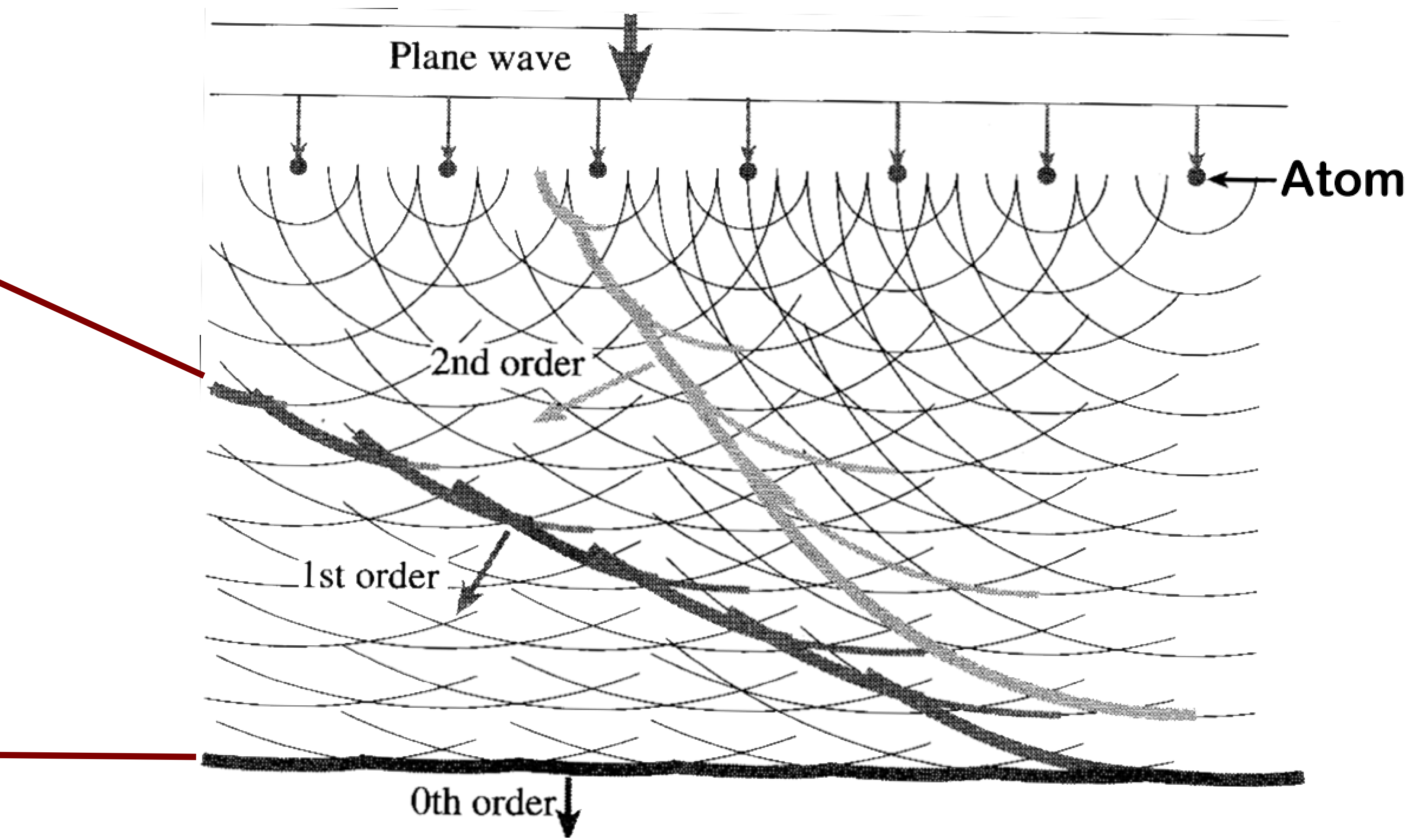
Total wave



$$\psi_{total}(\vec{r}') = \psi_{incident}(\vec{r}') + \psi_{scattered}(\vec{r}')$$

$$= \exp\left[2\pi i(\vec{k}_i \cdot \vec{r}')\right] + \frac{-m}{2\pi\hbar^2} \frac{\exp\left[2\pi i \vec{k}_d \cdot \vec{r}\right]}{|\vec{r}|} \int V_{atom}(\vec{r}') \exp\left[-2\pi i(\vec{K} \cdot \vec{r}')\right] d^3\vec{r}'$$

Coherence & Incoherence



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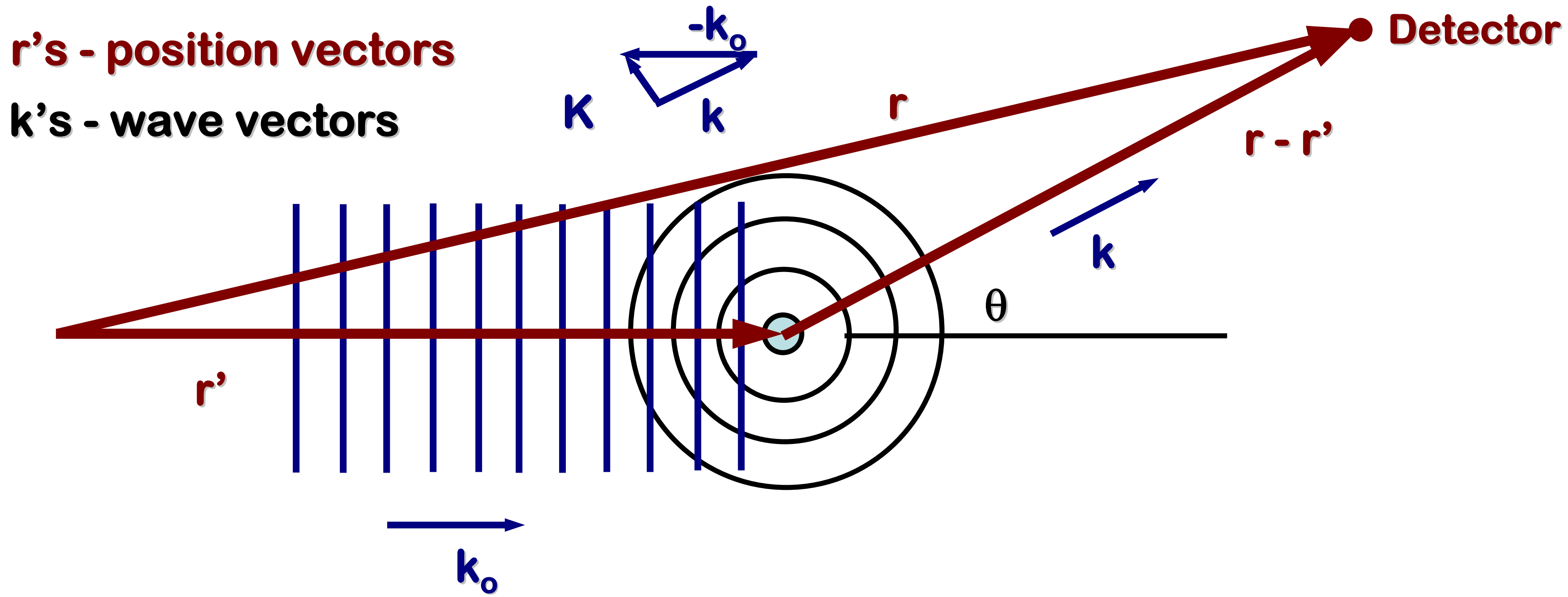

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Atomic form factor

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$$\text{w/ } f_{el}(\vec{K}) = \frac{-m}{2\pi h^2}\int V_{atom}(\vec{r}')\exp\left[-2\pi i(\vec{K}\cdot\vec{r}')\right]d^3\vec{r}'$$

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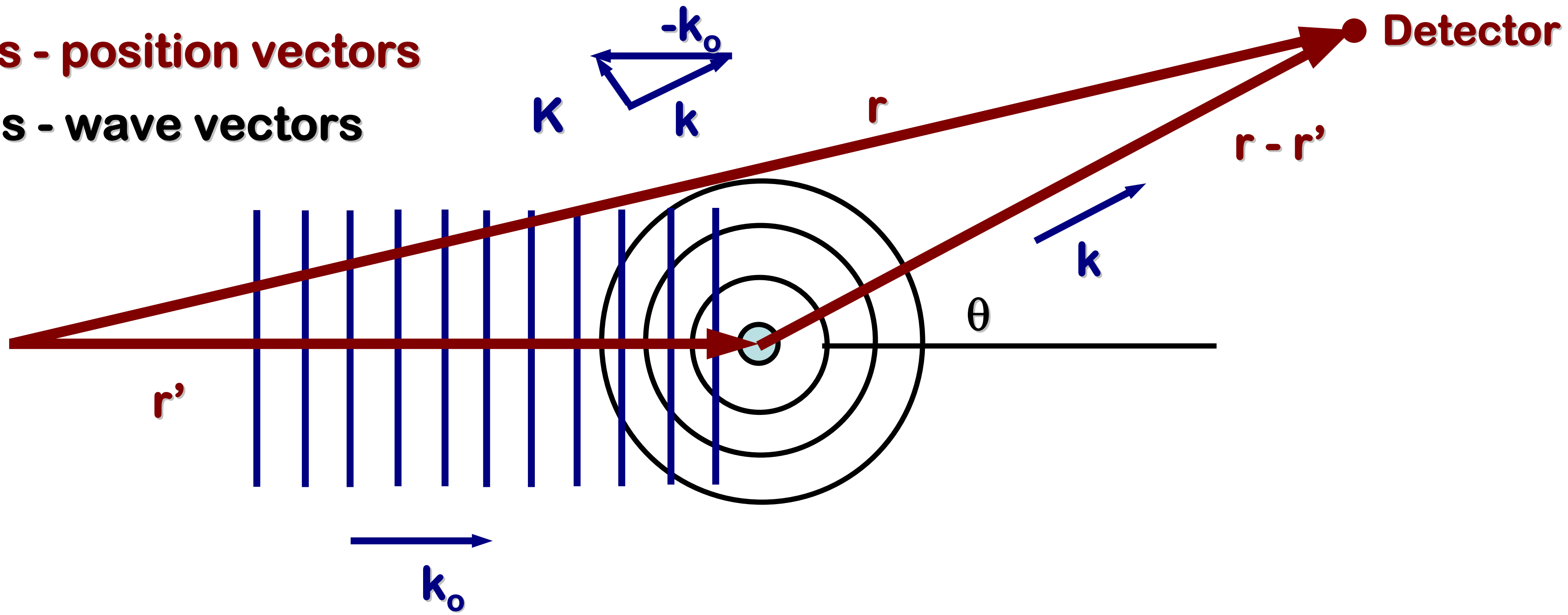
Total wave

r's - position vectors

k's - wave vectors



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