

Atomic scattering

Lecture 6

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Rutherford scattering

Experiment that uncovered the basic structure of the atom

If we want to investigate the nucleus (something small), we need a probe with a short wavelength

For short wavelength we need high energy

Nuclei \sim fm in size (say 10)

Light – $E = hc/\lambda = 12$ GeV

Electron – $E = 100$ MeV

Alpha particle – $E = 2$ MeV

Easier to use heavier particles

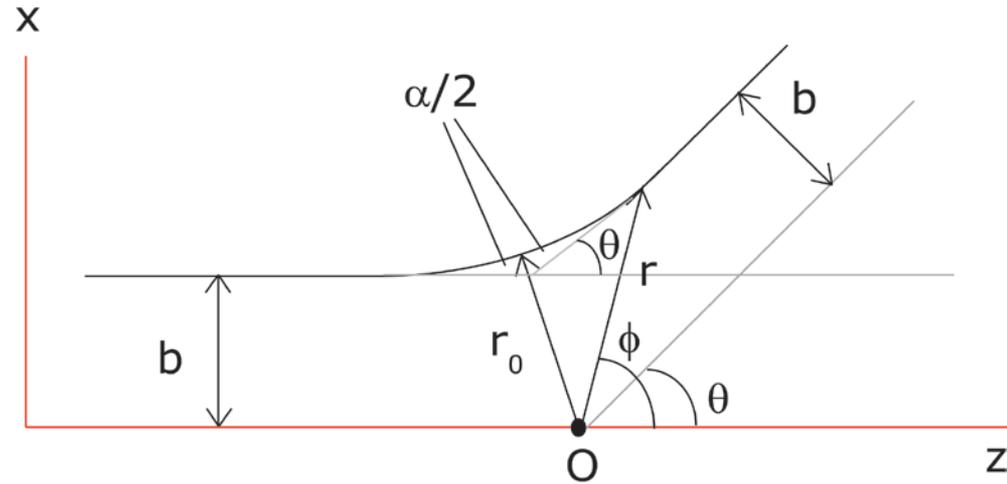
Rutherford scattering

$$\alpha = 2[\phi(r = \infty) - \phi(r = r_0)]$$

$$= 2 \int_{r_0}^{\infty} \frac{L}{mr^2} \left\{ \frac{2}{m} [E - V(r)] - \frac{L^2}{m^2 r^2} \right\}^{-1/2} dr$$

r_0 is given by

$$E - V(r) - \frac{L^2}{2mr^2} = 0$$



OK for electron scattering, but for nuclear scattering, replace m with μ (reduced mass). Also $E \rightarrow E_{\text{cm}}$ and $\theta \rightarrow \theta_{\text{cm}}$.

Now $V(r) = \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0 r}$ and we can substitute and rearrange the equations above

Rutherford scattering

Now we have: $r_0 = \frac{1}{2} \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0 E_{cm}} \left[1 + \sqrt{1 + \left(\frac{2b 4\pi\epsilon_0 E_{cm}}{Z_1 Z_2 e^2} \right)^2} \right]$ and

$$b = \frac{1}{2} \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0 E_{cm}} \cot(\theta_{cm}/2)$$

for $b=0$, we have $r_0 = \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0 E_{cm}}$ - minimum distance of closest approach

Call this "D"

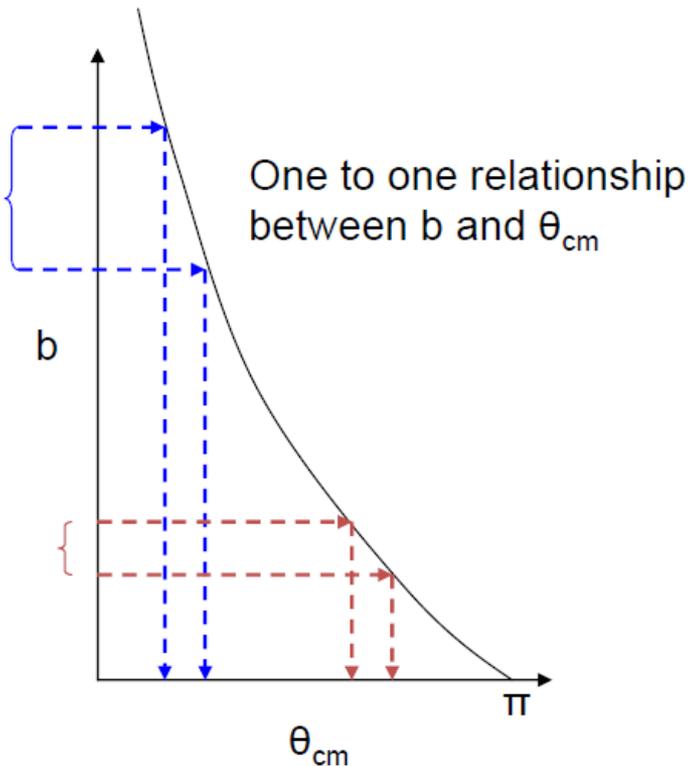
$$r_0 = \frac{D}{2} \left[1 + \sqrt{1 + \left(\frac{2b}{D} \right)^2} \right] \quad b = \frac{D}{2} \cot(\theta_{cm}/2)$$

Rutherford Scattering

$$b = \frac{D}{2} \cot(\theta_{cm}/2)$$

Small $\theta_{cm} \rightarrow$ large b (large l , angular momentum)

Where will Rutherford scattering peak?



Forward or backwards angles?

From earlier lecture (no. 2) we have

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta_{cm}} \left| \frac{db}{d\theta_{cm}} \right|$$

Rutherford Scattering

So we have:

$$\begin{aligned}\frac{d\sigma}{d\Omega}\Big|_{Ruth}^{cm} &= \frac{D}{16 \sin^4(\theta_{cm}/2)} \\ &= \left(\frac{Z_1 Z_2 e^2}{4\pi\epsilon_0}\right)^2 \frac{1}{E_{cm}^2} \frac{1}{16 \sin^4(\theta_{cm}/2)}\end{aligned}$$

result is identical to Q.M. formulation.

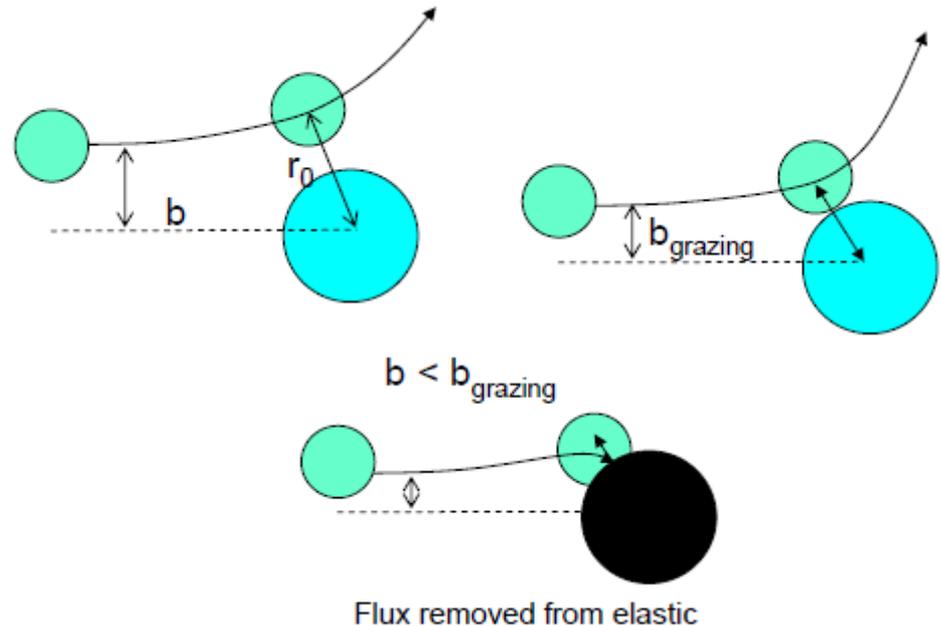
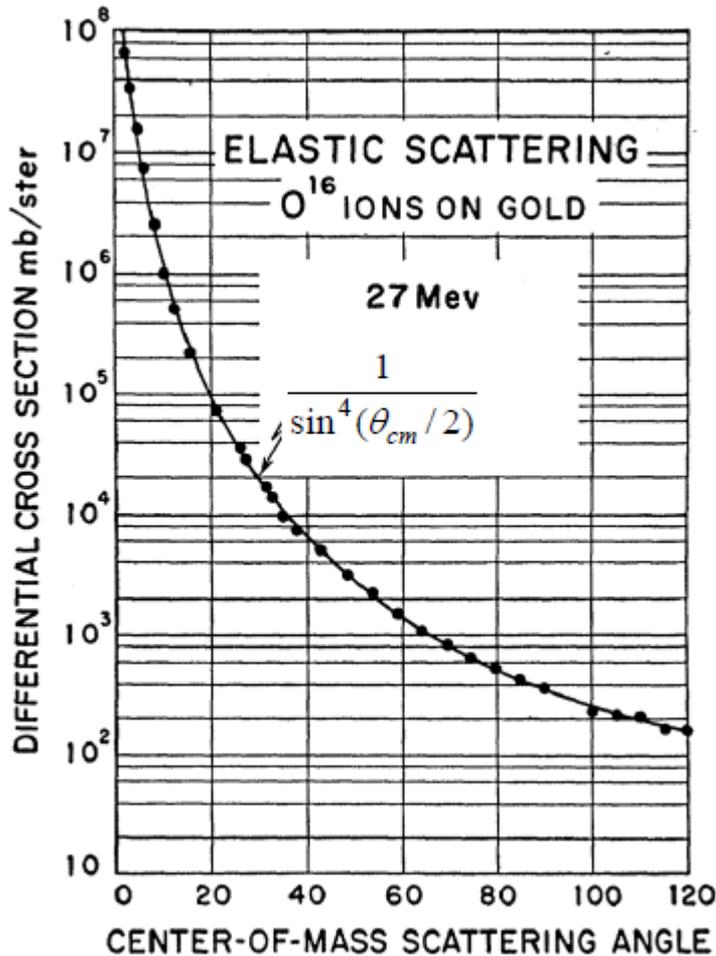
Cross section properties:

Strongly forward peaked

Inversely proportional to E_{cm}^2

For a fixed Z_1 , depends on $(Z_2)^2$

Rutherford scattering

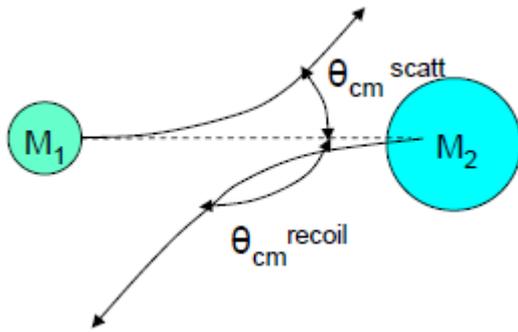


Below $b_{grazing}$, strong nuclear force becomes important

Classically, $\left. \frac{d\sigma}{d\Omega} \right|_{Ruth}^{cm} \rightarrow 0$

Rutherford Scattering

Applied in materials analysis:



Energy of scattered particle depends on mass of scattering nucleus

$$E_{lab}^{scat} = E_{lab}^{incident} \left[1 - \frac{2M_1M_2}{(M_1 + M_2)^2} (1 - \cos \theta_{cm}^{scat}) \right]$$

Characterise material composition

Good for detecting low mass impurities (ie: H)

Beyond the Born Approximation

How do we deal with the wave functions (target and projectile) before, during and after collision?

Projectile as a plane wave is only strictly good for high energies

Consider polarisation – charge cloud is distorted, but this then affects the incoming electron wave

Target wavefunction

“Exact” solutions known for H, but for more complex systems approximate methods are used to build target wavefunctions

Hartree-Fock approach – independent particle approximation, each electron interacts independently with the nucleus and an average of the other electrons

Hydrogen atom scattering

Simplest system for examining atomic collisions

Still can be complex, it is a three body problem

Can consider the scattering complex as a “two-electron” atom

Two electron system can be described using spatial eigenfunction and a spin eigenfunction (for the electron spins)

Full eigenfunction is a product of spatial and spin parts

$$\Psi(q_1, q_2) = \psi(r_1, r_2) \chi(1, 2)$$

q_i are the space and spin coordinates of electron i

Hydrogen atom scattering

As for helium atom, spatial functions satisfy the Schrödinger equation:

$$\left[-\frac{1}{2} \nabla_{r_1}^2 - \frac{1}{2} \nabla_{r_2}^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} \right] \psi(r_1, r_2) = E \psi(r_1, r_2)$$

Spin functions can be written $\alpha(1), \beta(1)$ and $\alpha(2), \beta(2)$

Each electron can be spin up or spin down

independent of the other

We get 4 separate spin states:

$$\chi_1(1,2) = \alpha(1)\alpha(2) \quad \uparrow\uparrow$$

$$\chi_2(1,2) = \alpha(1)\beta(2) \quad \uparrow\downarrow$$

$$\chi_3(1,2) = \beta(1)\alpha(2) \quad \downarrow\uparrow$$

$$\chi_4(1,2) = \beta(1)\beta(2) \quad \downarrow\downarrow$$

Hydrogen atom scattering

χ_1 and χ_4 are symmetric with respect to exchange

They are eigenstates of S^2 , where $S = S_1 + S_2$

χ_2 and χ_3 are neither symmetric or antisymmetric

Remember, symmetric means $\psi \rightarrow \psi$ under exchange of all coordinates

antisymmetric means $\psi \rightarrow -\psi$

in fact, antisymmetry is true for the exchange of coordinates ANY two particles

We can make symmetric and antisymmetric forms from linear combinations of χ_2 and χ_3

$$\chi_+ = \frac{1}{\sqrt{2}} [\chi_2(1,2) + \chi_3(1,2)] \quad \chi_- = \frac{1}{\sqrt{2}} [\chi_2(1,2) - \chi_3(1,2)]$$

Hydrogen atom scattering

We can now define 4 independent spin functions, labelled with total spin, S , and the spin projection, M_S

One is antisymmetric

$$\chi_{0,0}(1,2) = \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) - \beta(1)\alpha(2)]$$

Singlet spin function (spins parallel)

Three are symmetric

$$\chi_{1,1}(1,2) = \alpha(1)\alpha(2)$$

$$\chi_{1,0}(1,2) = \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) + \beta(1)\alpha(2)]$$

$$\chi_{1,-1}(1,2) = \beta(1)\beta(2)$$

Triplet spin function (antiparallel)

Hydrogen atom scattering

Pauli exclusion says that the TOTAL wavefunction must be antisymmetric under the exchange of coordinates for any two electrons

$$\Psi(q_1, \dots, q_N) \rightarrow -\Psi(q_1, \dots, q_N)$$

for a system of N electrons

For the “2-electron complex” in our scattering, we must combine symmetric spatial with antisymmetric spin and antisymmetric spatial with symmetric spin

Hydrogen atom scattering

Total wavefunctions

$$\Psi(q_1, q_2) = \psi_+(r_1, r_2) \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) - \beta(1)\alpha(2)]$$

$$\alpha(1)\alpha(2)$$

$$\Psi(q_1, q_2) = \psi_-(r_1, r_2) \times \frac{1}{\sqrt{2}} [\alpha(1)\beta(2) + \beta(1)\alpha(2)]$$
$$\beta(1)\beta(2)$$

Remembering that the spatial parts satisfy:

$$\left[-\frac{1}{2} \nabla_{r_1}^2 - \frac{1}{2} \nabla_{r_2}^2 - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{r_{12}} - E \right] \psi(r_1, r_2) = 0$$

origin is the proton (H^+) and r_1 and r_2 are the position vectors of the electrons

Hydrogen atom scattering

What are the boundary conditions?

Initial state of H atom is the ground state (1s), described by $\psi_{100}(r)$, the hydrogenic wavefunction

Total energy is given by: $E_{Tot} = E_1 + \frac{1}{2}k_1^2$

where E_1 is the ground state energy of H = -13.6 eV = -1/2 a.u. and $\frac{1}{2}k_1^2$ is the incident electron kinetic energy

In elastic scattering, the wave function where $r_1 \gg r_2$ will represent electron 1 moving with respect to a ground state H atom containing electron 2

Hydrogen atom scattering

Thus we have:

$$\psi_{\pm}(r_1, r_2) \xrightarrow{r_1 \rightarrow \infty} F_1^{\pm}(r_1) \psi_{100}(r_2)$$

and

$$\psi_{\pm}(r_1, r_2) \xrightarrow{r_2 \rightarrow \infty} \pm F_1^{\pm}(r_2) \psi_{100}(r_1)$$

where $F(r)$ is the free electron wavefunction (an incident plane wave and outgoing spherical wave – as is our usual boundary condition)

Take the incident direction as the z-axis, and let the amplitude of the wavefunction be unity

Hydrogen atom scattering

$$F_1^\pm(r) \xrightarrow{r_1 \rightarrow \infty} e^{ik_1 z_1} + f_1^\pm(k_1, \theta, \phi) \frac{e^{ik_1 r_1}}{r_1}$$

In this case, f^\pm is the scattering amplitude for the singlet (+) and triplet(-) states

$$f^+ \rightarrow \psi^+ \chi^-$$

$$f^- \rightarrow \psi^- \chi^+$$

Now, if the incident beam and the target are unpolarised (spin is randomly oriented), 3 times as many collisions occur in the triplet states, and:

$$\frac{d\sigma}{d\Omega} = \frac{1}{4} |f_1^+|^2 + \frac{3}{4} |f_1^-|^2$$

Hydrogen atom scattering

Now we have to calculate the scattering amplitudes

It is possible to do this exactly (in terms of the wavefunctions) but this is still very difficult

Typically, simplifications and approximations are made

Static-Exchange Approximation

Essentially includes only the “static” part of the Hamiltonian and the exchange part, but does not include “dynamic” polarisability effects

The electron-H elastic scattering wave function can then be written as a symmetrised product

Static-exchange approximation

$$\psi_{\pm}(r_1, r_2) = \left[F_1^{\pm}(r_1)\psi_1(r_2) \pm F_1^{\pm}(r_2)\psi_1(r_1) \right]$$

and F satisfies the equation:

$$\left(\nabla_1^2 + k_1^2 \right) F_1^{\pm}(r_1) = 2V_{11}(r_1)F_1^{\pm}(r_1) \pm 2 \int K_{11}(r_1, r_2) F_1^{\pm}(r_2) dr_2$$

K is the *exchange* potential and V_{11} is the static potential

$$\begin{aligned} V_{11}(r_1) &= \left\langle \psi_1 \left| -\frac{1}{r_1} + \frac{1}{|r_1 - r_2|} \right| \psi_1 \right\rangle \\ &= -\frac{1}{r_1} + \int \frac{|\psi_1(r_2)|^2}{|r_1 - r_2|} dr_2 \end{aligned}$$

Static-exchange approximation

For atomic hydrogen we have:

$$\psi_1 = \pi^{-1/2} e^{-r/2}$$
$$\Rightarrow V_{11}(r_1) = -\left(1 + \frac{1}{r_1}\right) e^{-2r_1}$$

The exchange potential is non-local and is given by:

$$K_{11}(r_1, r_2) = \psi_1^*(r_1) \psi_1(r_2) \left[\frac{1}{|r_1 - r_2|} - (E_{Tot} - 2E_1) \right]$$

In this approximation, the main processes that we leave out are the dynamic distortion of the target, and the loss of incident flux into elastic channels (above the first inelastic threshold)

Close coupling approach

Also called the coupled channels approach

In this approximation, the target wavefunction is considered to include additional configurations to account for the dynamic distortion

$$\psi_{\pm}(r_1, r_2) = \sum_{q=1}^N \left[F_q^{\pm}(r_1) \psi_q(r_2) \pm F_q^{\pm}(r_2) \psi_q(r_1) \right]$$

Now we have F_q , which are *channel wavefunctions* and represent different excited states of the atom and now we can write:

$$\left(\nabla_1^2 + k_q^2 \right) F_q^{\pm}(r_1) = 2 \sum_{q'=1}^N V_{qq'}(r_1) F_{q'}^{\pm}(r_1) \pm 2 \sum_{q'=1}^N \int K_{qq'}(r_1, r_2) F_{q'}^{\pm}(r_1) dr_2$$

Close coupling approach

There is now a set of N coupled equations where:

$V_{qq'}$ are the direct potentials

$K_{qq'}$ are the exchange potentials

This technique can do a good job for low energy electron scattering from light atoms

Atomic charge cloud distortion is represented by “virtual” excitation of closed channels

Also called “virtual states”

Born Approximation for Hydrogen

Recall the Born approximation:

$$f(\theta) = -\frac{2\mu}{\hbar^2} \int e^{ik_0(n_0 - n) \cdot r} U(r) dr$$

and $n \cdot n_0 = \cos\theta$

Now we can use the potential of an electron in the static field of the H atom in its ground state

$$U(r) = -e^2 \left(\frac{1}{r} + \frac{1}{a_0} \right) e^{-2r/a_0}$$

performing the integration we get:

$$f(\theta) = \frac{\frac{1}{2a_0} \left(\frac{2}{a_0^2} + k^2 \sin^2 \theta / 2 \right)}{\left(\frac{1}{a_0^2} + k^2 \sin^2 \theta / 2 \right)^2}$$

Born Approximation for Hydrogen

In the limit of small angle (θ), we get:

$$f(\theta) \rightarrow a_0$$

and

$$\frac{d\sigma}{d\Omega}(\theta = 0^0) = a_0^2$$

That is, the differential cross section at 0^0 is independent of energy in the Born approximation

We know that this is not the case – limitation of the approximations made

Spin dependent interactions

We have seen that collisions are a complex interplay of many different Coulomb interactions

Sometimes the scattering is dominated by one interaction, which shows up in the cross sections

- Polarisation

- Exchange

- Static interaction

This can mask more subtle effects, so how can we separate these out from everything else?

“Spin-tagging”

We can use electron spin to study the effects of spin-dependent interactions

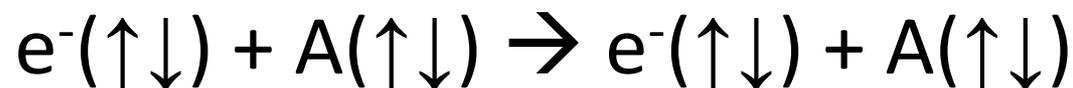
Create a spin-polarised beam of electrons – “tag” them

Study interactions like exchange and the spin-orbit interaction

Consider the following process:



if we consider the spin (for an unpolarised beam), we can write



Spin dependent interactions

In the previous example, there is no spin orientation of the incident, scattered or target particles

Cross section is then an average over the spins

$$\begin{aligned}\frac{d\sigma}{d\Omega} &= \frac{1}{2}|f|^2 + \frac{1}{2}|g|^2 + \frac{1}{2}|f - g|^2 \\ &= \frac{1}{4}|f + g|^2 + \frac{3}{4}|f - g|^2 \\ &= \frac{1}{4}|F^+|^2 + \frac{3}{4}|F^-|^2\end{aligned}$$

where f is the direct amplitude and g is the exchange amplitude (note there is a singlet and a triplet case)

Spin dependent interactions

We can directly study the effects of spin in scattering by using spin polarised beams

Consider a beam of 10 electrons

↑↑↑↑↓↓↓↓↓↓

We can define the polarisation as:

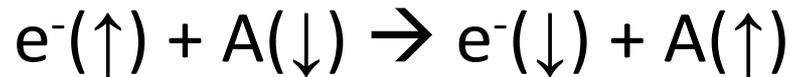
$$P = \frac{N(\uparrow) - N(\downarrow)}{N(\uparrow) + N(\downarrow)}$$
$$= 0.2$$

20% of the beam is completely polarised and 80% is unpolarised and we have

$$0 < |P| < 1$$

Spin dependent interactions

Now if we use polarised beam of spin up electrons and a polarised beam of spin down targets (atoms) we can look for differences in the polarisation of the scattered beam/target



in this case we can see that a spin flip has occurred

What can cause this?

Spin-orbit interaction

This is the interaction between the electron spin and the orbital angular momentum about the nucleus

Recall from previous lecture that we have:

$$\Delta E \propto \frac{Z}{r} \frac{dV}{dr} \mathbf{s} \cdot \mathbf{l}$$

Strength of the interaction depends on Z

This can change the polarisation of the scattered beam relative to the incident beam

We can consider the scattering of unpolarised electrons from mercury (Hg, $Z = 80$)