



### $3.1$ **DE BROGLIE WAVES** A moving body behaves in certain ways as though it has a wave nature  $3.2$ **WAVES OF WHAT?**

Waves of probability

#### $3.3$ **DESCRIBING A WAVE**

A general formula for waves

#### $3.4$ PHASE AND GROUP VELOCITIES

A group of waves need not have the same velocity as the waves themselves

#### $3.5$ PARTICLE DIFFRACTION

An experiment that confirms the existence of de Broglie waves

#### $3.6$ PARTICLE IN A BOX Why the energy of a trapped particle is quantized

#### $3.7$ **UNCERTAINTY PRINCIPLE I**

We cannot know the future because we cannot know the present

#### $3.8$ **UNCERTAINTY PRINCIPLE II**

A particle approach gives the same result

 $3.9$ APPLYING THE UNCERTAINTY PRINCIPLE A useful tool, not just a negative statement



- 1905 discovery of the *particle properties of waves*: A revolutionary concept to explain data.
- 1924 (Louis de Broglie's PhD thesis) speculation that *particles might show wave behavior*: An equally revolutionary concept without a strong experimental mandate.
	- **moving objects have wave as well as particle characteristics**
- 1927 The existence of de Broglie waves was experimentally demonstrated.
- The **duality principle** provided the starting point for Schrödinger's successful development of quantum mechanics.

### **3. 1 De Broglie Waves: Matter Waves**

- A moving body behaves in certain ways as it has a wave nature.
- A photon of light of frequency v has the momentum
- De Broglie suggested that Photon wavelength equation is a *completely general one that applies to material particles as well as to photons*.
- Part of de Broglie's inspiration came from Bohr's theory of the hydrogen atom, in which the electron is supposed to follow only certain orbits around the nucleus.
- Two years later Erwin Schrödinger used the concept of de Broglie waves to develop a general theory that he and others applied to explain a wide variety of atomic phenomena.
- The existence of de Broglie waves was confirmed in diffraction experiments with electron beams in 1927.



Louis de Broglie 1892-1987 Nobel Prize in Physics in 1929



(Photon wavelength)

 $h\nu$  \_

### **3. 1 De Broglie Waves: de Broglie wavelength**



• The momentum of a particle of mass m and velocity v is  $p = \gamma mv$ , and its **de Broglie wavelength** is accordingly  $\lambda = \frac{h}{\sqrt{2}}$  (de Broglie wavelength )  $\gamma mv$ γ is the relativistic factor:  $γ = \frac{1}{\sqrt{1 - v^2/c^2}}$ 

- In certain situations, a moving body resembles a wave and in others it resembles a particle.
- *Which set of properties is most apparent depends on how its de Broglie wavelength compares with its dimensions and the dimensions of whatever it interacts with*.



Find the de Broglie wavelengths of (a) a 46-g golf ball with a velocity of 30 m/s, and (b) an electron with a velocity of  $10<sup>7</sup>$  m/s.

### Solution

(a) Since  $v \ll c$ , we can let  $\gamma = 1$ . Hence

$$
\lambda = \frac{h}{mv} = \frac{6.63 \times 10^{-34} \text{ J} \cdot \text{s}}{(0.046 \text{ kg})(30 \text{ m/s})} = 4.8 \times 10^{-34} \text{ m}
$$

The wavelength of the golf ball is so small compared with its dimensions that we would not expect to find any wave aspects in its behavior.

(b) Again  $v \ll c$ , so with  $m = 9.1 \times 10^{-31}$  kg, we have

$$
\lambda = \frac{h}{mv} = \frac{6.63 \times 10^{-34} \text{ J} \cdot \text{s}}{(9.1 \times 10^{-31} \text{ kg})(10^7 \text{ m/s})} = 7.3 \times 10^{-11} \text{ m}
$$

The dimensions of atoms are comparable with this figure—the radius of the hydrogen atom, for instance, is 5.3  $\times$  10<sup>-11</sup> m. It is therefore not surprising that the wave character of moving electrons is the key to understanding atomic structure and behavior.

### **3. 1 De Broglie Waves**



## Example 3.2

Find the kinetic energy of a proton whose de Broglie wavelength is 1.000 fm= $1.000x10^{-15}$  m, which is roughly the proton diameter.

## Solution

A relativistic calculation is needed unless pc for the proton is much smaller than the proton rest energy of  $E_0 = 0.938$  GeV. To find out, we use Eq. (3.2) to determine pc:

$$
pc = (\gamma m v)c = \frac{hc}{\lambda} = \frac{(4.136 \times 10^{-15} \text{ eV} \cdot \text{s})(2.998 \times 10^8 \text{ m/s})}{1.000 \times 10^{-15} \text{ m}} = 1.240 \times 10^9 \text{ eV}
$$

$$
= 1.2410 \text{ GeV}
$$

Since  $pc > E_0$  a relativistic calculation is required. From Eq. (1.24) the total energy of the proton is

$$
E = \sqrt{E_0^2 + p^2 c^2} = \sqrt{(0.938 \text{ GeV})^2 + (1.2340 \text{ GeV})^2} = 1.555 \text{ GeV}
$$

The corresponding kinetic energy is

$$
KE = E - E_0 = (1.555 - 0.938) \text{ GeV} = 0.617 \text{ GeV} = 617 \text{ MeV}
$$

- Waves of *probability*.
	- In water waves, the quantity that varies periodically is the **height** of the water surface.
	- In sound waves, it is **pressure**.
	- In light waves, **electric and magnetic fields** vary.
	- *What is it that varies in the case of matter waves?*
- The quantity *whose variations make up matter waves* is called the **wave function**, symbol Ψ.
- Born came the basic concept that the wave function  $\Psi$  of a particle is probability of finding it.
- The wave function Ψ itself, however, has no direct physical significance. *By itself cannot be an observable quantity.*
- **|Ψ|<sup>2</sup> must represent probability density** for electrons (or other particles).
- For this purpose, atomic scattering (collisions of atoms with various particles) processes suggested.

Max Born 1882-1970 Nobel Prize in Physics in 1954







- $|\Psi|^2$ ; the square of the absolute value of the wave function, which is known as *probability density*.
- The probability of experimentally finding the body described by the wave function at the point x, y, z, at the time t is proportional to the value of  $|\Psi|^2$  there at t.
	- A large value of  $|\Psi|^2$  means the strong possibility of the body's presence,
	- while a small value of  $|\Psi|^2$  means the slight possibility of its presence.
- There is a big difference between the probability of an event and the event itself.
	- *Although we can speak of the wave function Ψ that describes a particle as being spread out in space, this does not mean that the particle itself is thus spread out.*



- When an experiment is performed to detect electrons, for instance, a **whole** electron is either found **at a certain time and place** or it is not; there is no such thing as a 20 percent of an electron.
- However, it is entirely possible for there to be a 20 percent **chance** that the electron be found **at that time and place**, and it is this likelihood that is specified by  $|\Psi|^2$ .
- While the wavelength of the de Broglie waves associated with a moving body is given by the simple formula  $\lambda = h/\gamma mv$ , to find their amplitude  $\Psi$  as a function of position and time is often difficult.
- A general formula for waves.
- How fast do de Broglie waves travel?
	- Since we associate a de Broglie wave with a moving body, we expect that this wave has the same velocity as that of the body?
- Call the de Broglie wave velocity as  $v_n=v$

• De Broglie phase velocity 
$$
v_p = v\lambda = \left(\frac{\gamma mc^2}{h}\right)\left(\frac{h}{\gamma mv}\right) = \frac{c^2}{v}
$$
 (de Broglie phase velocity)

- Because the particle velocity v must be less than the velocity of light c, the de Broglie waves always travel faster than light!
- In order to understand this <u>unexpected result</u>, we must look into the *distinction between phase velocity (wave velocity) and group velocity*.
- How waves are described mathematically?





- Fig. 3.1. If we choose t=0 when the displacement y of the string at x=0 is a maximum, its displacement at any future time t at the same place is given by the formula  $y = A\cos(2\pi\nu t)$ (3.4)
	- where A is the amplitude of the vibrations (that is, their maximum displacement on either side of the x axis) and ν their frequency.
	- *Equation (3.4) tells us what the displacement of a single point on the string is as a function of time t.*





Figure 3.1 (a) The appearance of a wave in a stretched string at a certain time. (b) How the displacement of a point on the string varies with time.



- 
- A complete description of wave motion in a stretched string, however, should tell us what y is at <u>any point</u> on the string at <u>any time.</u>

$$
y = A\cos\left(2\pi\nu\left(t - \frac{x}{v_p}\right)\right)
$$
 (3.5 Wave formula)

- To obtain such a formula, let us imagine that we shake the string at  $x=0$  when t=0, so that a wave starts to travel down the string in the  $+x$ direction (Fig. 3.2).
- Since the wave speed  $v_p$  is given by  $v_p = v \lambda$ , we have

$$
y = A\cos\left(2\pi\left(\nu t - \frac{x}{\lambda}\right)\right)
$$
 (Wave formula)

- Most widely used description of a wave, however, is still another form of Eq. (3.5). The quantities angular frequency  $\omega$  and wave number k are defined by the formulas.  $\omega = 2\pi\nu$  (Angular frequncy)  $k = \frac{2\pi}{\lambda} = \frac{\omega}{v_n}$  (Wave number)
	- The unit of  $\omega$  is the radian per second and unit of k is the radian per meter.
	- Angular frequency gets its name from uniform circular motion, where a particle that moves around a circle v times per second sweeps out  $2\pi v$  rad/s.
	- The wave number is equal to the number of radians corresponding to a wave train 1 m long, since there are  $2\pi$  rad in one complete wave.

 $y = A\cos(\omega t - kx)$ (3.9 Wave formula)



- A group of waves need not have the same velocity as the waves themselves.
- *The amplitude of the de Broglie waves that correspond to a moving body reflects the probability that it will be found at a particular place at a particular time.*
- de Broglie waves **cannot** be represented simply by a formula resembling Eq. (3.9), which describes an indefinite series of waves all with the same amplitude A.
- Instead, we expect the wave representation of a moving body to correspond to a **wave packet**, or **wave group**, like that shown in Fig. 3.3, whose waves have amplitudes upon which the likelihood of detecting the body depends.

Wave group

Figure 3.3 A wave group.



- A familiar example of how wave groups come into being is the case of beats.
- If the original sounds have frequencies of, say, 440 and 442 Hz, we will hear a fluctuating sound of frequency 441 Hz with two loudness peaks, called beats, per second.
- The production of beats is illustrated in Fig. 3.4.



Figure 3.4 Beats are produced by the superposition of two waves with different frequencies.

### **3. 4 Phase And Group Velocities: A wave group**



- A wave group: a *superposition* of individual waves of different wavelengths whose interference with one another results in the variation in amplitude that defines the group shape.
	- If the velocities of the waves are the same, the velocity with which the wave group travels is the common phase velocity.
	- However, if the phase velocity varies with wavelength, the different individual waves do not proceed together. This situation is called **dispersion**.
	- As a result, the wave group has a velocity different from the phase velocities of the waves that make it up. This is the case with de Broglie waves.

 $v_q = v$ (De Broglie group velocity )

The de Broglie wave group associated with a moving body travels with the same velocity as the body. The phase velocity v<sub>p</sub> of de Broglie waves is, as we found earlier,  $v_p = \frac{\omega}{l} = \frac{c^2}{r}$ (De Broglie phase velocity )

- This exceeds both the velocity of the body v and the velocity of light c, since v<c. *However,*  $v_p$  *has no physical significance because the motion of the wave group, not the motion of the individual waves that make up the group, corresponds to the motion of the body, and*  $v_g < c$  *as it should be.*
- The fact that  $v_p$ >c for de Broglie waves therefore does not violate special relativity.



An electron has a de Broglie wavelength of 2.00 pm =  $2.00 \times 10^{-12}$  m. Find its kinetic energy and the phase and group velocities of its de Broglie waves. Solution

(a) The first step is to calculate  $pc$  for the electron, which is

$$
pc = \frac{hc}{\lambda} = \frac{(4.136 \times 10^{-15} \text{ eV} \cdot \text{s})(3.00 \times 10^8 \text{ m/s})}{2.00 \times 10^{-12} \text{ m}} = 6.20 \times 10^5 \text{ eV}
$$

$$
= 620 \text{ keV}
$$

The rest energy of the electron is  $E_0 = 511$  keV, so

$$
KE = E - E_0 = \sqrt{E_0^2 + (pc)^2} - E_0 = \sqrt{(511 \text{ keV})^2 + (620 \text{ keV})^2} - 511 \text{ keV}
$$
  
= 803 keV - 511 keV = 292 keV

(b) The electron velocity can be found from

$$
E = \frac{E_0}{\sqrt{1 - v^2/c^2}}
$$

to be

$$
v = c \sqrt{1 - \frac{E_0^2}{E^2}} = c \sqrt{1 - \left(\frac{511 \text{ keV}}{803 \text{ keV}}\right)^2} = 0.771c
$$

Hence the phase and group velocities are respectively

$$
v_p = \frac{c^2}{v} = \frac{c^2}{0.771c} = 1.30c
$$

$$
v_{\sigma}=v=0.771
$$

**3 Electron Microscopes**

- The *wave nature of moving electrons* is the basis of the electron microscope, the first of which was built in 1932.
- The *resolving power* of any optical instrument is proportional to the wavelength of whatever is used to illuminate the specimen.
- In the case of a good microscope that uses visible light, the maximum useful magnification is about 500; higher magnifications give larger images but do not reveal any more detail.
- Fast electrons, however, have wavelengths very much shorter than those of visible light and are easily controlled by electric and magnetic fields because of their charge.



Figure 3. 5 Because the wavelengths of the fast electrons in an electron microscope are shorter than those of the light waves in an optical microscope, the electron microscope can produce sharp images at higher magnifications.



- In an electron microscope, current-carrying coils produce magnetic fields that act as lenses to focus an electron beam on a specimen and then produce an enlarged image on a fluorescent screen or photographic plate (Fig. 3.5).
	- The technology of magnetic "lenses" does not permit the full theoretical resolution of electron waves to be realized in practice.
	- For instance, 100-keV electrons have wavelengths of 0.0037 nm, but the actual resolution they can provide in an electron microscope may be only about 0.1 nm.
- However, this is still a great improvement on the ~200-nm resolution of an optical microscope, and magnifications of over 1,000,000 have been achieved with electron microscopes.



- An experiment that confirms the existence of de Broglie waves.
- A wave effect with no analog in the behavior of Newtonian particles is diffraction.
- In 1927 Clinton Davisson & Lester Germer and G. P. Thomson independently confirmed de Broglie's hypothesis by demonstrating that **electron beams are diffracted when they are scattered by the regular atomic arrays of crystals**. (All three received Nobel Prizes for their work)
- Classical physics predicts that the scattered electrons will emerge in all directions with only a moderate dependence of
	- their intensity on scattering angle and
	- even less on the energy of the primary electrons
- Using a block of nickel as the target, Davisson and Germer verified these predictions.
- In the middle of their work an accident occurred that allowed air to enter their apparatus and oxidize the metal surface. To reduce the oxide to pure nickel, the target was baked in a hot oven.
- *After this treatment*, the target was returned to the apparatus and the measurements resumed.



Figure 3.6 The Davisson-Germer experiment.

*Now the results were very different. Instead of a continuous variation of scattered electron intensity with angle, distinct maxima and minima were observed whose positions depended upon the electron energy!* 



• Typical polar graphs of electron intensity after the accident are shown in Fig. 3.7.



Figure 3.7 Results of the Davisson-Germer experiment, showing how the number of scattered electrons varied with the angle between the incoming beam and the crystal surface. The Bragg planes of atoms in the crystal were not parallel to the crystal surface, so the angles of incidence and scattering relative to one family of these planes were both 65° (see Fig. 3.8).

- The method of plotting is such that the intensity at any angle is proportional to the distance of the curve at that angle from the point of scattering.
- If the intensity were the same at all scattering angles, the curves would be circles (scattered electrons emerge in all directions) centered on the point of scattering.
- *De Broglie's hypothesis suggested that electron waves were being diffracted by the target, much as x-rays are diffracted by planes of atoms in a crystal.*

- Let us see whether we can verify that de Broglie waves are responsible for the findings of Davisson and Germer. In a particular case,
	- a beam of 54-eV electrons was directed perpendicularly at the nickel target and
	- a sharp maximum in the electron distribution occurred at an angle of 50° with the original beam.
	- The angles of incidence and scattering relative to the family of Bragg planes shown in Fig. 3.8 are both 65°.



Figure 3.8 The diffraction of the de Broglie waves by the target is responsible for the results of Davisson and Germer.

- The spacing of the planes in this family, which can be measured by xray diffraction, is 0.091 nm. The Bragg equation for maxima in the diffraction pattern is  $n\lambda = 2d\sin\theta$  here d=0.091 nm,  $\theta$ =65° and n=1.
- the de Broglie wavelength of the diffracted electrons is  $\lambda$ =0.165 nm.

Now we use de Broglie's formula  $\lambda = \frac{h}{\gamma m v}$  to find the expected wavelength of the electrons.



• The electron kinetic energy of 54 eV is small compared with its rest energy  $mc^2$  of 0.51 MeV, so we can let  $\gamma = 1$ . Since  $KE = 1/2mv^2$  the electron momentum *mv* is

$$
mv = \sqrt{2mKE}
$$
  
=  $\sqrt{(2)(9.1 \times 10^{-31} kg)(54 eV)(1.6 \times 10^{-19} J/eV)}$   
=  $4.0 \times 10^{-24} kg.m/s$ 

The electron wavelength is therefore

$$
\lambda = \frac{h}{\gamma m v} = \frac{6.63 \times 10^{-34} \text{ J.s}}{(1)(4.0 \times 10^{-24} \text{ kg.m/s}))} = 1.66 \times 10^{-10} \text{ m} = 0.166 \text{ nm}
$$

which agrees well with the observed wavelength of 0.165 nm.

• The Davisson-Germer experiment thus directly verifies de Broglie's hypothesis of the wave nature of moving bodies.



- **Why the energy of a** *trapped* **particle is quantized**.
- *The wave nature of a moving particle leads to some remarkable consequences when the particle is restricted to a certain region of space instead of being able to move freely*.
- The simplest case is that of a particle that bounces back and forth between the walls of a box, as in Fig. 3.9.
- From a wave point of view, a particle trapped in a box is like a standing wave in a string stretched between the box's walls (Fig. 3.10).
- In both cases the wave variable (transverse displacement for the walls of the box. string, wave function for the moving particle) must be 0 at the walls, since the waves stop there. (Boundary Condition)
- The possible de Broglie wavelengths of the particle in the box therefore are determined by the width L of the box, as in Fig.  $3.10$ .

$$
\lambda = \frac{2L}{n} \quad n = 1, 2, 3, \dots
$$





Figure 3.9 A particle confined to a box of width L. The particle is assumed to move back and forth



Figure 3.10 Wave functions of a particle trapped in a box L wide.

- 
- The kinetic energy of a particle of momentum mv is  $KE = \frac{1}{2}mv^2 = \frac{(mv)^2}{2m} = \frac{h^2}{2m\lambda^2}$

**can have are**  $E_n = \frac{n^2 h^2}{n}$   $n = 1, 2, 3, \ldots$  <sup>(3.18 Particle in a box)</sup> The particle has no potential energy in this model, the only energies it

- **Each permitted energy is called an energy level, and the integer n that specifies an energy level E<sup>n</sup> is called its quantum number.**
- We can draw three general conclusions from Eq. (3.18). These conclusions apply to any particle confined to a certain region of space, for instance an atomic electron held captive by the attraction of the positively charged nucleus.
- **1.A trapped particle cannot have an arbitrary energy, as a free particle can**. The fact of its confinement leads to restrictions on its wave function that allow the particle to have only certain specific energies and no others.
- **2.A trapped particle cannot have zero energy**. Since the de Broglie wavelength of the particle is  $\lambda = h/mv$ , a speed of v=0 means an infinite wavelength. But there is no way to reconcile an infinite wavelength with a trapped particle, so such a particle must have at least some kinetic energy.
- **3.Because Planck's constant is so small quantization of energy is considerable only when m and L are also small**. This is why we are not aware of energy quantization in our own experience.



## Example 3.4 & 3.5

An electron is in a box 0.10 nm across, which is the order of magnitude of atomic dimensions. Find its permitted energies.

Solution

Here  $m = 9.1 \times 10^{-31}$  kg and  $L = 0.10$  nm =  $1.0 \times 10^{-10}$  m, so that the permitted electron energies are

$$
E_n = \frac{(n^2)(6.63 \times 10^{-34} \text{ J} \cdot \text{s})^2}{(8)(9.1 \times 10^{-31} \text{ kg})(1.0 \times 10^{-10} \text{ m})^2} = 6.0 \times 10^{-18} n^2 \text{ J}
$$
  
= 38n<sup>2</sup> eV

The minimum energy the electron can have is 38 eV, corresponding to  $n = 1$ . The sequence of energy levels continues with  $E_2 = 152$  eV,  $E_3 = 342$  eV,  $E_4 = 608$  eV, and so on (Fig. 3.11). If such a box existed, the quantization of a trapped electron's energy would be a prominent feature of the system. (And indeed energy quantization is prominent in the case of an atomic electron.)

### A 10-g marble is in a box 10 cm across. Find its permitted energies. Solution

With 
$$
m = 10 \text{ g} = 1.0 \times 10^{-2} \text{ kg}
$$
 and  $L = 10 \text{ cm} = 1.0 \times 10^{-1} \text{ m}$ ,

$$
E_n = \frac{(n^2)(6.63 \times 10^{-34} \text{ J} \cdot \text{s})^2}{(8)(1.0 \times 10^{-2} \text{ kg})(1.0 \times 10^{-1} \text{ m})^2}
$$
  
= 5.5 × 10<sup>-64</sup>n<sup>2</sup> J

The minimum energy the marble can have is 5.5x10-64 J, corresponding to *n=*1. A marble with this kinetic energy has a speed of only 3.3x10-31 m/s and therefore cannot be experimentally distinguished from a stationary marble. A reasonable speed a marble might have is, say, 1/3 m/s-which corresponds to the energy level of quantum number *n=1030*!

- **We cannot know the future because we cannot know the present**.
- Wave group of Fig. 3.3: The particle that corresponds to this wave group may be located anywhere within the group at a given time.
	- The probability density  $|\Psi|^2$  is a **maximum in the middle** of the group, so it is most likely to be found there.
- Nevertheless, we may still find the particle anywhere that  $|\Psi|^2$ is not actually 0.
- *The narrower its wave group, the more precisely a particle's position can be specified (Fig. 3.12a).*
- However, the wavelength of the waves in a **narrow packet** is not well defined; there are not enough waves to measure  $\lambda$ accurately.
- This means that since  $\lambda = h/\gamma mv$ , the particle's momentum  $\gamma mv$ is not a precise quantity.
- *On the other hand, a wide wave group, such as that in Fig. 3.12b, has a clearly defined wavelength.*
- The momentum that corresponds to this wavelength is therefore a precise quantity.

11 March 2018 MSE 228 Engineering Quantum Mechanics © Dr.Cem Özdoğan <sup>the particle.</sup> 28 the particle.





Figure 3.12 (a) A narrow de Broglie wave group. The position of the particle can be precisely determined, but the wavelength (and hence the particle's momentum) cannot be established because there are not enough waves to measure accurately. (b) A wide wave group. Now the wavelength can be precisely determined but not the position of





#### 11 March 2018 MSE 228 Engineering Quantum Mechanics © Dr.Cem Özdoğan 29

- But where is the particle located? Thus, we have the uncertainty principle.
- It is impossible to know both the exact position and exact momentum of an object at the same time.
- This principle, which was discovered by Werner Heisenberg in 1927, is one of the most significant of physical laws.
- The de Broglie wavelength of a particle of momentum p is  $\lambda$ =h/p and the corresponding wave number is
- In terms of wave number, the particle's momentum is therefore  $p = \frac{hk}{2\pi}$

Hence an uncertainty  $\Delta k$  in the wave number of the de Broglie waves associated with the particle results in an uncertainty  $\Delta p$  in the particle's momentum according to the formula

$$
\Delta p = \frac{h\Delta k}{2\pi} \text{ Since } \Delta x \Delta k \ge \frac{1}{2}, \ \Delta k \ge \frac{1}{2\Delta x} \text{ and } \Delta x \Delta p \ge \frac{h}{4\pi} \qquad \text{(Uncertainty principle)}
$$

Werner Karl Heisenberg 1901-1976 Nobel Prize in Physics in 1932





- This equation states that the product of the uncertainty  $\Delta x$  in the *position of an object at some instant and the uncertainty*  $\Delta p$  *in its momentum component in the x direction at the same instant is equal to or greater than*  $h/4\pi$ *.* 
	- If we arrange matters so that  $\Delta x$  is small, corresponding to a narrow wave group, then  $\Delta p$  will be large.
	- If we reduce  $\Delta p$  in some way, a broad wave group is inevitable and  $\Delta x$  will be large.
- Since we cannot know exactly both where a particle is right now and what its momentum is, we cannot say anything definite about where it will be in the future or how fast it will be moving then.
- **We cannot know the future for sure because we cannot know the present for sure.**
- But we can still say that the particle is *more likely* to be in one place than another and that its momentum is *more likely* to have a certain value than another.

$$
\boxed{\Delta x \Delta p \geq \frac{\hbar}{2} \quad \text{ (Uncertainty principle)}}
$$

A measurement establishes the position of a proton with an accuracy of  $\pm 1.00x10^{-11}$  m. Find the uncertainty in the proton's position 1.00 s later. Assume v<<c.

Let us call the uncertainty in the proton's position  $\Delta x_0$  at the time  $t = 0$ . The uncertainty in its momentum at this time is therefore, from Eq. (3.22),

$$
\Delta p \geq \frac{\hbar}{2\Delta x_0}
$$

Since  $v \ll c$ , the momentum uncertainty is  $\Delta p = \Delta (mv) = m \Delta v$  and the uncertainty in the proton's velocity is

$$
\Delta v = \frac{\Delta p}{m} \ge \frac{\hbar}{2m \Delta x_0}
$$

The distance  $x$  the proton covers in the time  $t$  cannot be known more accurately than

$$
\Delta x = t \; \Delta v \ge \frac{\hbar t}{2m \; \Delta x_0}
$$

Hence  $\Delta x$  is inversely proportional to  $\Delta x_0$ : the more we know about the proton's position at  $t = 0$ , the less we know about its later position at  $t > 0$ . The value of  $\Delta x$  at  $t = 1.00$  s is

$$
\Delta x \ge \frac{(1.054 \times 10^{-34} \text{ J} \cdot \text{s})(1.00 \text{ s})}{(2)(1.672 \times 10^{-27} \text{ kg})(1.00 \times 10^{-11} \text{ m})}
$$
  
\n
$$
\ge 3.15 \times 10^3 \text{ m}
$$

This is 3.15 km—nearly 2 mi! What has happened is that the original wave group has spread out to a much wider one (Fig. 3.16). This occurred because the phase velocities of the component waves vary with wave number and a large range of wave numbers must have been present to produce the narrow original wave group. See Fig. 3.14.



- When a set of measurements is made of some quantity x in which the experimental errors are random, the result is often a Gaussian distribution whose form is the bell-shaped curve shown in Fig. 3.15.
- The standard deviation  $\sigma$  of the measurements is a measure of the spread of x values about the mean of  $x_0$ , where  $\sigma$  equals the square root of the average of the squared deviations from  $x_0$ .
	- If N measurements were made
	- The width of a Gaussian curve **at half** its maximum value is  $2.35\sigma$ .

$$
\sigma = \sqrt{\left(\frac{1}{N}\sum_{i=1}^{N}(x_i - x_0)^2\right)}
$$

(Standart deviation)

The Gaussian function f (x) that describes the curve is given by  $f(x) = \frac{1}{\sigma \sqrt{2\pi}} e^{-(x-x_0)^2/2\sigma^2}$ 

(Gaussian function)

where  $f(x)$  is the probability that the value x be found in a particular measurement.



11 March 2018 MSE 228 Engineering Quantum Mechanics © Dr.Cem Özdoğan 32



Figure 3.15 A Gaussian distribution. The probability of finding a value of x is given by the Gaussian function  $f(x)$ . The mean value of  $x$  is  $x_0$ , and the total width of the curve at half its maximum value is  $2.35\sigma$ , where  $\sigma$  is the standard deviation of the distribution. The total probability of finding a value of x within a standard deviation of  $x_0$  is equal to the shaded area and is 68.3 percent.



• The probability that a measurement lie inside a certain range of x values, say between  $x_1$  and  $x_2$ , is given by the area of the f (x) curve between these limits. This area is the integral

$$
P_{x_1x_2} = \int_{x_1}^{x_2} f(x) dx
$$

• An interesting question is *what fraction of a series of measurements*  has values within a standard deviation of the mean value  $x_0$ . In this case  $x_1 = x_0 - \sigma$  and  $x_2 = x_0 + \sigma$ , and

$$
P_{x_0 \pm \sigma} = \int_{x_0 - \sigma}^{x_0 + \sigma} f(x) dx = 0.683
$$

• Hence 68.3 percent of the measurements fall in this interval, which is shaded in Fig. 3.15. A similar calculation shows that 95.4 percent of the measurements fall within two standard deviations  $(2\sigma)$  of the mean value.



- **A particle approach gives the same result**.
- The uncertainty principle can be arrived at from the point of view of the particle properties of waves as well as from the point of view of the wave properties of particles.
- To measure the position and momentum of an object at a certain moment, we must **touch** it with something that will carry the required information back to us.
- Suppose we look at an electron using light of wavelength  $\lambda$ , as in Fig. 3.17.
- Each photon of this light has the momentum  $h/\lambda$ . When one of these photons bounces off the electron (which must happen if we are to "see" the electron), the electron's original momentum will be changed.
- The exact amount of the change  $\Delta p$  cannot be predicted, but it will be of the same order of magnitude as the photon momentum  $h/\lambda$ . Hence  $\Delta p = \frac{h}{\lambda}$ (3.23)



Figure 3.17 An electron cannot be observed without changing its momentum.



- The longer the wavelength of the observing photon, the smaller the uncertainty in the electron's momentum.
- A reasonable estimate of the minimum uncertainty in the measurement might be one photon wavelength, so that  $\Delta x > \lambda$ 
	- The shorter the wavelength, the smaller the uncertainty in location. However, if we use light of short wavelength to increase the accuracy of the position measurement, there will be a corresponding decrease in the accuracy of the momentum measurement because the higher photon momentum will disturb the electron's motion to a greater extent.
	- Light of long wavelength will give a more accurate momentum but a less accurate position.
	- Combining Eqs. (3.23) and (3.24) gives  $\Delta x \Delta p \geq h$
- Uncertanity Principle: A useful tool, not just a negative statement.
- Planck's constant h is so small that the limitations imposed by the uncertainty principle are *significant only in the realm of the atom.*

A typical atomic nucleus is about 5.0x10-15 m in radius. Use the uncertainty principle to place a lower limit on the energy an electron must have if it is to be part of a nucleus.

Solution

Letting  $\Delta x = 5.0 \times 10^{-5}$  m we have

$$
\Delta p \ge \frac{\hbar}{2\Delta x} \ge \frac{1.054 \times 10^{-34} \text{ J} \cdot \text{s}}{(2)(5.0 \times 10^{-15} \text{ m})} \ge 1.1 \times 10^{-20} \text{ kg} \cdot \text{m/s}
$$

If this is the uncertainty in a nuclear electron's momentum, the momentum  $p$  itself must be at least comparable in magnitude. An electron with such a momentum has a kinetic energy KE many times greater than its rest energy  $mc^2$ . From Eq. (1.24) we see that we can let KE =  $pc$ here to a sufficient degree of accuracy. Therefore

$$
KE = pc \ge (1.1 \times 10^{-20} \text{ kg} \cdot \text{m/s})(3.0 \times 10^8 \text{ m/s}) \ge 3.3 \times 10^{-12} \text{ J}
$$

Since 1 eV =  $1.6 \times 10^{-19}$  J, the kinetic energy of an electron must exceed 20 MeV if it is to be inside a nucleus. Experiments show that the electrons emitted by certain unstable nuclei never have more than a small fraction of this energy, from which we conclude that nuclei cannot contain electrons. The electron an unstable nucleus may emit comes into being at the moment the nucleus decays (see Secs. 11.3 and 12.5).

A hydrogen atom is  $5.3x10^{-11}$  m in radius. Use the uncertainty principle to estimate the minimum energy an electron can have in this atom.

### Solution

Here we find that with  $\Delta x = 5.3 \times 10^{-11}$  m.

$$
\Delta p \ge \frac{\hbar}{2\Delta x} \ge 9.9 \times 10^{-25} \text{ kg} \cdot \text{m/s}
$$

An electron whose momentum is of this order of magnitude behaves like a classical particle, and its kinetic energy is

$$
KE = \frac{p^2}{2m} \ge \frac{(9.9 \times 10^{-25} \text{ kg} \cdot \text{m/s})^2}{(2)(9.1 \times 10^{-31} \text{ kg})} \ge 5.4 \times 10^{-19} \text{ J}
$$

which is 3.4 eV. The kinetic energy of an electron in the lowest energy level of a hydrogen atom is actually 13.6 eV.





An "excited" atom gives up its excess energy by emitting a photon of characteristic frequency. The average period that elapses between the excitation of an atom and the time it radiates is  $1.0x10^{-8}$  s. Find the inherent uncertainty in the frequency of the photon.

### Solution

The photon energy is uncertain by the amount

$$
\Delta E \ge \frac{\hbar}{2\Delta t} \ge \frac{1.054 \times 10^{-34} \,\text{J} \cdot \text{s}}{2(1.0 \times 10^{-8} \,\text{s})} \ge 5.3 \times 10^{-27} \,\text{J}
$$

The corresponding uncertainty in the frequency of light is

$$
\Delta \nu = \frac{\Delta E}{h} \ge 8 \times 10^6 \text{ Hz}
$$

This is the irreducible limit to the accuracy with which we can determine the frequency of the radiation emitted by an atom. As a result, the radiation from a group of excited atoms does not appear with the precise frequency  $\nu$ . For a photon whose frequency is, say,  $5.0 \times 10^{14}$  Hz,  $\Delta \nu / \nu = 1.6 \times 10^{-8}$ . In practice, other phenomena such as the doppler effect contribute more than this to the broadening of spectral lines.



- *Another form of the uncertainty principle concerns energy and time*. We might wish to measure the energy E emitted during the time  $\Delta t$  in an atomic process.
- If the energy is in the form of EM waves, the limited time available restricts the accuracy with which we can determine the frequency ν of the waves.
- Let us assume that the minimum uncertainty in the number of waves we count in a wave group is one wave.
- Since the frequency of the waves under study is equal to the number of them we count divided by the time interval, the uncertainty  $\Delta v$  in our frequency measurement is  $\Delta \nu \geq \frac{1}{\Delta t}$

The corresponding energy uncertanity is  $\Delta E = h \Delta \nu \rightarrow \Delta E \Delta t \geq h$ 

• A more precise calculation based on the nature of wave groups changes this result to $\Delta E \Delta t \geq \frac{n}{2}$ (Uncertainties in energy and time)



1. Show that de Broglie wavelength of electron with having kinetic energy value of 100 keV is 0.0037.

KE=100 keV = 0.1 MeV which is comporable to electron restmass energy: 0.51 MeV = Relativistic Equations  $\theta$  E=KE + MC = KE+E  $QE^{2}=(mc^{2})^{2}+(pc)^{2}=E_{0}^{2}+(pc)^{2}$  $Pc = hV = h c$ ,  $\lambda = ?$  $k^{2}$   $(k^{2} + 5)^{2} = 5^{2} + (h^{2})^{2}$  $(0.1$ MeV + 0.5 MeV)<sup>2</sup>  $=(0.5$ MeV)<sup>2</sup> +  $((6.626 \times 10^{-34} \text{ s})/1.602 \times 10^{-19} \text{ eV})/3 \times 10^8 \text{ m/s}$  $\Rightarrow \lambda = [4.14 \times 10^{-15} \text{eV}_{+s}](3 \times 10^{8} \text{m/s})]^2 = [1.24 \times 10^{-7}$  $e^{-(\epsilon_{e} \sqrt{\kappa m})}$  $3.6 \times 10^{11}$ eV<sup>2</sup> 2.5 $\times10^{11}$ eV<sup>2</sup>  $\Rightarrow \lambda = \sqrt{1.40 \times 10^{-23}}$   $m^2 = 0.0037$  nm



2. An electron moves in the x direction with a speed of  $3.6x10^6$  m/s. We can measure its speed to a precision of 1%. With what precision can we simultaneously measure its x coordinate?

n-direction, speed of precision of 1% => Avr = 1/2 x + 100  $\Delta P_{\chi} = m \, \Delta V_{\chi} = (9.11 \times 10^{-31} kg)(6.6 \times 10^6 m/s) = 3.3 \times 10^{-26} kg m/s$  $\Rightarrow\Delta x\Delta p\geqslant \Delta\rightarrow\Delta x\cong\frac{6}{\Delta p_{\mathcal{L}}}=1.05\times10^{-3}\frac{m}{36}=3.18\times10^{-9}m=3.2 nm$ about 10 atoms in  $J \equiv kg m_{22}^{2}$ 



3. What kinetic energy (in electron volts) should neutrons have if they are to be diffracted from crystals with interatomic distance of 1.00 Å?

de Broglie wavelength should be in the order of interationic<br>dutance.  $\lambda \propto d$ .  $\lambda = 1.00 \text{ Å} \rightarrow p = \frac{h}{\lambda}$ ,  $\frac{D^2}{2m_\pi} = K E \begin{cases} m_{\pi} = 1.66 \times 10^{-27} \text{ kg} \\ h = 6.62 \times 10^{-3} \text{ J} \cdot \text{s} \end{cases}$ <br> $\lambda \propto \mu E = \frac{(h/\lambda)^2}{2mn} = \frac{(6.63 \times$ 



4. Show that the spread of velocities caused by the uncertainty principle does not have measurable consequences for macroscopic objects (objects that are large compared with atoms) by considering a 100-g racquetball confined to a room 15 m on a side. Assume the ball is moving at 2.0 m/s along the x axis

 $m = 0.1 kg$ <br>  $v = 2 m/s$ <br>  $\Delta x = 15 m$ <br>  $\Delta x = 15$ 



5. Estimate the kinetic energy of an electron confined within a nucleus of size  $1.0x10^{14}$  m by using the uncertainty principle.

election<br>
confined<br>  $\begin{pmatrix}\n\Delta x \Delta P_x \ge \frac{b}{2} \sim \Delta P_x \ge \frac{6.63 \times 10^{-3} g.s}{2 \cdot 2 \pi \cdot 7 \times 10^{-14} m}\n\end{pmatrix} \propto \begin{pmatrix}\n\Delta P_x \\
\Delta P_y\n\end{pmatrix} \propto \begin{pmatrix}\n\Delta P_y \\
\Delta P_z\n\end{pmatrix} \propto \begin{pmatrix}\n\Delta P_x \\
\Delta P_y\n\end{pmatrix} \propto \begin{pmatrix}\n\Delta P_y \\
\Delta P_z\n\end{pmatrix} \propto \begin{pmatrix}\n\Delta P_x \\
\Delta P$  $(a, p) = 2.2$  or  $h, 2$  and  $= 9.40$  MeV



6. Although an excited atom can radiate at any time from t=0 to t= $\infty$ , the average time after excitation at which a group of atoms radiates is called the **lifetime**,  $\tau$ , of a particular excited state. (a) If  $\tau = 1.0x10$ <sup>8</sup> s (a typical value), use the uncertainty principle to compute the line width  $\Delta v$  of light emitted by the decay of this excited state. (b) If the wavelength of the spectral line involved in this process is 500 nm, find the fractional broadening  $\Delta v/v$ .





7. (*a*) A charged pi meson has a rest energy of 140MeV and a lifetime of 26 ns. Find the energy uncertainty of the pi meson, expressed in MeV and also as a fraction of its rest energy. (*b*) Repeat for the uncharged pi meson, with a rest energy of 135MeV and a lifetime of 8*.*3x10-17 s. (*c*) Repeat for the rho meson, with a rest energy of 765MeV and a lifetime of  $4.4x10^{-24}$  s.





8. Find the quantized energy levels of an electron constrained to move in a one-dimesional atom of size 0.1 nm.

Particle in  $\left\{\n\begin{array}{l}\n2\pi r \Rightarrow n\lambda \\
\lambda = \frac{h}{p}\n\end{array}\n\right\}$  only  $k \in \infty$   $\in k\in -\frac{p^2}{2m} = \frac{h^2}{\lambda^2 2m} = \frac{h^2}{2\pi r^2} = \frac{h^2}{2\pi n^2} = \frac{h^2}{2\pi n r^2}$ <br>  $k = 0.1$ am<br>  $k \in -\frac{p^2}{2m}$ <br>  $\left\{\n\begin{array}{l}\n\lambda = \frac{h}{p}\n\end{array}\n\right\}$  $\Rightarrow$   $n=1 \rightarrow \frac{2}{2} = 38eV$ <br>  $n=2 \rightarrow \frac{2}{3} = 153eV$ <br>  $n=3 \rightarrow \frac{2}{3} = 344eV$ 



## Additional Materials