CHAPTER 15

More on the models of the atom

The limitations of classical physics gave birth to quantum physics

Introduction

This chapter will describe and discuss models of the atom, proposed by Louis de Broglie, Wolfgang Pauli and Werner Heisenberg. These models are collectively referred to as quantum mechanics, which itself stands as a brand new area of physics that parallels the classical Newtonian physics. Many of these concepts involve very complicated theories and sophisticated mathematics; however, for the scope of the HSC Physics course, only the main ideas will be described.

15.1 The wave–particle duality of light

For many centuries, light had always been thought of as waves, that is, it can undergo reflection, refraction, diffraction and interference, all of which are fundamental wave properties. However, as shown in Chapter 11, when Einstein was trying to explain the photoelectric effect theoretically in 1905, he had to assume that light behaved like particles, where each particle had the energy equal to Planck's constant multiplied by the light frequency, $E = hf$. This particle model of light successfully explained the photoelectric effect. The phenomenon that matter can behave as both a wave and a particle at the same time is known as **wave–particle duality**.

So the question is, how can something possess wave and particle characteristics at the same time? The answer lies in the fact that the wave model and particle model should be seen to complement each other to give a more complete description of a particular phenomenon, rather than to contradict each other. In terms of light, when one is dealing with properties such as reflection, deflection, refraction, diffraction and interference, the wave model of light applies. On the other hand, if one is explaining phenomena like the photoelectric effect, the particle model of light is more suitable. The two models do not contradict each other; rather, together they give rise to a better depiction of the overall properties of light.

This chapter expands on this idea: the wave–particle duality is not limited to light; rather, it can be generalised to other substances.

Relationship between the wave characteristics and the particle properties

To quantitatively describe wave–particle duality, a formula can be used to link the wavelength of the wave to the momentum of the particle, that is:

$$\lambda = \frac{h}{mc}$$

Where:

λ = wavelength of the light (m)
h = Planck's constant: 6.626×10^{-34} J s
m = mass of the photon (kg)
c = speed of the photon (light) = 3×10^{8} m s^{-1}
mc = momentum of the photon, measured in kg m s^{-1}

It is important to note that the left-hand side of the equation is 'wavelength', which is one feature of a wave, whereas the right-hand side contains 'momentum' which is an exclusive particle property.

15.2 Matter waves

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Worked example 26

■ *Describe the impact of de Broglie's proposal that any kind of particle has both wave and particle properties*

Louis de Broglie

As mentioned before, the wave-particle duality is not just limited to light or EMR. In fact, it can be generalised to all other substances. This principle was first proposed by Louis de Broglie (1892–1987) in 1924. He 'borrowed' the equation $\lambda = \frac{h}{mc}$ and generalised the equation by replacing the $\boldsymbol{c}$ (speed of light) by $\boldsymbol{v}$, the speed of any particle. The consequence of this transformation is that any particle that has a momentum can have a wavelength, and therefore can behave like a wave called the **matter wave**. This is particularly true for small particles like electrons, as we shall see in the examples.

■ *Solve problems and analyse information using:* $\lambda = \frac{h}{mv}$

Thus we have:

$$\lambda = \frac{h}{mv}$$

Where:

λ = wavelength of the matter wave (m)
h = Planck's constant: 6.626×10^{-34} J s
m = mass of the particle (kg)
v = speed of the particle (m s^{-1})
mv = momentum of the particle (kg m s^{-1})

Example 1

What is de Broglie's wavelength of an object with a mass of 1.00 kg moving at a velocity of 1.00 m s^{-1}?

Solution

$$\lambda = \frac{h}{mv}$$

$$\lambda = \frac{6.626 \times 10^{-34}}{1 \times 1}$$

$$= 6.63 \times 10^{-34} \text{ m}$$

This wavelength is too small to be observed! The consequence is that although all objects can possess wave characteristics, most of the wavelengths formed by massive objects are usually too small to be observed; therefore we usually cannot visualise them as waves (even with instruments).

Example 2

What is de Broglie's wavelength of an electron moving at 1.00×10^6 m s^{-1}?

Solution

$$\lambda = \frac{h}{mv}$$

$$\lambda = \frac{6.626 \times 10^{-34}}{(9.11 \times 10^{-31})(1.00 \times 10^6)}$$

$$= 7.27 \times 10^{-10} \text{ m}$$

This wavelength is reasonably large and can be detected by the right instruments.

Example 3

Calculate de Broglie's wavelength of an electron when it is accelerated by a voltage of 54 V.

Solution

In this case, in order to calculate the wavelength of this electron, we must know its momentum, and hence its velocity. To calculate the velocity, we need to use the fact that the kinetic energy gained by the electron (thus velocity) is derived from the electrical energy supplied by the voltage. Hence:

$$\frac{1}{2}mv^2 = qV$$

$$\frac{1}{2}mv^2 = q \times 54$$

$$mv^2 = 108q$$

$$v^2 = \frac{(108)(1.6 \times 10^{-19})}{9.11 \times 10^{-31}}$$

$$v^2 = \sqrt{\frac{(108)(1.6 \times 10^{-19})}{9.11 \times 10^{-31}}}$$

$$v = 4.4 \times 10^6 \text{ m s}^{-1}$$

Once we have velocity we can calculate the wavelength:

$$\lambda = \frac{h}{mv}$$

$$= \frac{6.626 \times 10^{-34}}{(9.11 \times 10^{-31})(4.4 \times 10^6)}$$

$$= 1.67 \times 10^{-10} \text{ m}$$

15.3 Proof for matter waves

- ***Define diffraction and identify that interference occurs between waves that have been diffracted***
- ***Describe the confirmation of de Broglie's proposal by Davisson and Germer***

Any kind of new proposal needs to be supported through experiments, and the concept of matter waves proposed by de Broglie could not be an exception. The experiment to confirm the existence of matter waves was performed by two scientists, Clinton J. Davisson (1881–1958) and Lester H. Germer (1896–1971), in 1927. In order to understand the experiment, we need to first study a basic wave property known as **diffraction**.

Diffraction

Definition

Diffraction is the bending of the waves as they pass around the corner of a barrier or as they move through obstacles such as a slit.

This concept is demonstrated in Figures 15.1 (a), (b) and (c).

Consider the situation where a wave is allowed to pass through two slits that are adjacent to each other, as shown in Figure 15.2. As we would expect, the waves will undergo diffraction. Furthermore, the diffracted waves will now make contact with each other; therefore, they will interact with each other to cause interference. Recall that when the crest of one wave meets the crest of another wave, they will combine to give an even bigger crest. A similar principle applies to two troughs; this is known as **constructive interference**. On the other hand, when a crest meets a trough, they will cancel each other out—this is known as **destructive interference**. Because waves have crests and troughs that alternate, there will be alternating constructive

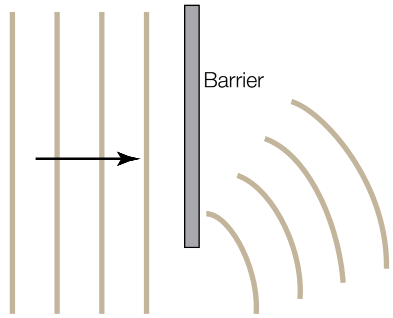

Figure 15.1 (a) Diffraction of a wave as it passes around a corner

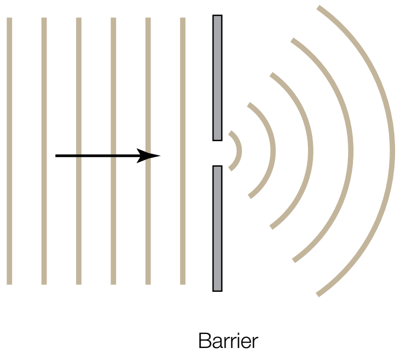

Figure 15.1 (b) Diffraction of a wave as it passes through a slit

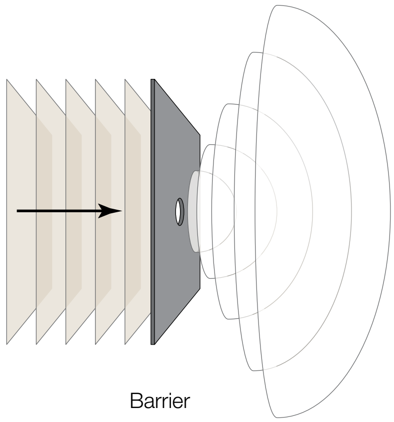

Figure 15.1 (c) Diffraction of a wave as it passes through a small circular hole

and destructive interferences throughout the region where the two waves are in contact, with the exact pattern determined by the size of the wavelength of the two waves (see Fig. 15.2). Furthermore, if the waves are visible light, then a series of dark and bright lines can be seen. In the case of sound waves, alternating loud and soft sounds can be heard. For any other waves, an alternating maximal and minimal signal intensity can be detected by instruments. Remember also that diffraction and interference are exclusive wave properties.

The experiment

In 1927, Davisson and Germer set up the experiment, similar to that shown in Figure 15.3. They fired energetic electrons towards a nickel crystal and studied the behaviour of these electrons as they scattered off the nickel surface.

The electrons were first accelerated using a voltage of 54 volts to achieve a high velocity and were then directed towards the nickel crystal. The electrons, on reaching the nickel crystal, would be scattered off different planes of the nickel crystal, similar to that in Bragg's experiment (described in Chapter 13). It is important to note that some of the returning (scattered) electrons would pass through the gaps between the nickel atoms, which act as many 'slits', so diffraction would occur. The situation was therefore similar to that shown in Figure 15.2 but more extensive. Consequently,

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Simulation: interference of light—interference patterns

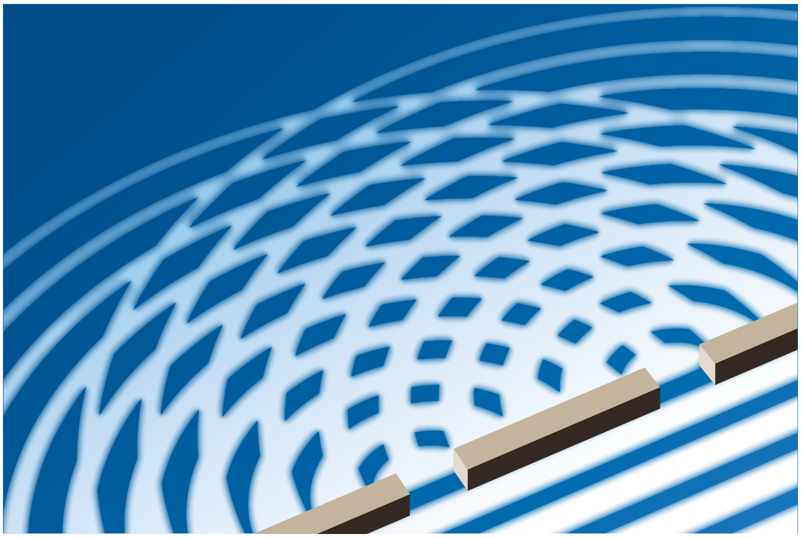

Figure 15.2 Interference pattern formed by two adjacent diffracted waves: note that the brighter regions represent constructive interference whereas the darker regions represent destructive interference

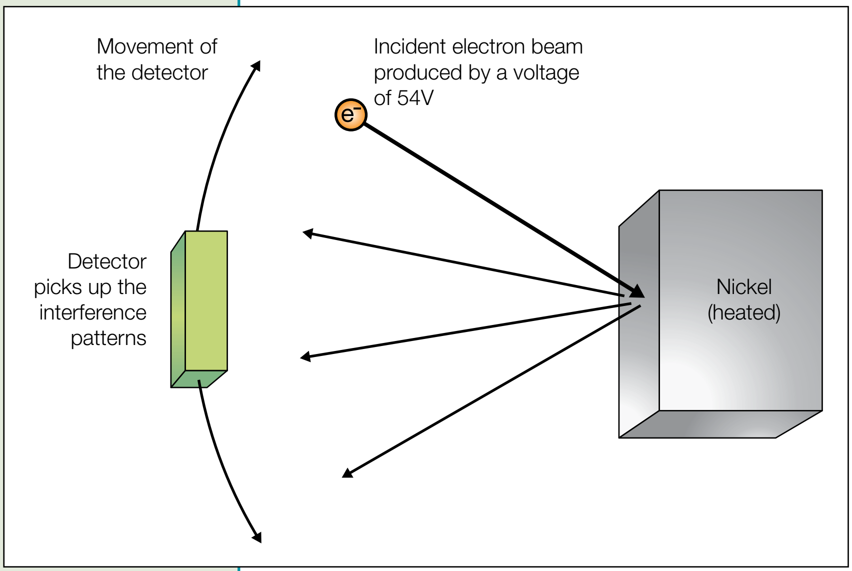

Figure 15.3 Davisson and Germer's electron-scattering experiment

interference patterns would be formed by the returning electrons. If a detector was run alongside the nickel crystal, a series of maxima and minima of electron intensity should be detected.

In their experiment Davisson and Germer were able to observe a series of maxima and minima of the scattered electrons, thus proving the wave nature of the electrons, and hence the existence of matter waves. Furthermore, from the interference pattern they were able to measure the wavelength of the electron waves that resulted from this diffraction pattern. The value agreed with the wavelength calculated using de Broglie's equation $\lambda = \frac{h}{mv}$ (refer to example 3 on page 263).

In summary, the experiment was successful not only in determining the existence of electron waves, and therefore matter waves, but also in confirming the validity of de Broglie's equation to describe these matter waves, $\lambda = \frac{h}{mv}$.

G. P. Thomson's electron diffraction experiment

Although G. P. Thomson's experiment is not addressed in the syllabus, it is appropriate to mention here. In 1928, G. P. Thomson, son of J. J. Thomson, passed an electron beam through a thin foil of gold. The electrons went through the thin foil and were scattered to land on the photographic film behind the foil, where they created an interference pattern. He compared the pattern to that obtained from using X-rays, which had been established to have wave characteristics, and saw the two patterns were remarkably similar. From this, he was able to confirm the wave nature of the electrons. Ironically, his father J. J. Thomson was awarded the Nobel Prize for proving the particle nature of electrons, whereas a couple of decades later, his son G. P. Thomson proved the wave characteristics of electrons.

15.4 Applying the matter waves to the electrons in an atom

■ *Explain the stability of the electron orbits in the Bohr atom using de Broglie's hypothesis*

De Broglie stated that electrons can behave as waves and this is true for all electrons including those found in the atoms. De Broglie went on to propose that:

Definition

The electrons in atoms behave like standing waves, which wrap around the nucleus in an integral number of wavelengths. They are known as **electron waves**.

The concept of standing waves is shown in Figure 15.4. Standing waves refer to waves that do not propagate but vibrate between two boundaries. The points that do not vibrate are called **nodes**, and the points that vibrate between maximum and minimum positions are known as **anti-nodes**. Also note a faster vibration will result in a higher frequency and hence more waves. If we pick any of the standing waves from Figure 15.4 (a) to (c) and join the waves from the head to the tail so that they form a closed loop, they resemble the electron waves that wrap around the nucleus.

Furthermore, as pointed out by de Broglie, the number of wavelengths for the electron waves wrapping around the nucleus must be an integer. This is because in order for the standing wave to wrap around the nucleus, the beginning point of the wave must be in phase with the end point of the wave, and this only occurs if the wave finishes with a complete wavelength. For non-integral wavelengths, the beginning and end position of the wave will be out of phase and consequently result in destructive interference, which diminishes the wave. Hence, for electrons in the first energy level, they have one wavelength as shown in Figure 15.5 (a), and for electrons in the second energy level, they have two wavelengths as shown in Figure 15.5 (b), and so on.

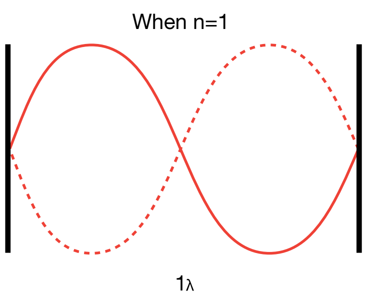

Figure 15.4 (a) A standing wave with one wavelength

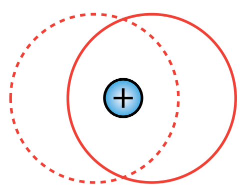

Figure 15.5 (a) An electron wave with one wavelength around the nucleus

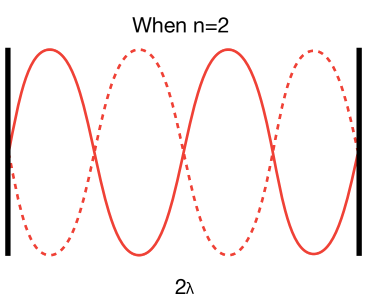

Figure 15.4 (b) A standing wave with two wavelengths

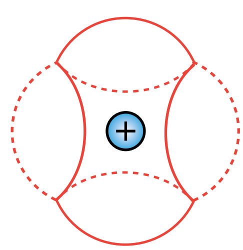

Figure 15.5 (b) An electron wave with two wavelengths around the nucleus

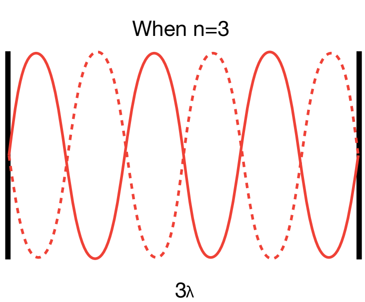

Figure 15.4 (c) A standing wave with three wavelengths

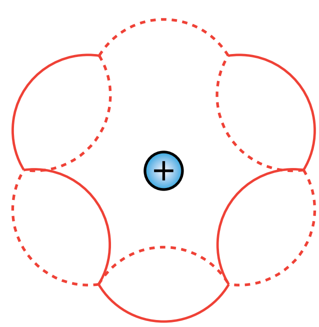

Figure 15.5 (c) An electron wave with three wavelengths around the nucleus

NOTE: It is incorrect to think that the sketches in Figure 15.5 represent the pathways for the electrons to move around the nucleus. The entire wave is actually one electron. Remember, electrons are now waves, not little moving particles!

The implications of de Broglie's electron wave model

With the electron wave model of the atom, it is now possible to explain why electrons, when in their own energy level, are stable and do not emit EMR. In other words, using de Broglie's model, Bohr's first postulate can be explained: as electrons are now standing waves, they are no longer moving charges, and hence will not emit any radiation. Furthermore, standing waves do not propagate, and therefore are stable and will not lose any energy.

Second, de Broglie's electron wave model enables a mathematical derivation for Bohr's third postulate—the quantisation of angular momentum, which Bohr proposed radically without any theoretical support:

The circumference = total length of the electron wave of the nth shell

$$2\pi r_n = n\lambda$$

$$\text{also } \lambda = \frac{h}{mv}$$

$$\therefore 2\pi r_n = \frac{nh}{mv}$$

$$mv(2\pi r_n) = nh$$

$$mvr_n = \frac{nh}{2\pi}$$

Thus, using de Broglie's theory of matter waves and the matter wave equation, we are able to theoretically derive Bohr's third postulate, thereby adding rationality to this postulate.

Historically, de Broglie's model and his matter wave equation $\lambda = \frac{h}{mv}$ also formed the foundation of a new area of physics known as **quantum mechanics**. Such physics was later expanded and perfected by the work of many physicists. Quantum mechanics involves complicated physics theory and mathematics. The work and the contributions of Wolfgang Pauli and Werner Heisenberg to the development of the model of the atom and quantum mechanics are discussed briefly.

Pauli and the exclusion principle

SECONDARY SOURCE INVESTIGATION

PFAs

H1, H3

PHYSICS SKILLS

H12.3 A, B, C, D
H12.4 F
H13.1 A, B, C, D, E
H14.1 A, B, E, F

- ***Gather, process, analyse and present information and use available evidence to assess the contributions made by Heisenberg and Pauli to the development of atomic theory***

In 1925, Wolfgang Pauli (1900–1958) proposed a theory for which he was famous—the exclusion principle.

Definition

The **exclusion principle** states that no two electrons in the same atom can have all four quantum numbers the same.


Wolfgang Pauli

The quantum numbers

In order to understand the exclusion principle, you must first examine the meaning of the four quantum numbers.

1. **The principal quantum number (n)**
   - This quantum number is related to the principal energy shells that Bohr proposed.
   - It takes the values of n = 1, 2, 3… z, where z is any integer.
   - For example, the electron in a hydrogen atom takes the value of n = 1. For a lithium atom, two electrons are in the first energy shell, thus both take the value of n = 1 and the other electron is in the second shell hence takes the value of n = 2.
2. **The orbital quantum number (*l*)**
   - This quantum number is related to the angular momentum and therefore to the orbital shape of the electrons.
   - They are also known as the sub-shells in chemistry.
   - They can take the values of *l* = 0, 1, 2… (n – 1). For example, when n = 1, *l* would take the value of 0. When n = 2, the *l* takes the value of 0 and 1. When n = 3, *l* can take the value of 0, 1 and 2.
   - Each of the orbital quantum numbers relates to a particular shape orbit and the corresponding angular momentum. For example, 0 is spherical in shape, and 1 is pear shaped. Electrons with different orbital quantum numbers will have a slight difference in their energy even if they are within the same energy shell (the same principal quantum number). This slight difference in energy explains the existence of hyperfine spectral lines.

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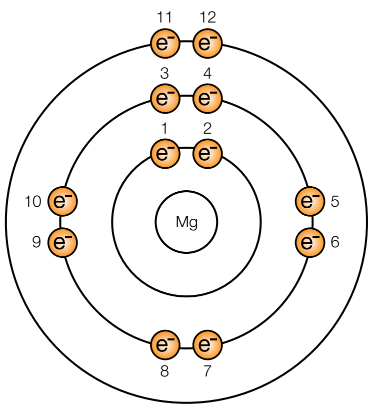
'Assess'

NOTE: Slight differences in energy result in slight differences in frequency, which constitute the hyperfine lines.

3. **The magnetic quantum number (m_l)**
   - This is the quantum number assigned to the magnetic orientation (moment) of the electron orbiting in the magnetic field.
   - It can take values of –*l*, …–2, – 1, 0, + 1, + 2 … +*l*. For example, when an electron is in the second energy level, n = 2. This electron can have two possible orbital shapes as *l* takes the values of 0 and 1. For *l* is 0, m_l is 0, correlating to 1 type of magnetic moment for this electron orbit. For *l* = 1, m_l can take the values of –1, 0, 1, correlating to 3 possible magnetic moments for this electron orbit.
   - The magnetic quantum number can also be used to explain the Zeeman effect. (Not required by the syllabus.)
4. **The magnetic spin quantum number (m_s)**
   - This quantum number is assigned to the spin of electrons about their own axis. Each electron can spin in two different ways, which are known as positive a half spin (+ ½) and negative a half spin (–½).

Pauli's exclusion principle

To understand the exclusion principle, examine it using an actual atom as an example. Say for a lithium atom, in which there are three electrons, we can assign one of the electrons to be n = 1, in which case *l* will be 0 and m_l will also be 0. The magnetic spin (m_s) for this electron can be assigned as either +½ or –½. Now for the second electron, if we assign it n = 1, then both *l* and m_l are again 0. It follows that in order to obey the **exclusion principle**, m_s must be –½ if the previous electron was assigned +½ and vice versa, to avoid having



1.	n = 1,	l = 0,	m_l = 0,	m_s = ? +1/2
2.	n = 1,	l = 0,	m_l = 0,	m_s = −1/2
3.	n = 2,	l = ?0,	m_l = 0,	m_s = ? +1/2
4.	n = 2,	l = ?0,	m_l = 0,	m_s = −1/2
5.	n = 2,	l = 1,	m_l = ?−1,	m_s = ? +1/2
6.	n = 2,	l = 1,	m_l = ?−1,	m_s = −1/2
7.	n = 2,	l = 1,	m_l = ?0,	m_s = ? +1/2
8.	n = 2,	l = 1,	m_l = ?0,	m_s = −1/2
9.	n = 2,	l = 1,	m_l = 1,	m_s = ? +1/2
10.	n = 2,	l = 1,	m_l = 1,	m_s = −1/2
11.	n = 3,	l = ?2,	m_l = ?−2,	m_s = ? +1/2
12.	n = 3,	l = ?1,	m_l = ?0,	m_s = −1/2

Figure 15.6 The quantum numbers for a magnesium atom

the same four quantum numbers for both electrons. Finally, for the third electron, it is now impossible to assign it n = 1 without it having to have the same four quantum numbers compared to one of the previous two electrons. Since electrons have to fill from a lower energy shell to a higher energy shell, it follows that this electron must be assigned n = 2. This logically explains why atoms can only hold a maximum of two electrons in the first shell.

Now let us look at a more complicated atom, such as magnesium. The electrons of the magnesium atom have been labelled from 1 to 12 and each electron has been assigned with a set of possible quantum numbers. Note that where a question mark is used, it represents the potential for an alternative quantum number, for instance for the m_s of the first electron to potentially be −½, but if that is the case, the second electron will have m_s = +½.

It is clear from Figure 15.6 that no two electrons in this atom have all four quantum numbers the same. It is also clear if the second shell is to hold more than eight electrons, then the exclusion principle would break down. This effectively explains why the electron configuration for a magnesium atom must be 2, 8, 2.

In summary, Pauli's exclusion principle provides a very solid theoretical background for why electrons have to be configured in the way they are in atoms: in other words, why the first electron shell only holds two electrons, whereas the second one only holds eight, and next one holds 18 and then 32 and so on. (Try to verify this by carrying out a similar exercise to that in Figure 15.6.) The principle also explains the regularity of the periodic table and the reason for atoms' position in the periodic table. Pauli's exclusion principle can be seen as a further advancement to Bohr's model in how to place electrons around the nucleus. Most electrons' behaviours can potentially be explained by using the quantum numbers and the exclusion principle. Consequently, Pauli's model can be seen as more comprehensive and complete compared to the earlier theories.

Pauli's other contributions

Wolfgang Pauli was also famous for the prediction of the existence of neutrinos (this is discussed in Chapter 16).

Heisenberg and the uncertainty principle

SECONDARY SOURCE INVESTIGATION

PFAs

H1, H3

PHYSICS SKILLS

H12.3 A, B, C, D
H12.4 F
H13.1 A, B, C, D, E
H14.1 A, B, E, F

- ***Gather, process, analyse and present information and use available evidence to assess the contributions made by Heisenberg and Pauli to the development of atomic theory***

Werner Heisenberg (1901–1976) in 1927 proposed the **uncertainty principle**, for which he won the Nobel Prize.

Definition

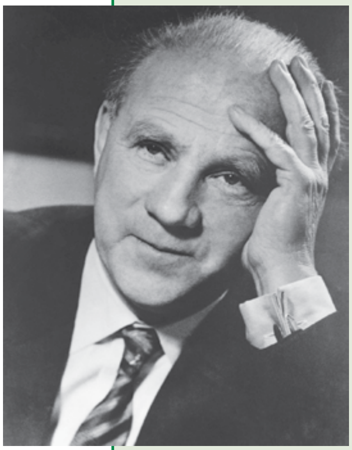
The **uncertainty principle** states that the product of the uncertainty in measuring the position and uncertainty in measuring the momentum of an object has to be always equal to or larger than a constant.

Mathematically, the equation is written as **$\Delta\rho.\Delta x \geq h/4\pi$**; where **$\Delta\rho$** is the uncertainty in the momentum measurements (kg m s^{-1}), **Δx** is the uncertainty in the measurements of positions (m) and h is Planck's constant.

It is important to point out that the uncertainty in this principle arises not as a result of the errors in measurements during the experiment, but rather as a result of the inherent properties of matter at atomic levels. The uncertainty principle is also a direct result of the wave-particle duality of matter.

In simple terms, the principle indicates that if one knows everything about the momentum of an object, then one would have absolutely no idea of its position. On the other hand, if one knows the position of an object for certain, nothing is known about its momentum and also its wavelength ($\lambda = \frac{h}{mv}$). In other words, one has to sacrifice some certainties in one quantity in order to know anything about the other.

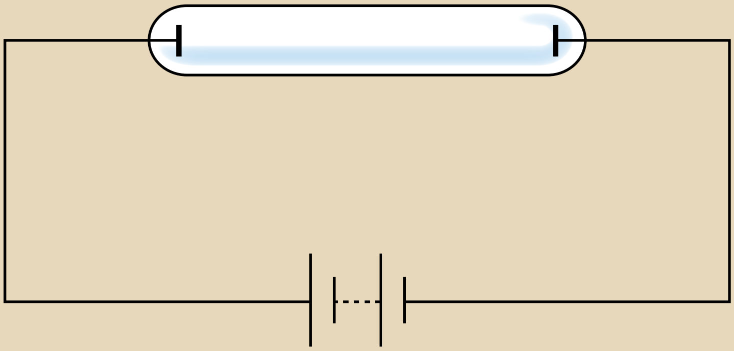
This is a new perspective in looking at matter at atomic levels: nothing can be measured absolutely and the momentum and position of any particles at atomic levels would all have to be assessed with some degree of uncertainty. This adds a further dimension to the electrons inside the atom, in addition to the standing wave theory and quantum numbers.


Werner Heisenberg

NOTE: The work done by Louis de Broglie, Wolfgang Pauli and Werner Heisenberg, as well as the contributions made by Max Born, Erwin Schrödinger and Paul Dirac, are collectively known as **quantum mechanics**, a new physics that is separate from Newtonian physics. It is a further advancement from the quantum theory proposed by Niels Bohr.

CHAPTER REVISION QUESTIONS

1. Define wave-particle duality.
2. Explain the meaning of matter waves.
3. (a) Calculate the wavelength of the matter wave when a tennis ball with a mass of 20.0 g is moving at a velocity of 2.00 m s^{-1}.
   (b) Calculate the wavelength of the matter wave when a proton is made to move at a velocity of 3.00 km s^{-1}.
   (c) Calculate the frequency of the matter wave when a neutron is made to move at 53.6×10^3 m s^{-1}.
4. When an electron is accelerated by a voltage, it achieves a high velocity such as in the case of a cathode ray tube (CRT) (see figure).



(a) Demonstrate, by drawing on the diagram, the direction in which the electron moves in the CRT.
(b) What is the wavelength of the matter wave of the electron when the voltage is set at 32.0 V?
(c) What is the required voltage to produce an electron wave with a wavelength of 1.32×10^{-10} m?

5. Electron microscopes are devices that use the wave characteristics of electrons to produce magnified pictures of minute objects.

   (a) One of the steps in the operation of an electron microscope is to focus the electrons and this is done by magnetic fields. Suppose beams of electrons travel from left to right parallel to each other each as shown in the diagram. Draw a possible pattern of magnetic field that can be used to focus these beams (to bring these beams to one point).

   (b) The electrons are accelerated by using a power source. Calculate the voltage required to produce electron waves with a wavelength of 0.102 nm.
   (c) Use the information in (b) to explain why an electron microscope is used to magnify things that are too small to be seen by a light microscope.

6. With the aid of a diagram, describe the experiment performed to prove the existence of matter waves. In your answer, you should mention the principle of interference and diffraction.

7. (a) Describe de Broglie's electron-wave model of atoms.
   (b) Evaluate why his model was successful. In your answer, you should discuss the inadequacies the model addressed and the improvements the model made.

8. (a) Define Pauli's exclusion principle.
   (b) Using the sodium and argon atoms as two examples, write down a set of possible quantum numbers for these two atoms; explain the meaning and the significance of the exclusion principle.

9. Define Heisenberg's uncertainty principle and describe its significance in the context of the models of the atoms.

10. Construct a table that describes chronologically all the events you know that are relevant to the development of the models of atoms.

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Answers to chapter revision questions