3   Wave properties of matter

In Lecture 1 we mapped out some of the principal interactions between photons and matter (electrons). At the quantum level, individual photons and electrons are described as particles in the various relationships used to describe phenomena such as the photo–electric effect and Compton scattering. We are building up a map of quantum interactions (Table 1). Under certain circum-

	particle	wave
electron	Thomson's experiment Photo–electric effect Compton effect	
low–energy photon	photo–electric effect	interference diffraction
high–energy photon	Compton effect Pair production	

Table 1: A simple map of quantum behaviour.

stances, low energy photons can act as particles or as waves. **Importantly, such photons never display both wave–like and particle–like properties in the same experiment (Two-slit experiment).**

The blank spaces in Table 1 provide the directions we must investigate in order to complete our simple quantum map: can high energy photons, X– and γ–rays, act as waves, and can electrons – classically viewed as matter particles – also act in a wave–like manner?

- X–ray diffraction – high energy photons can behave as waves.

- De Broglie suggests a relationship between momentum (mass) and wavelength – a wave–like description of matter?

- Electron scattering and transmission electron diffraction photography confirm wave phenomena in electrons.

- A wave mechanics primer.

- The uncertainty principle derived using wave physics.

- Bohr's complementarity principle and an introduction to the two slit experiment.

- The Copenhagen interpretation of quantum theory.

- A wave description of a particle in a box leads to quantised energy states.

3.1 X–ray diffraction

Roentgen identified X–rays in 1895 as a by–product of experiments using high–energy electron beams – the X-rays were produced via bremsstrahlung emission in the glass walls of the evacuation chamber. In the following decade, Charles Barkla demonstrated that X-rays demonstrated polarisation phenomena – an important clue that they might be an electromagnetic wave. However, it was very difficult to produce diffraction or interference effects with X–rays – a null result that was understood only if X–rays had very short wavelengths, e.g. 10^{-10}m or 10^{-11}m.

Electromagnetic waves produce diffraction or interference patterns when the wavelength is of the order of or smaller than the size of the grating rulings (diffraction) or aperture in a screen (interference). Max von Laue was the first to suggest that, as the interatomic spacing in certain crystals is of the order of 10^{-10}m, a suitably orientated crystal might act as a diffraction grating for X–rays.

The experimental set–up that confirmed Laue's prediction is shown in T–Rex Figure 5.1. The dots on the photographic screen are referred to as *Laue dots* and correspond to diffraction maxima produced by the three dimensional crystal structure. Laue's approach not only demonstrates the wave–like nature of X–rays but provides an important method for determining the structure of crystalline solids (and molecular material such as DNA).

Two generations of the Bragg family refined Laue's picture of X–ray diffraction into a simple geometric picture. T–Rex Figure 5.2 illustrates how a simple cubic crystal arrangement can be viewed as a series of interlocking planes with different orientations – **Bragg planes**. T–Rex Figure 5.3 shows how each set of Bragg planes is separated by an interatomic distance $D = d_1, d_2, \ldots$

The bright dots in a Laue diagram result from the constructive interference of X-rays scattered from successive Bragg planes. The numerical conditions for constructive interference are

1. The angle of incidence equals the angle of reflection.

2. The difference in path lengths between the two successively scattered waves must equal an integer number of wavelengths.

The geometry of X–rays scattering from a simple crystal is shown in T–Rex Figure 5.4. From this diagram and the above two conditions we derive **Bragg's law**

$$n\lambda = 2d\sin\theta \quad (n = \text{integer}). \tag{1}$$

T–Rex Figure 5.5 shows the apparatus used in a Bragg spectrometer. For a single crystal one obtains the patter of Laue dots seen in T–Rex Figure 5.1. However, if one grinds up the crystal into a powdered form one randomises the orientations of each series of Bragg planes. The effect of this is to rotate the scattering geometry shown in T–Rex Figure 5.4 through $360°$ – see T–Rex Figure 5.6 – with the effect that the Laue dot pattern becomes a series of concentric circles.

The above analysis is based upon classical wave physics. We have now demonstrated that both high– and low–energy photons display both particle– and wave–like properties.

T–Rex example 5.1: X–rays scattered from rock salt (NaCl) are observed to have an intense maximum at an angle of 20° from the incident beam. Assuming $n = 1$, what is the wavelength of incident radiation?

From T–Rex Figure 5.7 we see that the angle between the incident beam and the diffraction peak is 2θ. We can then use basic chemical data to compute the interatomic spacing d, if we assume that the volume occupied with one atom is d^3.

The number of molecules per unit volume is

$$\frac{\text{number of molecules}}{\text{volume}} = \frac{N_A \rho}{M}. \tag{2}$$

Inserting the values for NaCl, we obtain

$$\frac{N_A \rho}{M} = \frac{\left(6.02 \times 10^{23} \frac{\text{molecules}}{\text{mol}}\right)\left(2.16 \times 10^3 \frac{\text{kg}}{\text{m}^3}\right)}{58.5 \times 10^{-3} \frac{\text{kg}}{\text{mol}}}$$

$$= 2.22 \times 10^{28} \frac{\text{molecules}}{\text{m}^3}$$

$$= 4.45 \times 10^{28} \frac{\text{atoms}}{\text{m}^3}. \tag{3}$$

As NaCl has a simple, cubic structure, we may write

$$\frac{1}{d^3} = 4.45 \times 10^{28} \frac{\text{atoms}}{\text{m}^3}$$

$$d = 2.82 \times 10^{-10}\,\text{m} = 0.282\,\text{nm}. \tag{4}$$

Now that we know d we can re–arrange the Bragg law in terms of wavelength, i.e.

$$\lambda = \frac{2d \sin \theta}{n} = \frac{(2)(0.282\,\text{nm})(\sin 10°)}{1} = 0.098\,\text{nm}. \tag{5}$$

This analysis demonstrates how crystals of known properties act as a X–ray diffraction spectrograph. Conversely, by using X–rays of known wavelength, one can probe the geometry of the Bragg planes and thus learn about new crystal structures.

3.2   De Broglie and matter waves

By 1920 a picture was emerging of the dual nature of physical phenomena: energy was directly related to matter ($E = mc^2$), electromagnetic radiation sometimes behaved as a wave (interference, diffraction) and sometimes as a particle (photo–electric effect, Compton effect).

De Broglie was the first to suggest that matter might display both particle– and wave–like properties. It is all a question of scale; with X–rays we saw that wave–like effects only become apparent on scales of the order of the wavelength. De Broglie's advance was that the wavelength λ associated with a particle can be written as

$$\lambda = \frac{h}{p}, \tag{6}$$

where p is the momentum of the particle and h is Planck's constant. In the context of particles, λ is referred to as the **De Broglie wavelength** of the **matter wave** associated with the particle. We do not derive this relationship explicitly using wave mechanics, though we will show in Section 3.4 how a particle can be represented by a localised "wave packet". However, one can demonstrate a similar relationship for light of energy $E = hc/\lambda$ and momentum $p = E/c$, i.e.

$$\frac{hc}{\lambda} = pc \quad \text{or} \quad \lambda = \frac{h}{p}. \tag{7}$$

T–Rex example 5.2: calculate the De Broglie wavelength of 1) a tennis ball of mass 57g travelling at 25 ms^{-1} and 2) an electron of energy 50 eV.

1. For the tennis ball we may write

$$\lambda = \frac{h}{p} = \frac{6.626 \times 10^{-34}\,\text{Js}}{(0.057\,\text{kg})(25\,\text{ms}^{-1})} = 4.7 \times 10^{-34}\,\text{m}. \tag{8}$$

2. For the electron, we may re–arrange the equation into a more convenient form

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mK}} = \frac{hc}{\sqrt{2(mc^2)K}}$$

$$\lambda = \frac{1240\,\text{ev nm}}{\sqrt{(2)(511 \times 10^3\,\text{eV})(50\,\text{eV})}} = 0.17\,\text{nm}. \tag{9}$$

   Note that the low energy of the electron ensures that our use of the non–relativistic KE of the particle is reasonable.

3.2.1 Bohr's quantisation condition

The Bohr model of the hydrogen atom is partly based upon the assumption that the angular momentum of the electron located in a stationary state is an integer multiple of $h/2\pi$. We can view the stationary state associated with a wave–like electron as a one dimensional standing wave forming a circle about the nucleus (see T–Rex Figure 5.8). The mathematical condition for a standing wave of wavelength λ to exist at a radius r about the nucleus is

$$n\lambda = 2\pi r. \tag{10}$$

Inserting the De Broglie wavelength of the electron we obtain

$$2\pi r = n\lambda = n\frac{h}{p}. \tag{11}$$

The angular momentum of the electron is $L = rp$, which we can re–write as

$$L = rp = \frac{nh}{2\pi} = n\hbar. \tag{12}$$

So, from a theoretical perspective, De Broglie's concept of matter waves possessing a well–defined wavelength appears to provide an insight into the assumptions of the Bohr model.

3.3 Electron diffraction

Low energy electrons possess a De Broglie wavelength similar to X–rays. It is therefore reasonable to anticipate that they might generate diffraction effects in a similar fashion to X–rays.

Davisson and Germer were in the process of studying electron scattering from metal surfaces during the period when De Broglie developed his concept of matter waves. Their experimental set up is shown in T–Rex Figure 5.9 and consisted of an electron beam of energy 40–70 eV directed at a nickel target. Under normal circumstances nickel exists as a polycrystalline solid and the scattered electron beam shows a smooth variation of intensity versus angle ϕ.

However, a laboratory accident required the nickel target to be repeatedly heated and cooled in order to ensure a pure nickel sample – a process which created extended, uniform crystals of nickel on the surface. The electron scattering pattern now demonstrated a variable pattern as a function of beam energy, with a strong intensity peak evident at $\phi = 50°$ for a beam energy of 54 eV (T–Rex Figure 5.10).

Davisson and Germer's insight was to apply the Bragg law to their data. T–Rex Figure 5.11 shows the relationship between the incident electron beam and the nickel crystal. The angular relationships are slightly different to the original Bragg case. The Bragg law states that $n\lambda = 2d\sin\theta$ (where 2θ is the angle between the incident and exiting beams). However, from T–Rex Figure 5.11 we

have $\phi = \pi - 2\theta = 2\alpha$. As $\sin\theta = \cos(\phi/2) = \cos\alpha$, we can re–write the Bragg condition as $n\lambda = 2d\cos\alpha$. However, d is the lattice plane spacing and is related to the interatomic distance D by $d = D\sin\alpha$. Therefore, we can write

$$n\lambda = 2d\sin\theta = 2d\cos\alpha = 2D\sin\alpha\cos\alpha$$

$$n\lambda = D\sin 2\alpha = D\sin\phi \tag{13}$$

or

$$\lambda = \frac{D\sin\phi}{n}. \tag{14}$$

For nickel, the interatomic distance is $D = 0.215\,\text{nm}$. Assuming that the electron scattering peak at $50°$ corresponds to $n = 1$, then the electron wavelength is

$$\lambda = (0.215\,\text{nm})(\sin 50°) = 0.165\,\text{nm}. \tag{15}$$

T–Rex Example 5.3: How does this compare to the De Broglie wavelength of a 54 eV electron?

The De Broglie wavelength of an electron can be written in terms of the potential difference V_0 over which the electron is accelerated. For the KE of the electron we may write

$$\frac{p^2}{2m} = eV_0$$

$$p = \sqrt{2meV_0}. \tag{16}$$

Inserting this relationship into the expression for the De Broglie wavelength, we obtain

$$\begin{aligned}
\lambda &= \frac{h}{p} = \frac{hc}{pc} = \frac{hc}{\sqrt{2(mc^2)eV_0}} \\
&= \frac{1240\,\text{eV nm}}{\sqrt{(2)(511\times 10^3\,\text{eV})(eV_0)}} \\
&= \frac{1.226\,\text{nm V}^{1/2}}{\sqrt{V_0}} \\
&= \frac{1.226\,\text{nm V}^{1/2}}{\sqrt{54\text{V}}} = 0.167\,\text{nm}, \tag{17}
\end{aligned}$$

which is in very good agreement with the value for λ determined experimentally by Davisson and Germer. This first measurement was performed by scattering electrons off a metallic crystal target. Later experiments employed transmission electron diffraction – the electron beam was fired through a material – to produce diffraction patterns similar to X-ray images (see T–Rex Figure 5.12).

Reminder: the scattering experiments of Bragg and Davisson-Germer quote the angle of the exit beam in different ways – **that is the only difference**. Apparatus set up to reproduce Bragg scattering and Davisson-Germer scattering will work for both photons and electrons. Quoting the exit angle in a different way just means that you have to use the right formula for the lattice plane spacing as shown in Figure 1.
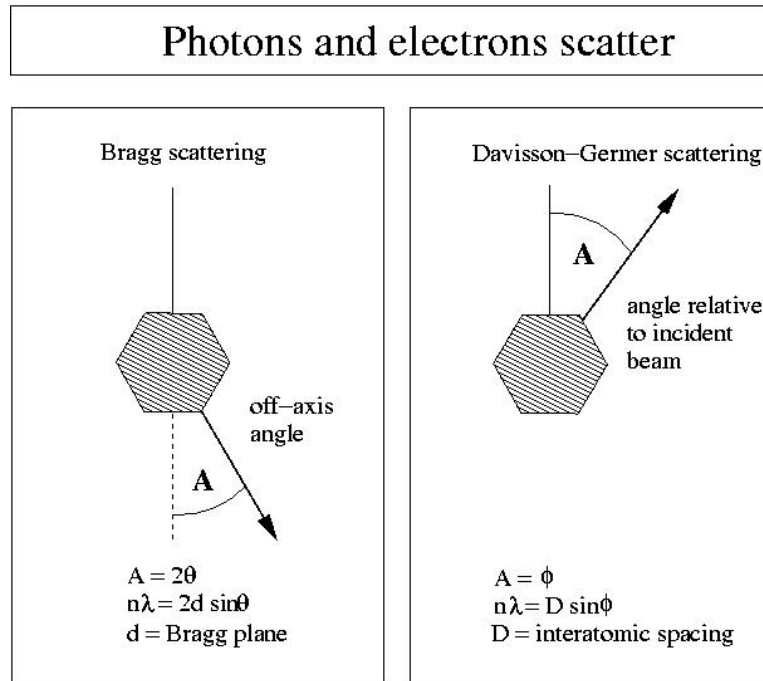

Figure 1: Bragg versus Davisson-Germer scattering.

3.4 Particles as localised wave packets

We need to refresh our knowledge of wave physics if we are to understand how a combination of waves can act as a particle.

A simple wave viewed at a fixed moment in time can be represented by a sinusoidal wave (see T–Rex Figure 5.10)

$$\Psi(x,t)|_{t=0} = A \sin\left(\frac{2\pi}{\lambda}x\right), \tag{18}$$

where $\Psi(x,t)$ represents the instantaneous amplitude or **displacement** of the wave as a function of position x and time t. Examples of displacement include the displacement of a violin string from equilibrium or the motion of air particles in the atmosphere. The term A is referred to as the **harmonic amplitude**.

At some later time the wave may have moved so we generalise the above expression, i.e.

$$\Psi(x,t) = A \sin\left[\frac{2\pi}{\lambda}(x - vt)\right]. \tag{19}$$

We define the **wavelength** λ as the distance between two adjacent points in the wave sharing the same phase and the **period** T as the time taken for the wave to travel a distance of one wavelength. As the velocity of points sharing the same phase is v we can write $\lambda = vT$ and note that the frequency $f = 1/T$ of a harmonic wave is the number of times a wave point (e.g. a crest) passes a reference position per second.

Travelling waves of the type shown above satisfy the wave equation

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 \Psi}{\partial t^2}. \tag{20}$$

The above wave equation describes mechanical waves, i.e. those whose movement is characterised by Newtonian mechanics. We can express the above general expression for a wave in a more general form using the **wave number** k and the **angular frequency** ω, i.e.

$$k \equiv \frac{2\pi}{\lambda} \quad \text{and} \quad \omega \equiv \frac{2\pi}{T}, \tag{21}$$

such that

$$\Psi(x,t) = A \sin(kx - \omega t). \tag{22}$$

The **phase velocity** v_{ph} can now be defined as the velocity of a point on a wave that has a given phase

$$v_{ph} = \frac{\lambda}{T} = \frac{\omega}{k}. \tag{23}$$

If a given wave does not have $\Psi = 0$ at $x = 0$ and $t = 0$, we introduce the **phase constant** ϕ as

$$\Psi(x,t) = A \sin(kx - \omega t + \phi). \tag{24}$$

If we select $\phi = \pi/2$, the wave becomes

$$\Psi(x,t) = A \cos(kx - \omega t). \tag{25}$$

Waves are combined in a linear fashion. The **principle of superposition** requires that we add the displacements of individual waves

$$
\begin{aligned}
\Psi(x,t) \;&=\; \Psi_1(x,t) + \Psi_2(x,t) \\[2ex]
&=\; A\cos(k_1 x - \omega_1 t) + A\cos(k_2 x - \omega_2 t) \\[2ex]
&=\; 2A\cos\left[\frac{1}{2}(k_1 - k_2)x - \frac{1}{2}(\omega_1 - \omega_2)t\right]\cos\left[\frac{1}{2}(k_1 + k_2)x - \frac{1}{2}(\omega_1 + \omega_2)t\right] \\[2ex]
&=\; 2A\cos\left(\frac{\Delta k}{2}x - \frac{\Delta \omega}{2}t\right)\cos(k_{av}x - \omega_{av}t),
\end{aligned}
\tag{26}
$$

where $\Delta k = k_1 - k_2$, and $k_{av} = (k_1 + k_2)/2$, etc. Examples of linear wave superposition are shown in T–Rex Figure 5.14. Equation 26 is simply the product of two wave terms: the first term describes the **envelope** within which the "average" wave described by the second term oscillates.

The superposition of two waves is still continuous in space. To create a **wave packet** – a superposition of waves that is localised in space – one has to combine a larger number of waves. However, the properties of the envelope term in Equation 26 indicate some of the properties of a wave packet. If w consider two consecutive points where the envelope term is zero we create a localised region $\Delta x = x_2 - x_1$. At some fixed time the interval $\Delta k \cdot x/2$ evaluated at x_2 and x_1 must represent a phase difference of π. Another way of putting this is that $\Delta x = x_2 - x_1$ represents half an envelope wavelength. We can write

$$\frac{1}{2}\Delta k x_2 - \frac{1}{2}\Delta k x_1 \;=\; \pi$$

$$\Delta k(x_2 - x_1) = \Delta k \Delta x \;=\; 2\pi. \tag{27}$$

We can obtain a similar relationship by considering the time interval over which the wave packet is localised, i.e.

$$\Delta \omega \Delta t = 2\pi \tag{28}$$

This is a simple indication of how **uncertainty** is inherent in any attempt to describe localised phenomena (e.g. particles) as a wave packet. If one wishes to determine a precise position of the particle/wave packet (Δx small), a large range of wave numbers (Δk large) is required. Similarly, if we wish to know the precise time at which the particle is at a given location (Δt small), the wave packet must have a large range of frequencies ($\Delta \omega$ large).

A Gaussian wave packet provides a useful description of a localised particle. At a time $t = 0$ a Gaussian wave packet can be written as

$$\Psi(x,0) = \psi(x) = Ae^{-\Delta k^2 \Delta x^2}\cos(k_0 x), \tag{29}$$

where Δk is the width of a Gaussian distribution of wave numbers k used to form the packet (see T–Rex Figure 5.16). If $\psi(x)$ is a measure of the probability of finding the particle at some point x to $x + \mathrm{d}x$ then with a Gaussian wave packet there is a high chance of finding the particle between $x = 0 \pm \Delta x/2$ – the particle is localised. Gaussian wave packets provide a good description of particles as the product $\Delta k \Delta x$ is minimised, in this case $\Delta k \Delta x = \frac{1}{2}$.

3.5   The uncertainty principle from wave physics

De Broglie postulated the existence of matter waves – a view that was subsequently confirmed experimentally. We have seen that by using a sum of two waves to represent a particle we achieve the condition $\Delta k \Delta x = 2\pi$ – the localisation of a wave packet always comes at the cost or requiring

a large set of wave numbers. In the limit of a Gaussian wave packet we achieve the minimum condition $\Delta k \Delta x = 1/2$. We might therefore write that when describing matter as a wave effect we must always satisfy

$$\Delta k \Delta x \geq \frac{1}{2}. \tag{30}$$

The De Broglie wavelength of a particle is $\lambda = h/p$, therefore we may rewrite the wavenumber as

$$k = \frac{2\pi}{\lambda} = \frac{2\pi}{h/p} = p\frac{2\pi}{h} = \frac{p}{\hbar} \tag{31}$$

and

$$\Delta k = \frac{\Delta p}{\hbar}. \tag{32}$$

For the case of a Gaussian wave packet, we now have

$$\Delta k \Delta x = \frac{\Delta p}{\hbar}\Delta x = \frac{1}{2} \tag{33}$$

or

$$\Delta p \Delta x = \frac{\hbar}{2}. \tag{34}$$

Werner Heisenberg first presented the **uncertainty principle** in 1927 (he actually used a different kind of quantum theory – based upon matrix mechanics – but the two approaches are complementary). Strictly speaking, p is a vector, therefore we write the uncertainty principle as

$$\Delta p_x \Delta x \geq \frac{\hbar}{2}. \tag{35}$$

This is the lowest possible limit upon our knowledge of Δp_x and Δx if we describe a particle using wave mechanics (or indeed any other form of quantum mechanics). However, the uncertainty principle does not limit the precision of combinations such as Δp_y and Δx, or Δp_x and Δz.

By considering a Gaussian wave packet at fixed location (e.g. $x = 0$) we can formulate a similar uncertainty relation of the form

$$\Delta \omega \Delta t \frac{1}{2}. \tag{36}$$

As $E = hf$, we may write

$$\Delta E = h\,\Delta f = h\,\frac{\Delta \omega}{2\pi} = \hbar \Delta \omega. \tag{37}$$

Therefore

$$\Delta \omega = \frac{\Delta E}{\hbar} \quad \text{and} \quad \Delta \omega \Delta t = \frac{\Delta E}{\hbar}\Delta t = \frac{1}{2} \tag{38}$$

and we may write Heisenberg's uncertainty principle in the form

$$\Delta E \Delta t \geq \frac{\hbar}{2}. \tag{39}$$

In fact, given the units of Planck's constant (energy $\times$ time) the uncertainty principle can be expressed for any pair of conjugate variables for which the product shares the same dimension as Planck's constant.

T–Rex Example 5.9: Treat the hydrogen atom as a one dimensional entity of length $l = 2a_0$ and determine the electron's minimum KE.

If the electron is confined to a length l, then we know the position to within $\Delta x \leq l/2$. The uncertainty principle specifies that Δp_x is limited by

$$\Delta p_x \geq \frac{\hbar}{2\Delta x} \geq \frac{\hbar}{l}. \tag{40}$$

If we assume that the electron is non–relativistic we can write $KE = p_x^2/2m$. Given that Equation 40 represents the minimum possible electron momentum, the minimum KE is

$$KE_{min} = \frac{p_{min}^2}{2m} = \frac{(p = 0 \pm \Delta p_x)^2}{2m} \geq \frac{\hbar^2}{2ml^2}. \tag{41}$$

Therefore, if the electron is localised within an atom of diameter l it cannot have zero energy. We can rearrange the above expression to answer the original question, i.e. computing KE_{min} for a one dimensional atom of length $l = 2a_0$, such that

$$
\begin{aligned}
KE_{min} &= \frac{\hbar^2}{2ml^2} = \frac{(\hbar c)^2}{2mc^2(2a_0)^2} \\[2mm]
&= \frac{(197\,\text{eV nm})^2}{(2)(511\,\text{keV})(2 \times 0.0529\,\text{nm})^2} = 3.4\,\text{eV}.
\end{aligned}
\tag{42}
$$

If we attempted the calculation in three dimensions, the answer would be larger by approximately a factor three. Therefore, this simple analysis provides a reasonable value for the ground state energy for an electron in the hydrogen atom.

3.6   Wave versus particle behaviour: Bohr's complementarity principle

Light can act as both a particle and wave. So can matter – as demonstrated by electrons. This phenomena is referred to as **wave–particle duality**.

So what determines whether a photon or an electron will behave as a particle or as a wave? Can it do both? The best answer to this question is given by **Bohr's complementarity principle**:

It is not possible to describe physical observables simultaneously in terms of both particles and waves.

The key here is that **physical observables** are quantities such as position, velocity, momentum and energy – quantities that can be measured in an experiment. Until we construct an experiment we cannot say whether the thing being observed is particle or wave – it has a dual nature.

The consequences of Bohr's complementarity principle is that no single photon or electron will behave as both a particle and a wave in any single experiment. It will either behave 100% as a wave (e.g. interference) or 100% as a particle (e.g. photo–electric effect etc.).

The complementarity principle is just that – an unproven principle. However, it has never been proven to be untrue. The best demonstration of complementarity in action is given by an examination of the two–slit experiment for either electrons or photons.

3.7   The two-slit experiment

The concepts behind the two–slit experiment are illustrated just as well by photons or electrons. The basic geometry of the two–slit experiment is shown in T–Rex Figure 5.18.

If we start by considering a classical wave motion incident upon the double slit, then we may describe the wave displacement as $\Psi(y, t)$. In this simple case Ψ might represent the displacement of water in a tank from the equilibrium position. The incident wave motion is converted into two sets of wavelets by the double slits and upon reaching the distant screen the wave height of the interfering wavelets is equal to $\Psi_{12} = \Psi_1 + \Psi_2$. The energy received (intensity) at any point y along the screen is equal to $\Psi_{12}^2 = (\Psi_1 + \Psi_2)^2$. The condition for constructive interference (maximum intensity) is $n\lambda = d\sin\theta$. If we block off one of the two slits then the wave height of the single wavelet is $\Psi_{12} = \Psi_1$ and the wave intensity is $\Psi_{12}^2 = \Psi_1^2$ (and vice versa if we block of slit 1 and leave slit 2 open). In this case no interference pattern is observed.

Feynman contrasted the above wave example of the two slit experiment with a 100% particle version - bullets fired at an armoured screen by a wayward gunner. The probability of a bullet going through slit 1 and hitting a particular point on the screen (measured perhaps by a whole stack of boxes containing sand) is N_1 – the number of bullets hitting the small detector at y in some fixed time interval – with N_2 defined similarly for slit 2. The total number of bullets received as a function of location y along the slit is $N_{12} = N_1 + N_2$ – note that no interference occurs (consistent with our "real world" picture of particle interactions).

We now consider an electron beam in a laboratory. The electron beam is not infinitely narrow and so when the electrons impact upon the two closely spaced slits we do not know which slit they go through. At the detector screen we measure the number of electrons arriving a some point between y and $y + \mathrm{d}y$ – exactly as we did for bullets. However, we now see that $N_{12} \neq N_1 + N_2$. The result is shown in T–Rex Figure 5.20 and the electrons produce an interference pattern exactly as if they were behaving as waves, i.e. we see a result of the form $N_{12} = \Psi_{12}^2 = (\Psi_1 + \Psi_2)^2$. We can go further and block off slit 2, noting that $\Psi_{12}^2 = \Psi_1^2$ (and vice versa).

What does Ψ^2 represent? In this case Ψ^2 represents the probability of detecting an electron at some location y to $y + \mathrm{d}y$ along the detector screen – it is an observable quantity. Following the same approach, Ψ_1^2 is the probability of detecting an electron at y to $y + \mathrm{d}y$ that has gone through slit 1 and we can make a similar definition for Ψ_2^2. For completeness we call Ψ_1 and Ψ_2 the **wave**

functions representing the electrons travelling through slit 1 and 2 respectively. The wave function alone is **not an observable quantity**.

Now we slow down the rate at which electrons arrive at the slit to the point at which only one electron arrives at a time. The result is shown in T–Rex Figure 5.19 – though only one electron goes through the slit at a time, if we wait long enough, the same interference pattern as before is observed. Therefore, **what is a single electron "interfering" with?** In the case of a single electron, Ψ_1 represents the wave function of the electron passing through slit 1 and Ψ_2 represents the wave function **of the same electron** passing through slit 2. The two wave function travel to the screen and upon detection we realise the observable quantity $\Psi_{12}^2 = (\Psi_1 + \Psi_2)^2$. This is one of the fundamental examples of the "weirdness" of quantum mechanics, the electron is represented by two wave functions – one for each possible path – that are not observable *en route*. **The electron effectively passes through both slits**. Only when we detect the electron at the screen do evaluate Ψ^2 – the observable.

Now we will try to "cheat" the experiment. We will observe which slit the electron passes through by shining a light on the slits. As an electron passes through either slit 1 or slit 2 we will see an associated flash of light at that slit.

Turning on the light immediately turns off the interference pattern. One way of interpreting this effect is that light has momentum which is in turn imparted to the observed electron, altering its path and the resultant interference pattern. Consider the momentum of the photons used to make the observation. To be sure what slit the electron passed through we must use a photon wavelength that is smaller than the slit separation d, i.e.

$$p_{ph} = \frac{h}{\lambda_{ph}} > \frac{h}{d} \tag{43}$$

However, the condition for interference to occur is that the electron wavelength must be of the order of or smaller than the slit separation, i.e.

$$p_{el} = \frac{h}{\lambda_{el}} \sim \frac{h}{d}. \tag{44}$$

The problem is that, by shining light on the slits, we impart momentum to the electron – we force it to act like a particle – and change its trajectory – wiping out the wave behaviour indicated by the interference pattern.

Note that we cannot fine tune the light to minimise the intrusion into the experiment. If we decrease the photon momentum, the wavelength of light increases to the point where we cannot tell which slit the electron went through. If we turn down the intensity of the light beam (less photons) we get an intermediate pattern: electrons that avoid being struck by a photon act like waves and show the interference pattern; electrons that are struck be photons behave like bullets and the interference pattern is lost.

However, a more general interpretation is that, in a particular experiment, all possible paths are travelled by the electron wave function. The particular path taken only becomes reality through the act of observation. **The wave function is a "virtual" quantity that only generates an observable quantity during the act of observation.** In the two slit experiment, when we observe the electron passing through a particular slit, e.g. slit 1, the probability of the electron passing through slit 1 must be $\Psi_1^2 = 1$ and the probability of the electron passing through slit 2 is $\Psi_2^2 = 0$. The probability of the electron hitting a particular point on the screen now behaves as if $\Psi^2 = \Psi_1^2 + \Psi_2^2$. No interference now occurs and the single electron wave function behaves exactly like the bullets in the earlier example. In a sense, we force the electron to "choose" between the possible wave functions – the wave function collapses to the observed value.

We can push this interpretation further. Wheeler proposed a version of the two slit experiment that using lenses to separate the electron path through each slit to large distance before bringing them together again to create the interference pattern. Shining light on the electrons cannot now "smear out" the interference pattern. However, bouncing light off the electrons still destroys the interference pattern. The wave function still collapses under observation. So if we see the electron go along the path corresponding to slit 1 – Ψ_1 collapses upon observation – how does Ψ_2 know to disappear? Discuss and submit answers on postcard to Nobel committee.

3.8   The Copenhagen interpretation

What does quantum theory tell us about the fundamental nature of the physical world? The following three ideas are one interpretation of the "meaning" of quantum theory:

1. The Heisenberg uncertainty principle.

2. The Bohr complementarity principle.

3. The statistical interpretation of Born – based upon probabilities determined by the wave function.

We have discussed points (1) and (2). Point (3) has been hinted at during the discussion of the two slit experiment and requires further definition now.

To describe particles as matter waves we use the wave function Ψ – in general $\Psi(x, y, z, t)$ may be a complex quantity. However, the wave function alone has no physical significance. The quantity $\Psi^*\Psi = |\Psi^2|$ is a **probability density** and is **observable**. It represents the probability of finding the particle in a given unit volume at a given instant of time, i.e. the probability of finding the particle between x and $x + \mathrm{d}x$ at a time t is

$$P(x)\mathrm{d}x = |\Psi(x, t)^2|\,\mathrm{d}x. \tag{45}$$

Because the particle has to exist *somewhere* we can **normalise** the wave function using the following condition

$$\int_{-\infty}^{\infty} P(x)\,\mathrm{d}x = \int_{-\infty}^{\infty} |\Psi(x,t)^2|\,\mathrm{d}x = 1. \tag{46}$$

In general, the wave function can be a superposition of wave functions each describing the possible outcomes of an experiment. In the case of the two slit experiment, we have a superposition of two wave functions: one where the electron goes through slit 1 and one where the electron goes through slit 2. As a predictive tool, quantum mechanics concerns itself only with the outcome of experiments – the process of observation forces the wave function to choose a final wave function randomly from the available possibilities. Observation collapses the wave function. However, prior to any observation we can say nothing about the definite state of the particle. As Heisenberg said when referring to the two slit experiment, "The path of the electron comes into existence only when we observe it."

Expressed formally, the Born interpretation states that experimental results are based upon **probability** – in this case determined via the wave function. This view contradicted the idea that physics is **deterministic** – based upon fixed rules of cause equals effect. For example, Newtonian mechanics is a completely deterministic theory: a fixed set of initial conditions always produces the same outcome. This is what led Einstein to state, "God does not play dice" – the world is not governed by probabilities. To which Born replied, "Einstein, don't tell God what to do" – i.e. why should quantum theory match our common sense?

Perhaps the best quote is provided by Richard Feynman, Nobel prize winning quantum physicist, "I don't understand quantum physics".

3.9   Putting it all together: a particle in a box

Describing the physics of a particle in a box brings together a number of the ideas presented in this topic and forms the beginning of a purely quantum theory of the atom. We will use

- De Broglie's assertion that matter can be represented as a wave function Ψ of wavelength $\lambda = h/p$.

- The interpretation of the term $|\Psi^2|$ as the probability of finding the particle in a unit volume at a given time.

We consider a particle of mass m confined within a one dimensional box of length l (when computing exact values we will take $l = 0.1$ nm). We have already demonstrated using the uncertainty principle that such a particle cannot have zero KE.

If we consider the particle at some fixed time t then the wave function $\Psi(x,t) = \psi(x)$. In order to describe a physically reasonable situation we introduce a couple of restrictions:

1. The value of the wave function $\psi(x) = 0$ for $|x| > l/2$. This is the same as stating that the probability of finding the particle outside the box is zero.

2. The wave function $\psi(x)$ must be continuous.

3. The wave function $\psi(x)$ must take only one value at each x.

In order to satisfy these condition the range of permitted wave function must satisfy

$$\frac{n\lambda}{2} = l \quad \text{or} \quad \lambda_n = \frac{2l}{n}, \tag{47}$$

where $n = 1, 2, 3, ...$ is an integer. We will consider the wave function as a sinusoidal wave of wavelength λ. The range of permitted wavelengths is quantised and the wave functions will feature terms based upon $\sin(n\pi x/l)$ (see T–Rex Figure 5.23). If we assume that there is no potential term and treat the particle energy non–relativistically we may write

$$E = \text{KE} = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2}. \tag{48}$$

Using the above condition for λ_n, we obtain

$$
\begin{aligned}
E_n &= \frac{h^2}{2m}\left(\frac{n}{2l}\right)^2 = n^2 \frac{h^2}{8ml^2} \quad (n = 1, 2, 3, ...) \\
&= n^2 \frac{(hc)^2}{8mc^2l^2} \\
&= n^2 \frac{(1240\,\text{eV nm})}{(8)(511\,\text{keV})(0.1\,\text{nm})^2} \\
&= n^2\,(38\,\text{eV}).
\end{aligned}
\tag{49}
$$

The permitted energy states are quantised: the first three energy levels are $E_1 = 38$ eV, $E_2 = 152$ eV, and $E_3 = 342$ eV. Zero energy is not permitted – this is demonstrated either using the uncertainty principle (a less refined calculation than the present one) or by considering that $E = 0$ implies that $n = 0$ and $\psi_0 = 0$ at all values of x – the particle could not exist in this state.

The probability of observing the particle in state n located between x and $x + dx$ is

$$P_n \, dx \propto |\psi_n(x)|^2 \, dx. \tag{50}$$

The lowest energy state is E_1 and the most probable location of the particle in this state is in the middle of the box (T–Rex Figure 5.23).

3.10   Summary

- Wave–particle duality is a fundamental characteristic of both light and matter. Experiment forces a given electron/photon to choose between the two options.

- The uncertainty principle imposes a fundamental limit on the precision with which we can determine "conjugate variables", e.g. position & momentum, energy & time.

- The wave function is not directly observable: only the term $|\Psi^2|$ has physical meaning – it represents an observable probability.

- In a given experiment Ψ represents a superposition of wave functions representing all possible outcomes. The act of observation collapses this superposition to just one outcome.

- The above ideas form the Copenhagen interpretation of quantum theory: **uncertainty**, **complementarity**, and **probability**.