



## **Maths for Chemists 1**

### *Physics Skills: Waves and Electromagnetic Radiation*

Dr Meghan Halse

Email: [meghan.halse@york.ac.uk](mailto:meghan.halse@york.ac.uk)

Office: C/A 061

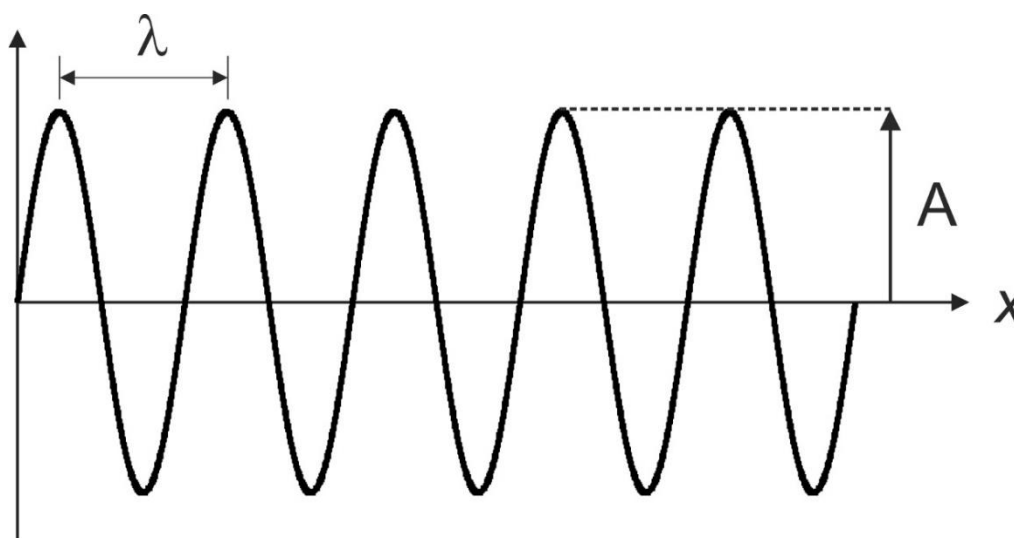
Phone: 01904 32 2853

## Waves and Oscillations

Waves are a type of periodic motion or oscillation that occur throughout the physical sciences. In Chemistry waves and oscillations are particularly important in **Quantum Mechanics** and **Spectroscopy**.

### Definition of a wave

Consider a wave travelling through space along the x axis.



How do we describe the features of this wave?

Variable	Name	Definition	Base units
$\lambda$ (lambda)	Wavelength	Distance between two wave crests	m
$A$	Amplitude	Height of a wave crest	
$\nu$ (nu)	Frequency	The number of wave crests that pass a single point per unit time	Hz ( $s^{-1}$ )
$\tilde{\nu}$	Wavenumber	The number of wavelengths per unit distance	$m^{-1}$
$c$	Speed	Speed of the wave travelling through space	$m\ s^{-1}$

How are **wavelength**, **frequency** and **velocity** related?

$$c = \lambda \nu$$

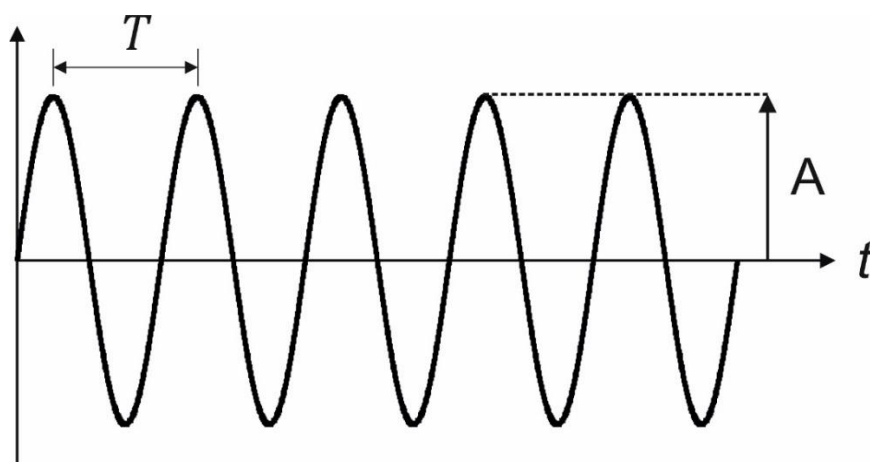
How are **wavelength** and **wavenumber** related?

$$\tilde{\nu} = \frac{1}{\lambda}$$

What is the relationship between **wavenumber** and **frequency**?

$$\tilde{\nu} = \frac{\nu}{c}$$

Consider a wave travelling through time.



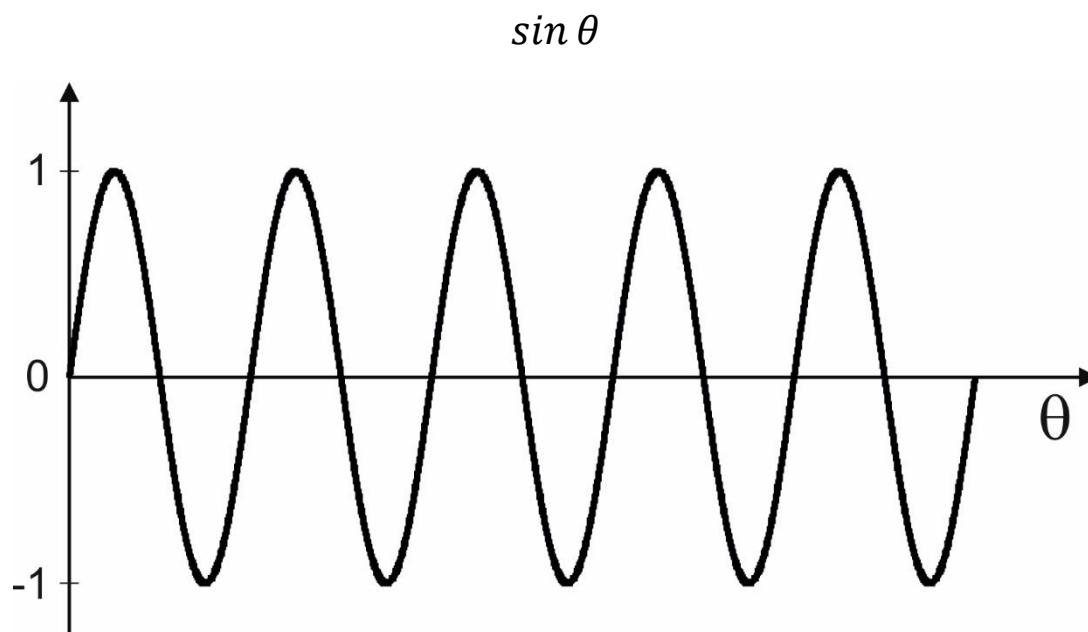
Variable	Name	Definition	Units
$T$	Period	Time between two crests of the wave (time to complete a single oscillation)	s
$A$	Amplitude	Height of a wave crest	
$\nu$ (nu)	Frequency	The number of complete waves (full oscillations) within a second	Hz ( $s^{-1}$ )

How are **period** and **frequency** related?

$$T = \frac{1}{\nu}$$

### Wave Equation

Consider the sine function. This function defines a wave where the position along the wave is defined by an angle:  $\theta$ .



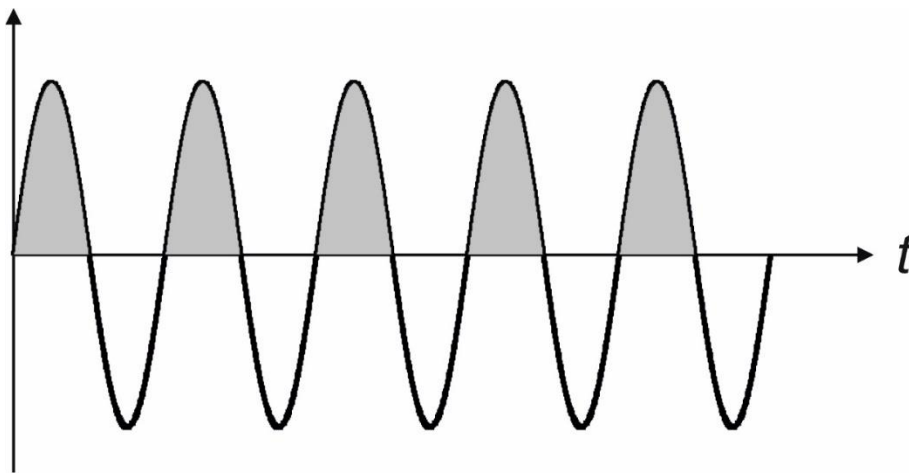
## Phase ( $\theta$ )

The **phase** defines the point in the cycle. It is the name given to the angle,  $\theta$ , in the sine function of the wave equation. It can be defined by units of **radians** or **degrees**. In mathematics **radians** is usually the unit used.

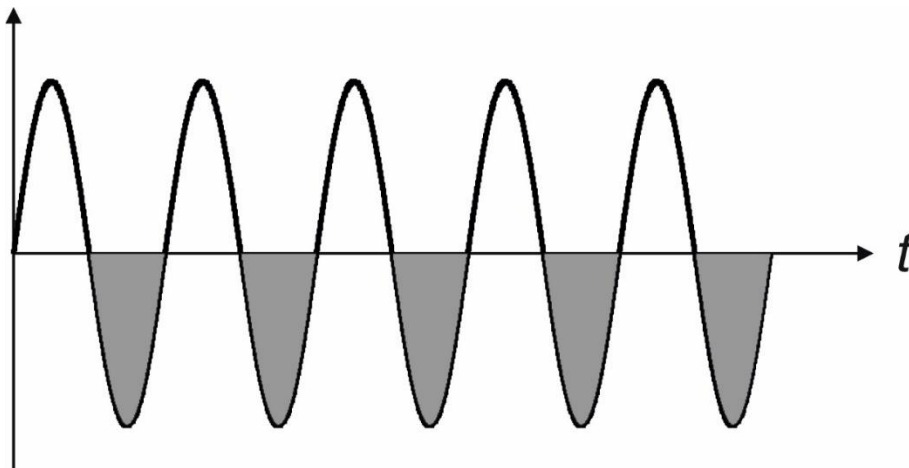
Remember:

$$2\pi \text{ radians} = 360^\circ = \text{one full cycle}$$

Regions of **positive** amplitude can be said to have **positive phase**.



Regions of **negative** amplitude can be said to have **negative phase**.



For a wave oscillating with **time** we define the phase,  $\theta$ , as the product of the **frequency** and **time**.

$$\theta = 2\pi\nu t = \omega t$$

$$\sin(\theta) = \sin(2\pi\nu t) = \sin(\omega t)$$

The **angular frequency**,  $\omega$ , is the frequency in units of **radians s<sup>-1</sup>**. It is related to the **frequency**,  $\nu$ , in **Hz (s<sup>-1</sup>)** by  $2\pi$ .

$$\omega = 2\pi\nu$$

For a wave travelling through **space** we define phase,  $\theta$ , as the product of the **wavenumber** and **position** ( $x$ ).

$$\theta = 2\pi\tilde{\nu}x = Kx$$

$$\sin(\theta) = \sin(2\pi\tilde{\nu}x) = \sin(Kx)$$

$K$  has units of **radians m<sup>-1</sup>** and is related to the **wavenumber**  $\tilde{\nu}$  in **m<sup>-1</sup>** by  $2\pi$ .

$$K = 2\pi\tilde{\nu}$$

For a wave travelling through time and space we need to include both factors.

$$\theta = 2\pi\nu t + 2\pi\tilde{\nu}x = \omega t + Kx$$

$$\sin(\theta) = \sin(2\pi\nu t + 2\pi\tilde{\nu}x) = \sin(\omega t + Kx)$$

## Principle of superposition

One of the key special features of waves is how they interact with each other. Waves can pass through each other and come out the same as they went in. However, in the interaction region where the waves overlap we see interesting and important effects.

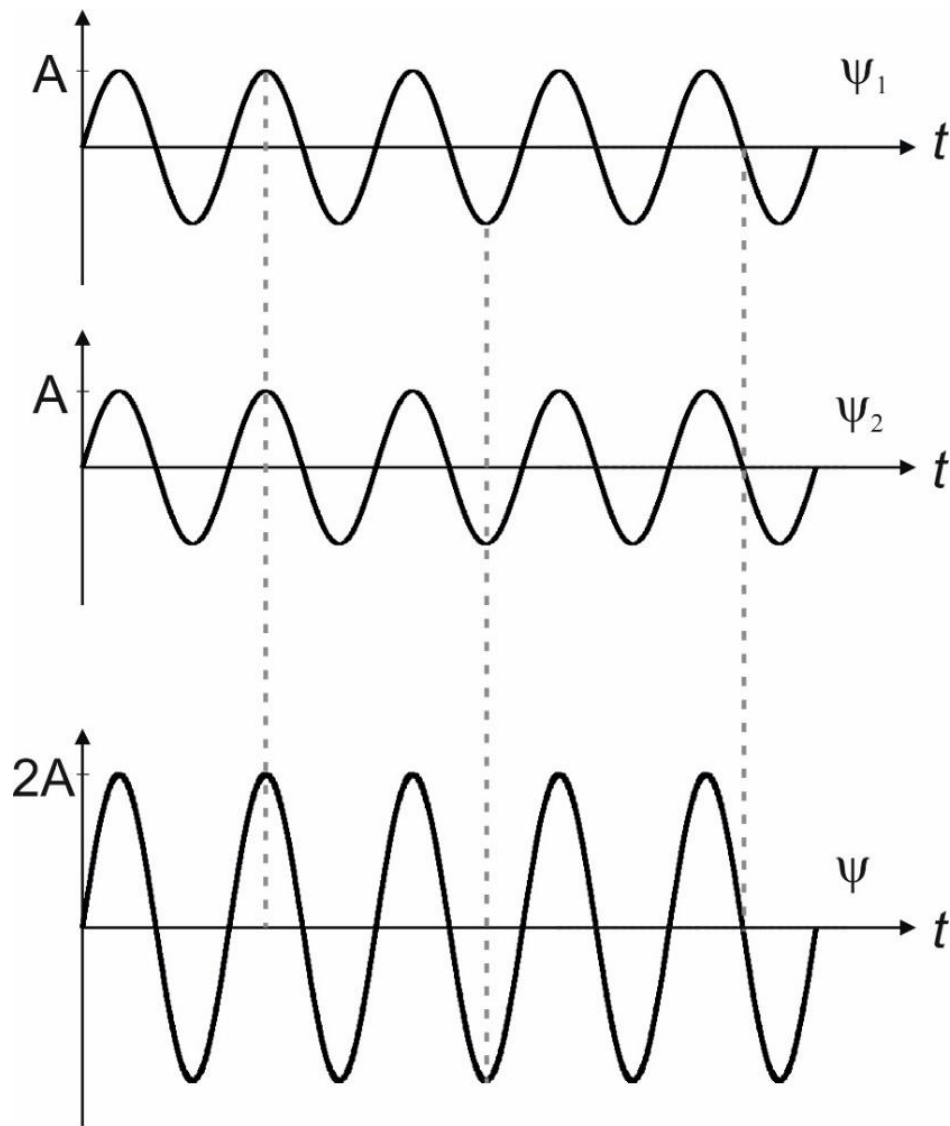
Mathematically, the interaction of two waves  $\psi_1$  and  $\psi_2$  in the region where they overlap can be written as a sum.

$$\psi = \psi_1 + \psi_2$$

How the two waves interact will depend on their relative **frequency**, **wavelength** and **phase**.

## Constructive interference

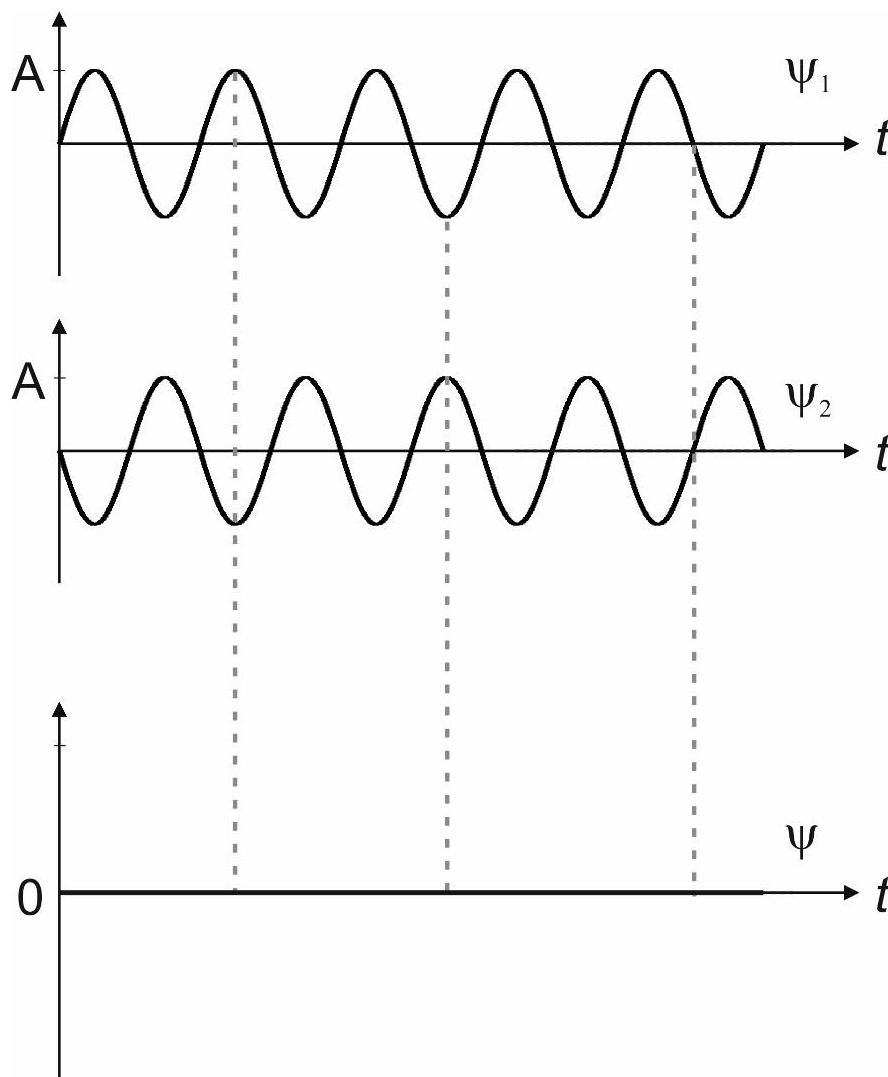
If the peaks and troughs of two waves line up, then the waves add up. This is **constructive interference**. This requires the two waves to have the same **frequency** and the same **phase** ( $\Delta\theta = 0$ ). Positive and negative regions line up leading to a net increase in amplitude.



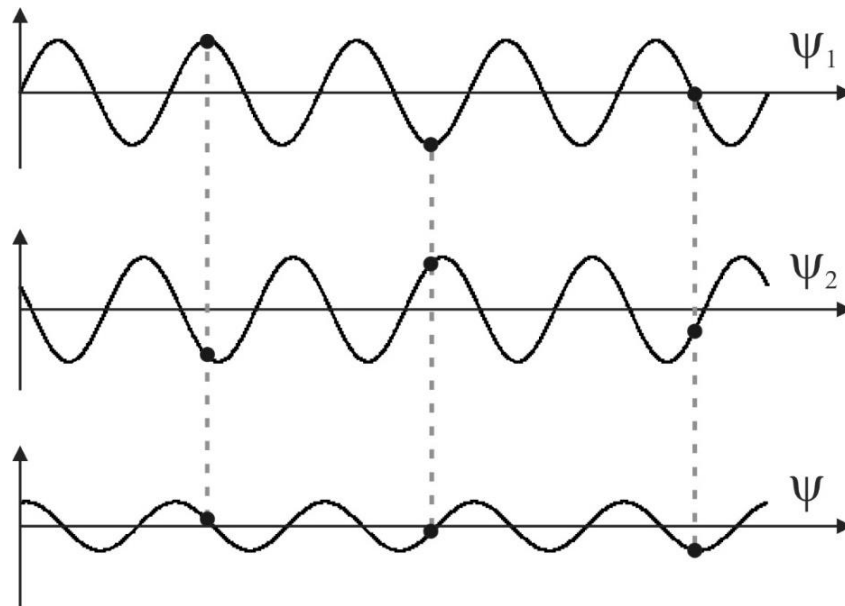


**Destructive interference**

If the peaks and troughs of two waves do not line up (i.e. if the waves have different phases) then the waves will not perfectly add up and will at least partially cancel out. This is **destructive interference**. If positive regions of one wave match perfectly with negative regions of the other wave there is complete cancellation. This means that the difference in their phases is  $\Delta\theta = \pi$  ( $180^\circ$ ). We call this having **opposite phase**.



In most cases the waves will not have completely opposite phases ( $-\pi < \Delta\theta < \pi$ ) and so will not completely add up or completely cancel out. There will either be partial addition or partial cancellation.

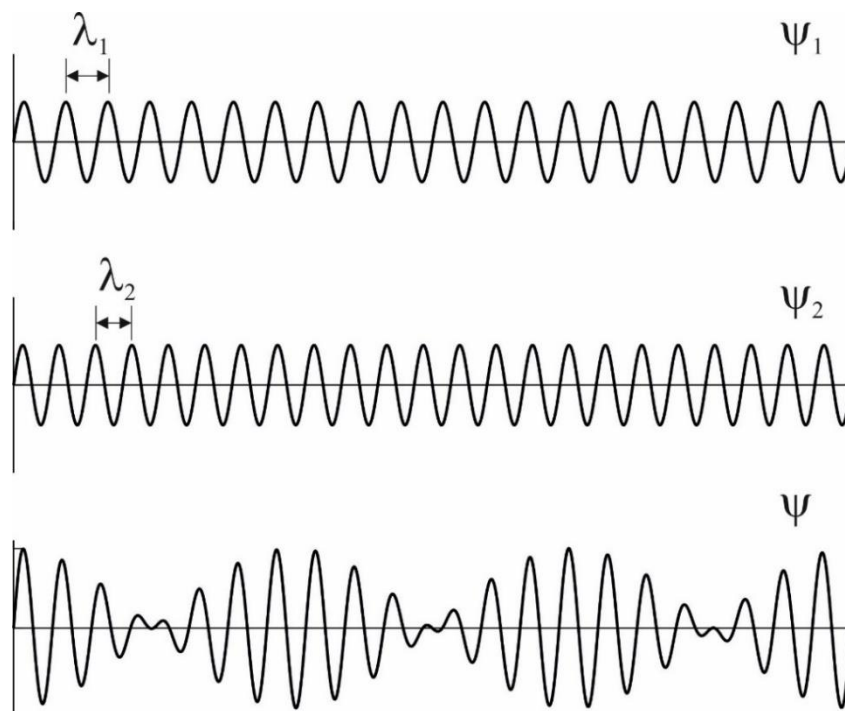


The sum,  $\psi$ , has the same frequency as  $\psi_1$  and  $\psi_2$  but a different **phase** and **amplitude**.

### Beat patterns

What happens when waves of different frequencies interact?

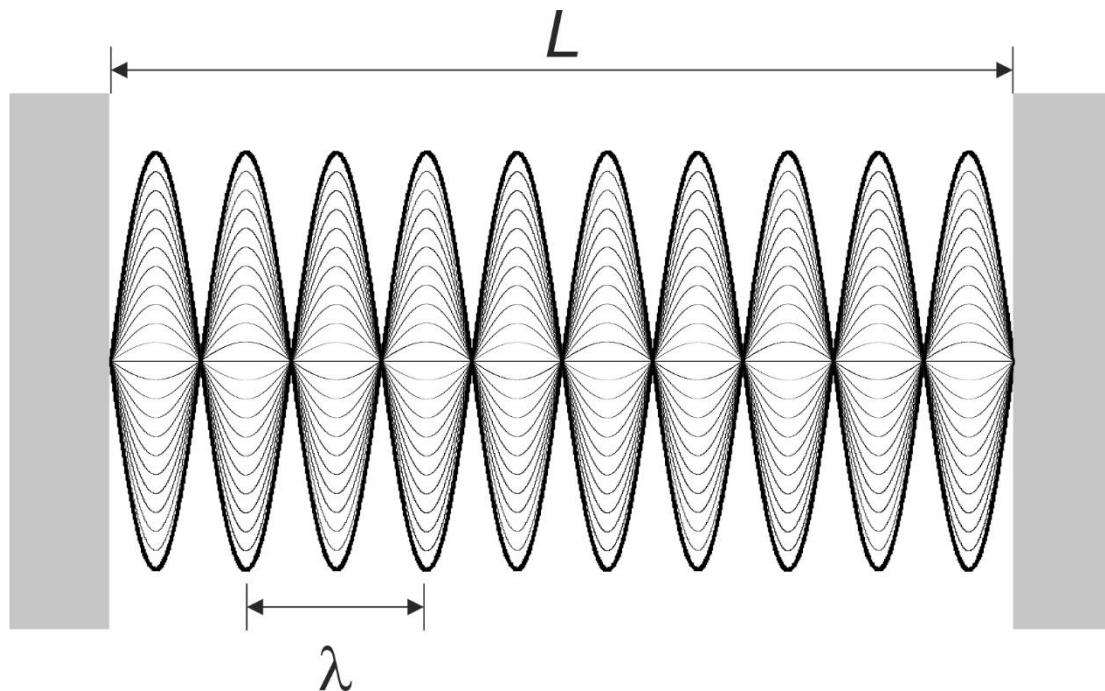
Consider two waves,  $\psi_1$  and  $\psi_2$ , with **different** frequencies,  $\nu_1$  and  $\nu_2$  and wavelengths  $\lambda_1$  and  $\lambda_2$ . These waves combine to form a **beat pattern**.



## Standing waves

A standing wave is a wave that oscillates in time but is fixed in space. It can be visualised as a vibrating string where the ends are fixed. Another classic example of a standing wave is a **particle in a box**.

The standing wave arises from **constructive interference** of waves travelling backwards and forwards along the string.



In order for **constructive interference** to occur, the wave must go through **zero** at both **ends** of the string.

Therefore, the **length** of the string ( $L$ ) must be an **integer multiple** of **half the wavelength**.

$$L = \lambda \frac{n}{2}$$

$$n = 1, 2, 3 \dots$$

Therefore, the **wavelength** has to fulfil the following

$$\lambda = \frac{2L}{n}$$

$$n = 1, 2, 3 \dots$$

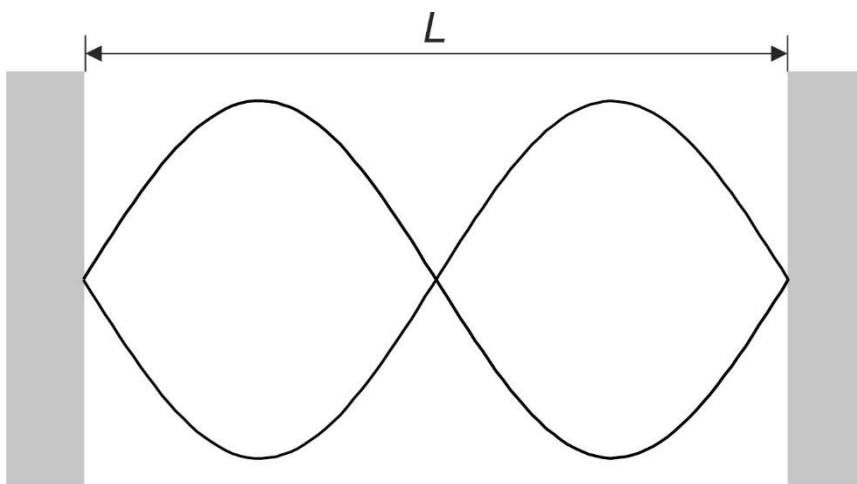
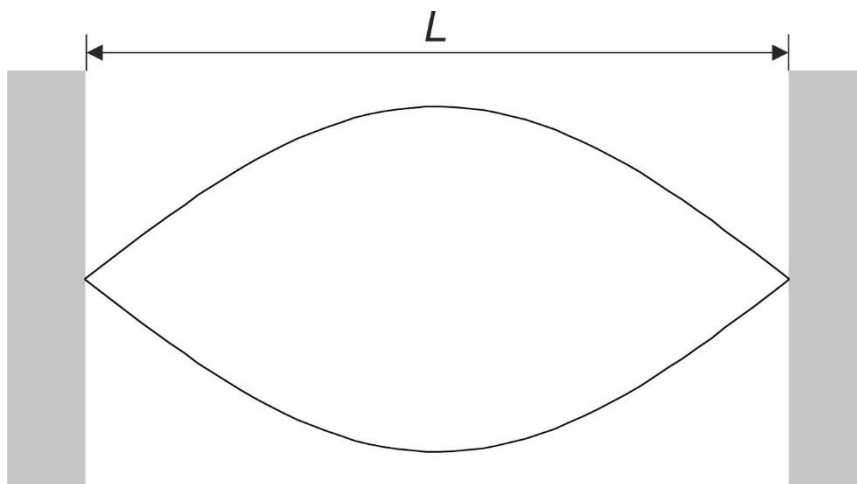
How does this relate to **frequency**?

$$v = \frac{nc}{2L}$$

$$n = 1, 2, 3 \dots$$

How many **nodes** are there in the standing wave?

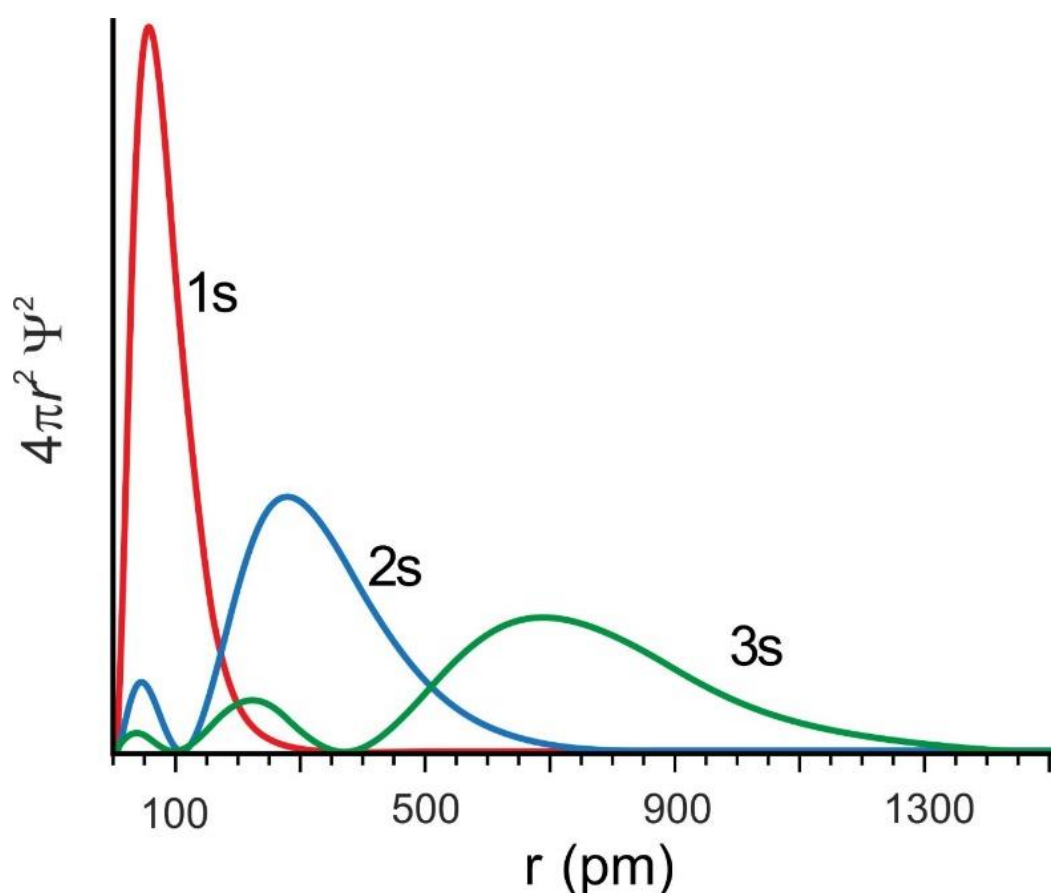
$$\text{number of nodes} = n - 1$$



## Practical Application: Radial Distribution Functions

The form of atomic and molecular **orbitals** are a consequence of the principles of standing waves and interference. The wavelike properties of electrons mean that **constructive interference** leads to orbitals with very specific, **quantised** frequencies.

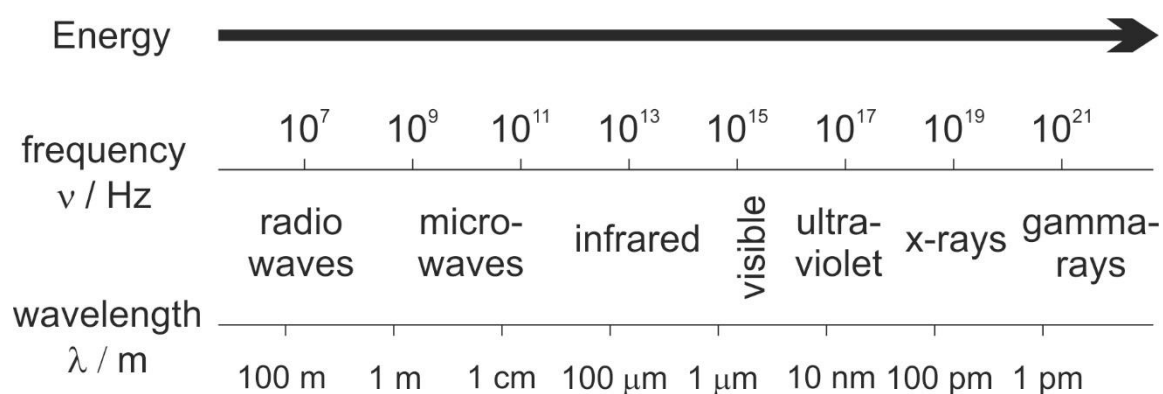
The atomic orbitals can be visualised in 1D using the **radial distribution function**. These are essentially standing waves, with a number of nodes that is related to the quantum number,  $n$ .



## Electromagnetic (EM) Radiation

One of the applications of waves in Chemistry is in the idea of the **wave-particle duality** of light. Visible light is just one type of **electromagnetic (EM) radiation**. Wave-particle duality tells us that EM radiation behaves both like a wave and like a particle.

### Electromagnetic spectrum



Electromagnetic radiation travels at the speed of light,  $c = 2.998 \times 10^8 \text{ m s}^{-1}$ . This constant relates the **frequency** and **wavelength** of EM radiation.

$$c = \lambda \nu$$

The energy associated with EM radiation is defined by **Planck's constant**, which defines the amount of energy (J) per unit frequency.

$$h = 6.626 \times 10^{-34} \text{ J s}$$

$$E = h\nu = \frac{hc}{\lambda} = hc\tilde{\nu}$$

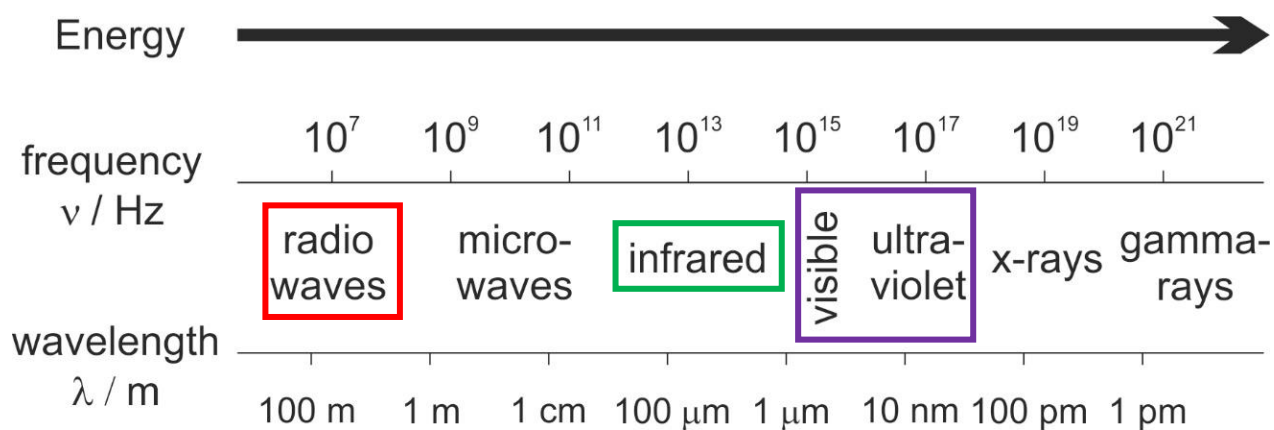
Energy is directly proportional to **frequency** (and **wavenumber**) and indirectly proportional to **wavelength**.

For angular frequency,  $\omega$ , the relationship uses the **reduced Planck's constant** ("h-bar")

$$\hbar = \frac{h}{2\pi} = 1.055 \times 10^{-34} \text{ J s}$$

$$E = \hbar\omega$$

### Practical Application: Spectroscopy



**kHz - GHz**

$$E = h\nu = \frac{hc}{\lambda} = hc\tilde{\nu}$$

nm

**NMR Spectroscopy**

**IR Spectroscopy**

**UV-vis Spectroscopy**