1 STRUCTURE OF THE ATOM

LECTURE 1

Content

In this lecture we will discuss the evidence that existed pre-1900 that matter is not continuously divisible into smaller and smaller units, and that there in fact exists a fundamental 'building block' known as the **atom**.

We will then look at two classic experiments, Thomson's measurement of the specific charge of the electron and Millikan's oil drop experiment, that atoms contain yet smaller particles (**electrons**) that carry the fundamental unit of electric charge.

Outcomes

At the end of this lecture you will:

- know the evidence for the existence of atoms and subatomic particles (electrons)
- be able to describe experiments to measure the charge and the specific charge of the electron
- be able to calculate these quantities from typical experimental data

> **atom** *n* the smallest particle of an element that can take part in a chemical reaction. [Gr *atomos*, undivided]
>
> *Chambers English Dictionary*

> 'The only things existing are atoms and empty space. All else is mere opinion'
>
> *Democritus, 450BC*

By *c*1900 there was already a range of observations suggesting a particulate composition of matter:

- *Chemical Evidence*—**Dalton** observed that elements combined in specific ratios (1803).
  Mendeleev grouped elements in the Periodic Table (1869).
- *Brownian Motion*—The botanist Robert **Brown** observed under a microscope (1827) that pollen grains suspended in a fluid move about randomly. This effect was explained by **Einstein** (1905) in terms of collisions between the pollen grains and particles of the fluid undergoing thermal motion.
- *Kinetic Theory*—J. C. **Maxwell** and Ludwig **Boltzmann** (1850s) explained the physical properies of gases by assuming atomic or molecular composition

But almost nothing was known about the internal structure of these particles. Effects such as radioactivity suggested an internal structure. A number of ‘classic’ experiments though, gradually built up a picture of the atom.

Of course nowadays we can ‘see’ single atoms, either with a Scanning Tunnelling Microscope or fluorescing in an atom trap.

1.1 DISCOVERY OF THE ELECTRON: THOMSON'S EXPERIMENT

1.1.1 THE EVIDENCE

- **Faraday** (1833, 1834) showed, in electrolysis experiments, that matter and electricity are equivalent, and units of positive and negative charge existed
- **Stoney** (1874, 1891) suggested a natural unit of electricity he called the *electron*
- **Cathode Rays** emanating from a cathode when electricity passes through a rarefied gas consist of particles with negative charge but with mich higher *specific charge* (i.e. charge to mass ratio, e/m) than ions from electrolysis

So ... what are these particles? What is their charge? What is their mass?

1.1.2 THE EXPERIMENT

> ‘The immeasurable of today may be the measurable of tomorrow’
>
> *J. J. Thomson*

In 1897, **J.J. Thomson** designed an experiment to measure the charge to mass ratio e/m of the particles in a Cathode Ray Tube. The beam of cathode rays was accelerated by the applied PD between the cathode and anode; a *transverse* electric field was then applied to the beam as it passes through a pair of deflecting plates.

Thompson used several different electron sources:

- cathode rays from cathodes of Al, Pt and Fe
- photoelectrons emitted by Zn
- thermionic emission from a carbon filament

His value for e/m was very inaccurate, but significantly:

- e/m was much larger—by a factor of 1000—from the value expected, given known masses of atoms. This indicated that the particles in the cathode rays were very light
- The ratio e/m was virtually *independent of the source* so the particles must be considered a fundamental constituent of matter and were called **electrons**
- When the experiment was run in reverse, much heavier particles (ions) were found. These differed from atom to atom, but the lightest (for hydrogen) was called the **proton**

The present accepted value for the specific charge of the electron is:

$$e/m = (-1.75882012 \pm 0.00000015) \times 10^{11}\ \mathrm{C/kg}$$

source: `http://physics.nist.gov`

1.1.3 THE APPARATUS

This is a slightly simplified version, but contains the fundamental elements of Thomson's experiment. It is also the principle behind the **Cathode Ray Oscilloscope** you are familiar with from the laboratories.

The electric field that deflects the particle between the plates is:

$$E = \frac{V}{d} = \frac{\text{Voltage drop between plates}}{\text{Distance between plates}} \; . \tag{1}$$

Since the force experienced by the charged particle is

$$F = ma = \text{charge} \times \text{field} = eE, \tag{2}$$

the transverse displacement as they leave the field, y_1, is given by

$$y_1 = \frac{1}{2}at_1^2 = \frac{1}{2}\frac{eE}{m}{t_1}^2 = \frac{1}{2}\frac{e}{m}\frac{V}{d}\left(\frac{l}{v_0}\right)^2 \tag{3}$$

where t_1 is the time taken to traverse the plates.

Now find the velocity of the particle in the transverse y direction as it leaves the region of electric field. In the x direction (longitudinal) there is no acceleration so particles move at constant speed v_0. So on leaving the field:

$$v_y = at_1 = \frac{eE}{m}t_1 = \frac{eE}{m}\frac{l}{v_0} = V\frac{e}{m}\frac{l}{d \times v_0} \ . \tag{4}$$

Hence the total deflection in the y direction is:

$$\begin{aligned} y_2 &= y_1 + v_y t_2 \qquad (5) \\ &= y_1 + v_y \times \left(\frac{L}{v_0}\right) \\ &= \left(\frac{e}{m}\right) \times V \times \underbrace{\frac{l}{d \times v_0^2}\left(\frac{1}{2}l + L\right)}_{constant} \end{aligned}$$

So measuring V and y_2 we can determine the specific charge e/m since:

$$y_2 = \mathrm{const}\frac{e}{m}V \tag{6}$$

The value of the constant is determined by the dimensions of the apparatus (l, L, d) and the initial velocity of the particles, v_0.

Thomson used a magnetic field to determine v_0. For electric and magnetic fields perpendicular ('crossed fields') the net force on the particle is:

$$F = eE - ev_0 B \tag{7}$$

and so by adjusting the strengths of the fields until there is zero net force and thus zero deflection of the beam we may deduce that

$$v_0 = \frac{E}{B}. \tag{8}$$

1.2 MILLIKAN'S OIL DROP EXPERIMENT

1.2.1 QUANTISATION OF ELECTRIC CHARGE

Robert **Millikan** (1909) measured the rate of fall of droplets of oil through air in the presence of an electric field.

Droplets are sprayed through the nozzle into the space between the plates of a condenser. The droplets are positively charged ($+ve$ by friction at the nozzle). The charge can be modified by irradiating the apparatus with X-rays which ionise the air molecules, M:

$$M \overset{X-ray}{\longrightarrow} M^{+} + e^{-} \tag{9}$$

and the electrons are taken up by the oil droplets which reduces their positive charge.

The droplet has charge q, so we have:

$$F = \underbrace{M'g}_{effective\ weight} - \overbrace{qE}^{electrostatic} - \underbrace{\beta v}_{viscosity} \tag{10}$$

NB: M' is the effective mass of the drop and takes into account the bouyancy which acts upwards:

$$M' = M_{oil} - M_{air} = \frac{4}{3}\pi r^{3}(\rho_{O} - \rho_{A}) \tag{11}$$

and ρ_O, ρ_A are the densities of oil and air respectively.

The viscous force is the Stokes Drag on a spherical object falling through a fluid with velocity v, and the constant of proportionality is:

$$\beta = 6\pi\eta r \tag{12}$$

where r is the radius of the drop, η is the coefficient of viscosity.

First we set $E = 0$. The drop falls and it reaches terminal velocity when:

$$M'g = \beta v_1 \tag{13}$$

since gravitational acceleration is balanced by viscous drag.

Now, turn on the electric field: the drop moves upwards. The terminal velocity in this case is reached when:

$$qE = M'g + \beta v_2 \; . \tag{14}$$

Substituting the no field case, Eq. (13), into the expression above, we have:

$$qE = \beta(v_1 + v_2) \; . \tag{15}$$

To calculate β we need to know r. This can be obtanied as a function of v_1 using equations:

$$r = \sqrt{\frac{9\eta v_1}{2g\left(\rho_O - \rho_A\right)}} \; . \tag{16}$$

Now one can alter the charge in the drop, with a burst of ionizing radiation and make many measurements. Millikan observed a drop for hours, repeating the experiment many times. The charge q was found to change by *integral units of a basic charge e* which was found to be $e = 1.6 \times 10^{-19}\,\mathrm{C}$.

This is further evidence that electric charge is *quantised*, i.e. occurs in discrete amounts, that are integral multiples of e. It also establishes the electron as the fundamental unit of charge.

Combining this with Thomson's value for e/m the mass of the electron is

$m = 9.10 \times 10^{-31}$ kg

($\simeq$ 1840 times lighter than a positive hydrogen ion). This explains Thomson's observation that the measured value of e/m for the electron was much larger than that expected from (much heavier) atoms.

LECTURE 1 SUMMARY

- matter is made of atoms
- atoms contain smaller, lighter particles called electrons
- electrons carry the fundamental unit charge, $e = 1.6 \times 10^{-19}$C
- electric charge is quantised in units of e
- Thomson's apparatus may be used to measure the ratio e/m
- Millikan's oil drop experiment may be used to measure e

LECTURE 2

Content

In this lecture we will look at **collisions** and **scattering** of particles. Collisions provide the standard tool for probing atomic and molecular structure. We will discuss total collisional cross-sections, and elastic and inelastic scattering.

We will then examine the famous **Rutherford Scattering** experiment (which you may be familiar with from Lab 2) and the evidence it provides for the structure of the atom being a massive positively charged nucleus surrounded by negatively charged electrons.

Outcomes

By the end of this lecture you will:

- know the definition of the total collisional cross section
- know and be able to use the Beer-Lambert Law
- be able to qualitatively explain data from electron and positron scattering experiments
- describe the Franck-Hertz experiment and use data from it to calculate the wavelength of spectral lines
- describe experimental evidence for the concentration of mass and positive charge in the nucleus of the atom, i.e. the Rutherford experiment

1.3 COLLISIONAL CROSS-SECTIONS

1.3.1 TOTAL COLLISIONAL CROSS-SECTION

Early estimates for the “size” of atoms came from the experiments of **Lennard** (1895–1903). He studied the collisions of a beam of electrons as it passed through a gas. From the decrease of the intensity of such a beam it is possible to estimate the effective cross-sectional area—the total cross-section, denoted σ_T below—presented by a target to an incoming projectile. It is a measure of their *overall interaction probability.*

> **Important Definition**:
> The Total Collisional Cross-Section, σ_T, is the effective area, normal to the direction of incidence, provided by a target to an incoming projectile.

N.B. ‘effective’ is the key word here. For a hard disk of radius R the effective area = actual area = πR^2. But long-range electrostatic forces mean that atoms actually interact when they are relatively far from each other.

Consider a beam of particles of type ‘A’. These could be anything: electrons, positrons, elephants....

The intensity of the beam, I is the number of particles per unit area per unit time, and so has units $\mathrm{m}^{-2}\mathrm{s}^{-1}$.

The beam is incident on a slab of material containing target particles of type ‘B’. Again these could be anything - atoms in a solid, for example.

The density of target particles, that is the number of particles per unit volume, is n which has units m^{-3}.

The fraction of incident particles scattered or lost from the beam must be proportional to the number of target particles:

$$dI/I \propto -n dx \ . \tag{17}$$

We introduce a constant of proportionality (which will be the collisional cross section):

$$dI/I = -n\sigma_T dx \ . \tag{18}$$

N.B. σ_T must have units of area.

The unit of σ is the **barn**: $1\mathrm{barn} = 10^{-28}\,\mathrm{m}^2$ but is never used in atomic and molecular physics because typical magnitudes for atomic σ_T are $\sim 10^{-20}\,\mathrm{m}^2$.

Now integrate over the length of the target material:

$$\int_{I_0}^{I(l)} dI/I = -n\sigma_T \int_0^l dx = -nl\sigma_T \ . \tag{19}$$

If the initial intensity of the beam is I_0, then,

$$\ln(I(l)/I_0) = -nl\sigma_T \ . \tag{20}$$

So, we get the **Beer-Lambert** law:

$$I(l) = I_0 \exp(-nl\sigma_T) \ . \tag{21}$$

σ_T is the effective area presented by each target particle, B, to the incoming projectile, A.

Its values depend on the projectile and its velocity (e.g., consider the interaction time and also $\lambda_{\mathrm{DB}} = h/p$, etc) as well as the target. It does not represent the '*physical*' size of the atom, since the interaction is '*soft*'.

'Softer' for ions, 'harder' for neutrals. **Why ?**

Two charged particles interact by Coulomb potential which decays as $V(r) \sim 1/r$.

Two neutrals interact by a Van der Waals type potential which decays much more abruptly, as $V(r) \sim 1/r^6$

Hence the 'effective area' is much smaller for the two neutral particles since the potential is much more 'short-ranged'.

1.3.2 Example

A beam of electrons of energy 20 eV scatter off Xe atoms of density $3 \times 10^{19}\ \mathrm{m}^{-3}$. The beam of electrons is measured to be attenuated by 18% across a 20 mm cell. What is the total collisional cross-section ?

1.3.3 e^-, e^+ and Ps scattering from He and Ar atoms

An example of research carried out at UCL.

Ps is **positronium** - a bound state of an electron and a positron orbiting each other.

The picture below shows measurements of σ_T for:

$e^- + \mathrm{He}$	$e^+ + \mathrm{He}$	$\mathrm{Ps} + \mathrm{He}$
$e^- + \mathrm{Ar}$	$e^+ + \mathrm{Ar}$	$\mathrm{Ps} + \mathrm{Ar}$

From Garner, Ozen and Laricchia (1998) *Nucl. Instrum. Meth.*, **B143**, 162

Comparing targets for a given projectile, clearly:

$\sigma_T(\mathrm{Ar}) > \sigma_T(\mathrm{He})$

Why?

Comparing projectiles for a given target, **at low Energy**:

$\sigma_T(e^-) >> \sigma_T(e^+)$

Let's see why. Qualitatively, some of the interactions between projectile and targets are:

- **static** interaction with undisturbed target. The projectile sees a partially screened nucleus.

  For e^- interaction is attractive (negative)
  For e^+ interaction is repulsive (positive)

- **polarization** electron charge cloud is distorted by approaching projectile.

  Interaction is attractive in *both* cases

So, at **at low Energy**, the interactions are additive for the e^- but they approximately cancel for e^+ and the cross section is larger for electrons.

But **at high Energy**, $\sigma_T(e^-) \simeq \sigma_T(e^+)$. This is because the importance of polarization decreases - it takes time to distort the cloud charge. The magnitude of the static interaction is the same for both projectiles and hence the cross sections are similar.

$\sigma_T(e^-) \simeq \sigma_T(e^+) \simeq \frac{1}{2}\sigma_T(\mathrm{Ps})$

So, the magnitude of σ_T depends on the *target*, the *projectile* and its *energy*.

By measuring σ_T we can obtain information about the projectile and the target.

What about the Ps? For the Ps the centres of mass and charge coincide. This means that the static interaction and the polarization (to first order) are zero.

Nevertheless, $\sigma_T(Ps) \neq 0$. This is because there are other interactions, some of which we will discuss later on in the course. However, note at **at high Energy**:

$$\sigma_T(Ps) \simeq \sigma_T(e^-) + \sigma_T(e^+)$$

as if the e^- and e^+ interact separately with the target!

At **low Energy** the behaviour is even more surprising. It is not fully understood yet and further investigations, both theoretical and experimental are in progress.

Professor Laricchia's group in UCL has the only Ps beam in the world!!

1.3.4 INELASTIC CROSS-SECTIONS

So far, what we have done is to consider collisions which change the direction of the scattered particles. Atoms also have *internal structure*. Their electronic energies are quantised into energy levels E_1, E_2,... (energy spectrum). If an atom is in its ground electronic state and the collisional energy $E > E_2 - E_1$ then the collision may result in an exchange of kinetic and internal energy. The electron may be excited into a higher lying state.

Hence we define also:

- a total inelastic cross-section σ_{ij} from quantum level i to level j;

They can also be calculated from the Schrödinger equation. The classic **Franck-Hertz** experiment [1] (Nobel prize in 1925) was the first demonstration of this effect.

Electrons are ejected from the heated cathode and accelerated through potential V_1 to the wire grid, acquiring a kinetic energy $mv^2/2 = eV_1$.

Electrons that pass through the grid are collected by the plate causing a current to flow that is measured on the ammeter. The potential of the plate is slightly lower than the grid, i.e. there is a small *retarding potential* (this idea may be familiar from the photoelectric effect experiment in Lab 2).

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[1] James Franck & Gustav Hertz *Verhand. Deut. Physik Ges.*, **16**, 512, (1914)

The tube is filled with mercury vapour and the current measured as a function of the accelerating voltage V_1, i.e. the kinetic energy.

For **low** energies the collision is **elastic** - only the direction of the electron is changed in the collision with the massive mercury atom.

Above a certain energy (i.e. voltage V_1) threshold the electron has enough kinetic energy to excite the mercury atom. The electon's kinetic energy is transferred into internal energy of the excited mercury atom. The collision is **inelastic**. The slow moving electron now does not have enough energy to overcome the retarding potential and there is a sharp drop in the current at the ammeter.

Franck and Hertz observed this to occur at $V_1 = 4.9$V. So what is the energy of the transition from ground to first excited state in mercury? What is the wavelength?

answer:

kinetic energy of electron that is *just* enough to excite mercury atom, $E = eV_1$, so $E = 4.9$eV$= 7.8 \times 10^{-19}$J.

$E = hc/\lambda$ so $\lambda = 7.8{\times}10^{-19}/hc = 253$nm (or in wavenumbers 39500cm^{-1}.

1.4 THOMSON'S 'PLUM PUDDING' MODEL OF THE ATOM

Thomson discovered the electron, but his proposed model of where in the atom the electrons originated was wrong. His idea was that the electrons were embedded in a massive, positively charged component. This model didn't last long because it didn't fit the *experimental evidence*.

1.5 RUTHERFORD SCATTERING

Between 1906 and 1913, **Geiger**, **Marsden** and **Rutherford** carried out experiments on the scattering of α-particles by thin metallic foil (Rutherford had discovered that α-particles emitted in radioactive decay by, e.g. Radon were helium (He^{2+}) nuclei).

You may also have performed this experiment in Lab 2.

Most of the α-particles were only weakly deflected ($\theta < 1^\circ$) but remarkably a few scattered by $\theta > 90^\circ$ (i.e., back-scattered).

> "As if a 15-inch shell had been fired at a piece of paper and it bounced back at you"
>
> *Ernest Rutherford*

From this experiment it was concluded that most of the atom's mass and positive charge is concentrated over a small region $r \sim 10^{-14}$ m—the **nucleus**—whereas for the atom, $r \sim 10^{-10}$ m.

LECTURE 2 SUMMARY

- the collisional cross section is a measure of the interaction probability of a projectile and a target.
- it is related, but not equivalent to the size of the particles
- the Beer-Lambert law describes attenuation due to scattering
- scattering can be elastic or inelastic
- particle scattering is a powerful tool in physics
- the Franck-Hertz experiment uses inelastic scattering to demonstrate quantisation of energy levels
- Rutherford scattering demonstrates the concentration of mass and positive charge in the nucleus of the atom

LECTURE 3

Content

In this lecture we will examine particle scattering in more detail. We will consider the relation between *total* and *differential* cross section, and then move on to a *quantum* treatment of scattering, where the incoming particles must be treated as waves.

Outcomes

At the end of this lecture you will:

- know the difference between total and differential cross section
- be able to calculate the total cross-section from the form of the differential cross section
- appreciate the importance of a quantum description of scattering
- describe scattering events in terms of incoming plane waves and outgoing spherical waves

1.6 DIFFERENTIAL CROSS-SECTION

Clearly, the total cross-section is a very crude indicator of the details of the collision. We fire a beam at a target and we count how many projectiles emerge unscattered versus the number lost. We find that the number ‘lost’ increases exponentially with the density of the target and with its length. We defined our cross-sections by considering a beam coming in from a definite direction, but the scattered particles go off in every possible direction.

The total cross-section tells us nothing about *where* the scattered particles went. The direction of the scattered particles is given by the **differential cross section**.

> **Important Definition**:
> The Differential Cross-Section is the particle flux scattered by each target nucleus into solid angle $d\Omega$, divided by the incoming intensity.

N.B. *flux* means particles per unit time (units are s^{-1})
intensity means particles per unit time per unit area (units are $\mathrm{s}^{-1}\mathrm{m}^{-2}$).

A note about solid angle: to visualise solid angle think of a sphere. Draw a circle on the surface, and it *subtends* a solid angle, Ω, equal to the area divided by the square of the radius of the sphere. The unit of solid angle is the **steradian** (a dimensionless unit). The whole surface of the sphere subtends a solid angle of 4π steradians.

1.6.1 Back to Rutherford Scattering

What Rutherford found was that the flux scattered in a particular direction was:

$$dN \propto Nnld\Omega \,. \tag{22}$$

where N is the incident flux, n and l are the target density and thickness respectively and $d\Omega$ is the element of solid angle:

Introducing a constant of proportionality (which we will later call the differential cross section, and with a bit of foresight denote $\frac{d\sigma}{d\Omega}$):

$$dN = \frac{d\sigma}{d\Omega} Nnld\Omega \,. \tag{23}$$

This differential cross-section determines how many particles are scattered into a given direction (θ, ϕ).

1.7 RELATION BETWEEN TOTAL AND DIFFERENTIAL CROSS-SECTION

If we count the scattered particles over all possible directions we get back the total cross-section. To do this we integrate over solid angle...

$$\sigma = \int \frac{d\sigma}{d\Omega}(\theta, \phi) d\Omega \tag{24}$$

where $d\Omega = \sin\theta d\theta d\phi$, so. . .

$$\sigma = \int_0^{2\pi} d\phi \int_0^{\pi} \frac{d\sigma}{d\Omega}(\theta, \phi) \sin\theta d\theta \ . \tag{25}$$

(N.B. $\int d\Omega = 4\pi$.)

There is an important simplification for the case of interatomic collisions. In this case, since we have cylindrical symmetry, $d\sigma/d\Omega$ does not depend on ϕ.

So we have:

$$\sigma = 2\pi \int_0^{\pi} \frac{d\sigma}{d\Omega}(\theta) \sin\theta d\theta \ . \tag{26}$$

1.7.1 Example: The Rutherford Formula

Rutherford obtained a formula for the differential cross-section for the scattering of a charged projectile (charge Z_1) off a target (charge Z_2) assuming pure Coulomb forces.

$$\frac{d\sigma}{d\Omega}(\theta) = \underbrace{(\frac{1}{4\pi\epsilon_0}\frac{Z_1 Z_2}{4E})}_{K}^{2}(\sin\theta/2)^{-4} \; . \tag{27}$$

The formula explained his famous α-particle colliding-with-nuclei experiment, but failed at high energy, when the finite size of the nucleus becomes important, i.e., he assumed $V \sim -1/r$ which becomes infinite at $r = 0$.

Question: What is the *total* cross-section ?

The problem has cylindrical symmetry, so:

$$\sigma_T = 2\pi K \int_0^\pi \frac{\sin\theta}{\sin^4(\theta/2)} d\theta \tag{28}$$

where K is the collection of constants.

$$\sigma_T = 4\pi K \int_0^\pi \frac{\sin(\theta/2)\cos(\theta/2)}{\sin^4(\theta/2)} d\theta \tag{29}$$

where the identity $\sin\theta = 2\sin(\theta/2)\cos(\theta/2)$ has been used. Cancel a factor of $\sin(\theta/2)$ and make the substitution $u = \sin(\theta/2)$, such that $u = 0$ when $\theta = 0$, $u = 1$ when $\theta = \pi$, and $\frac{du}{d\theta} = \frac{\cos(\theta/2)}{2}$. This leads to:

$$\sigma_T = 4\pi K \int_0^1 \frac{2}{u^3} du \tag{30}$$

and so:

$$\sigma_T = -4\pi K \left[\frac{1}{u^2}\right]_0^1 \rightarrow \infty \tag{31}$$

What does that mean?

It just means that scattering will occur, but in calculating the total scattering cross section we have lost the *directional information* contained in the differential cross section, which told us that most of the scattering is at very small angles.

1.7.2 Examples of differential cross-sections vs. angle

See accompanying figures (lecture handout labelled **fig. 1.4**).

Note that there is not a monotonic change in $\frac{d\sigma}{d\Omega}$ with increasing angle, θ, rather that there is a series of maxima and minima. What could be causing this?

We expect *diffraction effects* if the dimension of the object is similar to the de Broglie wavelength of the projectile: $\lambda_{\mathrm{DB}} \geq h/p$.

Low energy ($E \leq 150\,\mathrm{eV}$) e^- scatter from atoms
high energy ($E \leq 1\,\mathrm{GeV}$) e^- scatter from nuclei
So note how the different energies of electrons can be used to probe *atomic* or *nuclear* structure - despite there being several orders of magnitude difference in the size.

This is confirmed by the figures which all show diffraction-like patterns (that is, bright and dark bands from constructive and destructive interference).

In fact, this analogy holds semi-quantitatively: *cf* diffraction of light by a circular disc of diameter D. The *Airy disc formula* gives the position of the first minimum at

$$\theta = \sin^{-1}\left(\frac{1.22\,\lambda}{D}\right) \qquad \lambda = \frac{h}{\sqrt{2mE}}\,. \tag{32}$$

Can use data from figures to read off θ to obtain D get

$$\text{atomic radius: } r(\mathrm{Kr}) \sim 10^{-10}\,\mathrm{m}$$

$$\text{nuclear radii: } r(^{16}\mathrm{O}, ^{12}\mathrm{C}) \sim 10^{-14}\,\mathrm{m}$$

1.8 QUANTUM CROSS-SECTIONS

So far we have defined cross-sections in terms of numbers of particles lost from a beam, or scattered in a particular direction. A proper quantum treatment must allow for the *wave nature* of atoms - we have just seen how important this is in describing experimental data.

We could describe an atom as a wavepacket interacting with some potential and evolving in time, but in general this is difficult to solve for.

Far more practical is a *time-independent* treatment where we replace the incoming beam of particles by **plane waves**. The scattered particles are described as outgoing **spherical waves**.

These solutions are obtained from the **time-independent Schrödinger equation**:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(\underline{r}) = E\psi(\underline{r}) \; . \tag{33}$$

Note that the potential is *'central'*, i.e. it depends only on $r = |\underline{r}|$ not on $\underline{r}$ for collisions between atoms or between electrons and atoms. Think about why this is the case.

We look for solutions which, as $r \Rightarrow \infty$, take the form:

$$\psi(\underline{r}) = \underbrace{e^{ikr}}_{\text{plane wave}} + \underbrace{f(\theta,\phi)\frac{e^{ikr}}{r}}_{\text{spherical waves}} \quad , \tag{34}$$

for which the wavenumber, k, is related to the energy, E, by:

$$E = \frac{p^2}{2m} = \frac{(\hbar k)^2}{2m} \tag{35}$$

and so:

$$k = \sqrt{\frac{2mE}{\hbar^2}} \ . \tag{36}$$

Unfortunately for the general case we must use a computer!

$f(\theta, \phi)$ is the **scattering amplitude** which determines the probability of scattering in a given direction for a given energy. Sounds familiar?

It can be shown rigorously that, in fact, $f(\theta, \phi)$ gives the differential cross-section:

$$|f(\theta,\phi)|^2 = \frac{d\sigma}{d\Omega}(\theta,\phi) \ . \tag{37}$$

Hence we can calculate the total cross section from the Schrödinger equation:

$$\sigma = \int |f(\theta,\phi)|^2 d\Omega \ . \tag{38}$$

For *inelastic* quantum scattering we would look for solutions for which the outgoing waves have different energy (different wave-number) from the incoming waves, i.e.,

$$\psi(\underline{r}) = \underbrace{e^{ik_i z}}_{\text{plane wave}} + \underbrace{f_{ij}(\theta,\phi)\frac{e^{ik_f r}}{r}}_{\text{spherical waves}} \quad . \tag{39}$$

An aside:

Why is this solution so different from the hydrogen atom solution derived in the previous quantum course ?

- $E > 0$.
- Hence we do not have bound state solutions, i.e., $\psi \neq 0$ for $r \Rightarrow \infty$.
- So we don't get discrete eigenvalues E_n but a continuously varying eigenvalue E.

We could do the one-dimensional scattering problem (an electron scattering off a proton, in a way equivalent to hydrogen) analytically, just like the bound state problem, by changing the boundary conditions as described above. We then get the Rutherford formula directly from the Schrödinger equation. But the analytical treatment is complicated (mainly because the potential $1/r$ is so long ranged that the solution does not tend to the form in Eq. (34) until r is very large indeed).

LECTURE 3 SUMMARY

- the total cross section σ_T does not contain information about the *direction* of scattering, for this we need the differential cross section, $\frac{d\sigma}{d\Omega}$.
- These are related by $\sigma_T = \int \frac{d\sigma}{d\Omega}(\theta, \phi) d\Omega$
- the wave nature of the scattering particles is important, leading to a quantum treatment being necessary
- a quantum description of scattering is made using incoming plane waves and outgoing spherical waves

END OF SECTION SUMMARY

This is the end of the first section *'Introduction to atoms and atomic structure'*. By now you should know the evidence for the existence of atoms and electrons - in fact, I hope you knew atoms existed well before we started this course! - but now you should be able to describe the experimental evidence for this, for the internal structure of atoms and for phenomena such as the quantisation of electronic charge.

You should be able to appreciate the importance of scattering techniques for probing atomic (and nuclear!) structure and the significance of parameters such as the total and differential cross sections.

We will consolidate your knowledge from this section before moving on to the next part of the course - *'One electron atoms'*.