PH 101: Physics I

Module 3: Introduction to Quantum Mechanics

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Recap

- **Bohr's model to explain the atomic spectra**

  --The angular meomentum is quantized.

  --The orbit is stationary in nature.

- **De Broglie Hypothesis:**

  --Wave-particle duality:

  --Every particle or system of particles *can* be defined in quantum mechanical terms and therefore have wave-like properties.

  --The quantum wavelength of an object is:

$$\lambda = h/p \qquad (p \text{ is momentum})$$

  --Typical macroscopic objects

  masses ~ kg; velocities ~ m/s $\rightarrow p \approx 1$ kg·m/s

  $\lambda \approx 10^{-34}$ meters (too small to matter in macro environment!!)

  --Typical "quantum" objects

  electron (10^{-30} kg) at thermal velocity (10^5 m/s) $\rightarrow \lambda \approx 10^{-8}$ m

  so λ is 100 times larger than an atom: very relevant to an electron!

- --Derivation of the Bohr's postulate of quantization of orbital angular momentum using De-Broglie Hypothesis.

  Wave nature of electron is required to understand the quantized angular momentum.

Understanding particle & wave nature

Experiment with a gun (bullets as particles):

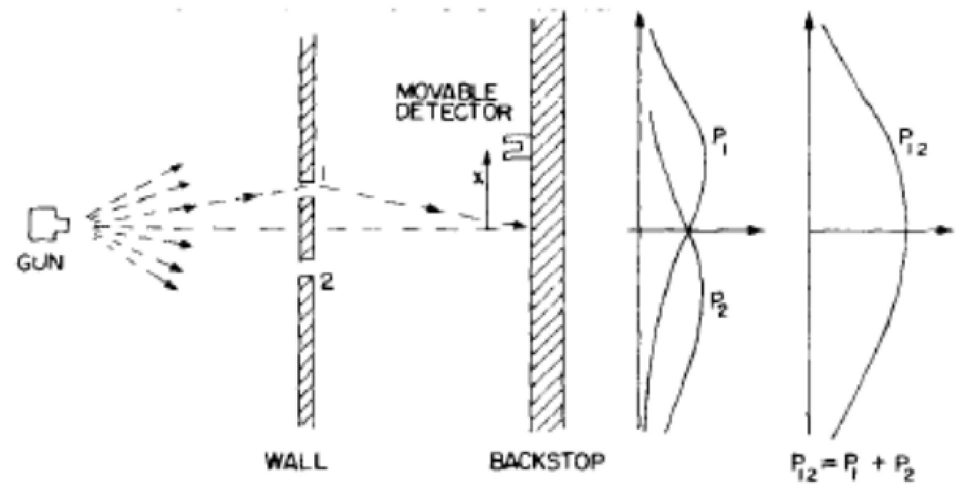
Detector counts number of bullets.

P_1: probability when hole 2 is closed.

P_2: probability when hole 1 is closed.

P_{12}: probability when both holes are open.

Result: No interference.



Experiment with water wave:

Detector records intensity of the wave.

I_1: intensity when hole 2 is closed.

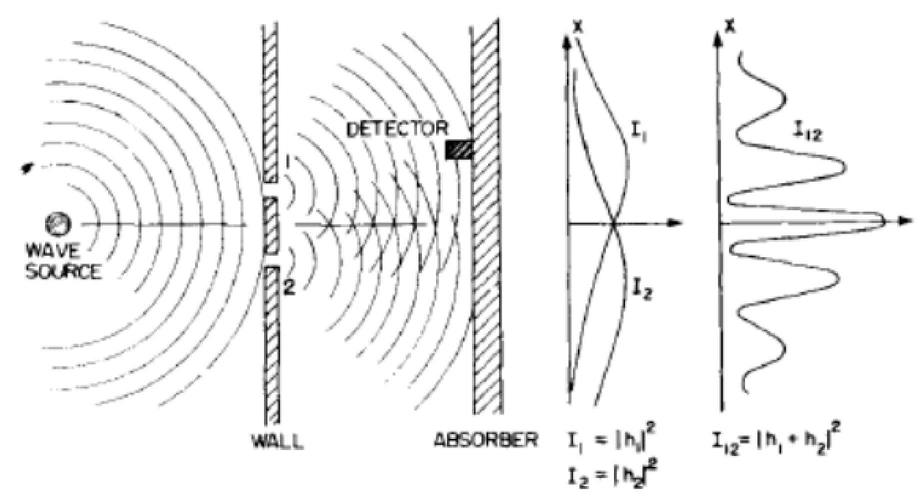
I_2: intensity when hole 1 is closed.

I_{12}: intensity when both holes are open.

$$|h_1 + h_2|^2 = |h_1|^2 + |h_2|^2 + 2|h_1||h_2| \cos \delta,$$

$$I_{12} = I_1 + I_2 + 2\sqrt{I_1 I_2} \cos \delta.$$

Result: Constructive interference.



Double-slit Experiments

Experiment with electrons:

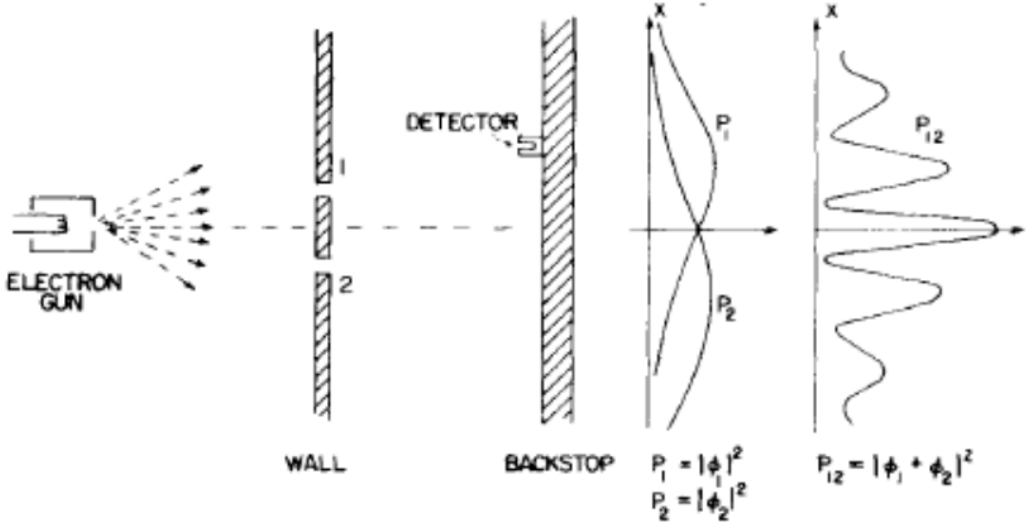
Detector records intensity of the wave.

P_1: probability when hole 2 is closed.

P_2: probability when hole 1 is closed.

P_{12}: probability when both holes are open.

Result: An interference !!!



$$P_{12} \neq P_1 + P_2.$$

Conclusion: the electrons arrive in lumps, like particles, and probability of arrival of these lumps is distributed like the distribution of the intensity of a wave. In this sense electrons behave like a particle and a wave.

Check this link for Particle-Wave Duality explanation

http://www.youtube.com/watch?v=DfPeprQ7oGc

Representation of Matter through waves

$$\Psi(x, t) = A \sin(kx - \omega t)$$

OR

$$\Psi(x, t) = A \cos(kx - \omega t)$$

$$k \equiv \frac{2\pi}{\lambda} \quad \text{and} \quad \omega = \frac{2\pi}{T}$$

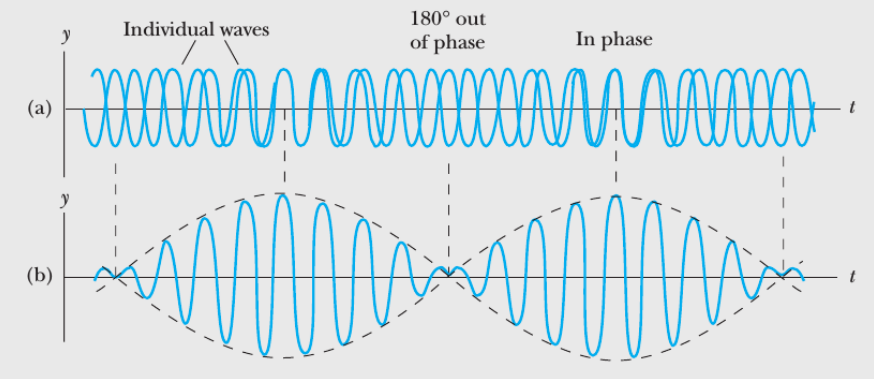
$$v_{\text{ph}} = \frac{\lambda}{T} = \frac{\omega}{k}$$

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

These waves are solutions of classical wave equation.

The wave equation is a linear equation, this means sum of any two waves with different frequencies and amplitude should also be a solutions of this equation. This is called the principle of superposition.

Consider the superposition of two waves as shown in the figure.



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

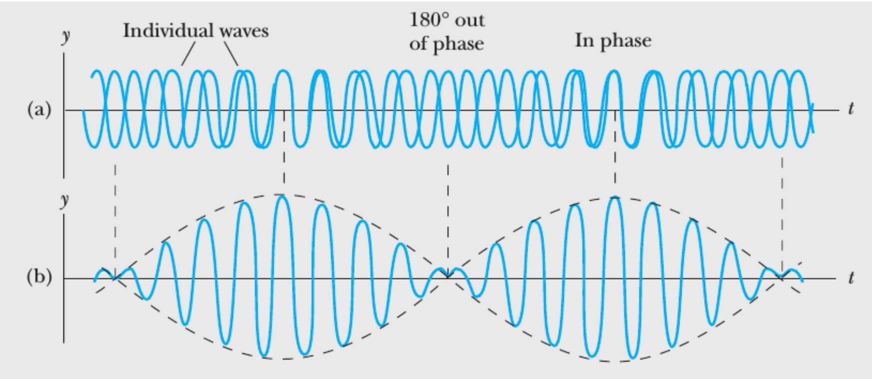
Using $\cos\alpha + \cos\beta = 2\cos\frac{1}{2}(\alpha + \beta)\cos\frac{1}{2}(\alpha - \beta)$

where $\Delta k = k_1 - k_2$, $\Delta\omega = \omega_1 - \omega_2$, $k_{\text{av}} = (k_1 + k_2)/2$, and $\omega_{\text{av}} = (\omega_1 + \omega_2)/2$

Here the solid blue line shows the sum of two waves and the black dashed line denotes an envelope which denotes the maximum displacement of the combined wave. The combined wave Ψ oscillates within the envelope with the wave number k_{av} and angular frequency ω_{av}.

Representation of Matter through waves

Consider the superposition of two waves as shown in the figure.



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

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where $\Delta k = k_1 - k_2$, $\Delta\omega = \omega_1 - \omega_2$, $k_{av} = (k_1 + k_2)/2$, and $\omega_{av} = (\omega_1 + \omega_2)/2$

Here the solid blue line shows the sum of two waves and the black dashed line denotes an envelope which denotes the maximum displacement of the combined wave. The combined wave Ψ oscillates within the envelope with the wave number k_{av} and angular frequency ω_{av}.

The envelope is described by the cosine factor in the front which has the wave number $\Delta k/2$ and angular frequency $\Delta\omega/2$.

The individual waves Ψ_1 and Ψ_2 move with their own phase velocities ω_1/k_1 and ω_2/k_2.

The combined wave has the phase velocity $v_p = \omega_{av}/k_{av}$

Combining many such waves gives rise to a pulse or **wave packet** which moves at the **group velocity** $v_{gr} = \Delta\omega/\Delta k$

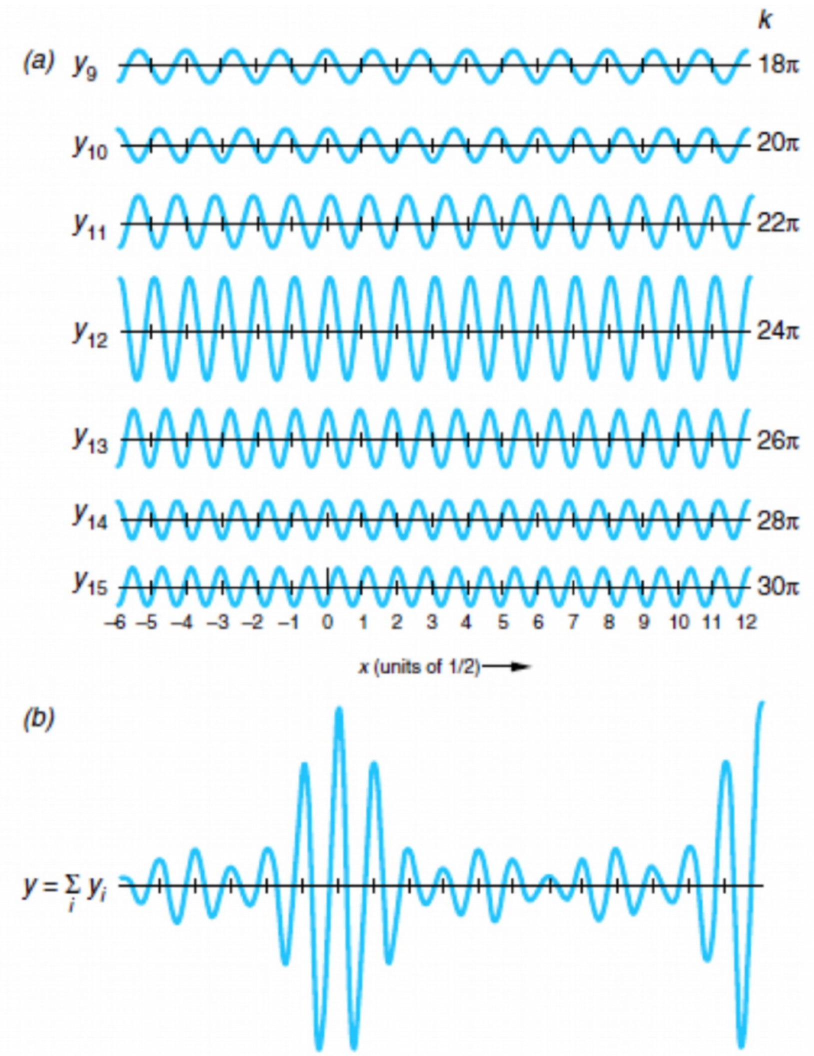
This group velocity which describes the speed of the envelope is important when dealing with the wave packets.

Representation of Matter through waves

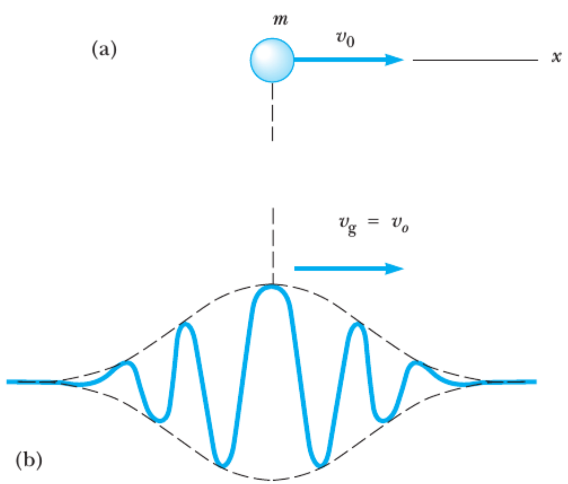
Combining many such waves gives rise to a pulse or **wave packet** which moves at the **group velocity** $v_{gr} = \Delta\omega/\Delta k$

This wave packet is more localised in space as shown in the figure.

This group velocity which describes the speed of the envelope is important when dealing with the wave packets.



Matter particle moving with velocity v_0

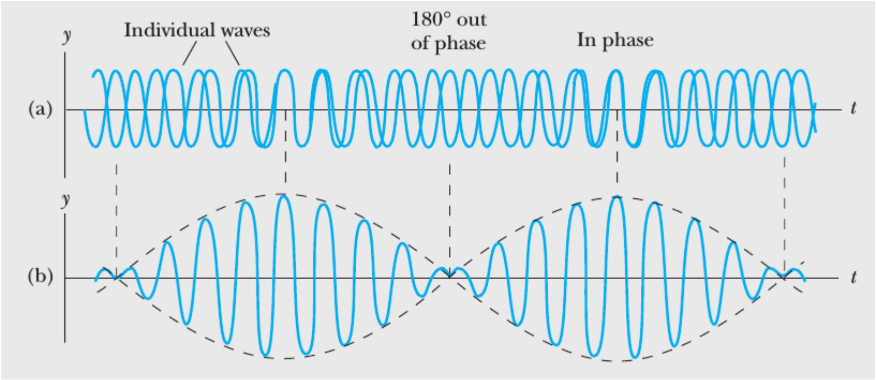


Wave representation of Matter particle moving with velocity v_0

Representation of Matter through waves

In principle one can generalise the previous calculation to obtain the form of the most general wave packet.

However, we can obtain an interesting insight about the wave packet by simply considering the superposition of two waves which can also be generalised to many waves.



$$\Psi(x,\ t) \quad = 2A\cos\left(\frac{\Delta k}{2}x - \frac{\Delta\omega}{2}t\right)\cos(k_{av}x - \omega_{av}t)$$

where $\Delta k = k_1 - k_2$, $\Delta\omega = \omega_1 - \omega_2$, $k_{av} = (k_1 + k_2)/2$, and $\omega_{av} = (\omega_1 + \omega_2)/2$

Note that we can identify a region $\Delta x = x_2 - x_1$ where x_1 and x_2 represent two consecutive points where the envelope is zero for a given value of t.

This is possible when the quantity $\dfrac{\Delta k}{2}x$ is different by a phase of π for the values x_1 and x_2. i.e

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

$$\Delta x \Delta p = h$$

$$\Delta k \Delta x = 2\pi$$

Similarly for a given value of x we can obtain the time Δt over which the wave is localised which gives rise to

$$\Delta\omega\Delta t = 2\pi \qquad\qquad \Delta E \Delta t = h$$

Representation of Matter through waves

When we consider the superposition of many waves to form a wave packet we have a continuous spread of ω and k.

In this case the group velocity is defined as $v_{gr} = \dfrac{d\omega}{dk}$

We can rewrite the phase and group velocities as

$$v_p = \frac{E}{p} \text{ and } v_{gr} = \frac{dE}{dp}$$

Check !!!

Phase velocity of Photon

$E = pc \Rightarrow v_p = E/p = c$

Phase velocity of particles

K.E of a particle of mass m moving at speed v is $E = p^2/2m$

$\therefore$ the phase velocity of the de Broglie wave associated with this is

$$v_p = E/p = p/2m = v/2$$

For a relativistic particle of rest mass m_0 moving with velocity $v \sim c$

$$E = \frac{m_0 c^2}{\sqrt{1 - v^2/c^2}}$$

$$p = \frac{m_0 c}{\sqrt{1 - v^2/c^2}}$$

$\therefore u = E/p = c^2/v = cc/v$

Since $v << c$, $c/v > 1$

$\therefore u > c$

Representation of Matter through waves

When we consider the superposition of many waves to form a wave packet we have a continuous spread of ω and k.

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We can rewrite the phase and group velocities as

$$v_p = \frac{E}{p} \text{ and } v_{gr} = \frac{dE}{dp}$$

Check !!!

For photons

$$v_{gr} = \frac{dE}{dp} = c$$

For non-relativistic particles

$$E = p^2/2m$$

$$v_{gr} = \frac{dE}{dp} = p/m = v$$

For relativistic particles

$$E = \sqrt{c^2p^2 + m_0^2c^4}$$

$$v_{gr} = \frac{dE}{dp} = \frac{2c^2p}{2\sqrt{p^2c^2 + m_0^2c^4}}$$

$$\Rightarrow v_{gr} = c^2p/E = v$$

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

Solution: The first step is to calculate pc for the electron, which is

$$pc = \frac{hc}{\lambda} = \frac{(4.136 \times 10^{-15} eV.s)(3.00 \times 10^{8} m/s)}{2.00 \times 10^{-12} m} = 6.20 \times 10^{5} eV = 620 keV$$

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

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

(b) The electron velocity can be found from

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

$$v = c\sqrt{1 - \frac{E_0^2}{E^2}} = 0.771c$$

Hence, $v_p = \omega/k = c^2/v = c^2/0.771c = 1.30c$

and $v_g = v = 0.771c$

In January 1926, Schrödinger published in Annalen der Physik the paper "Quantisierung als Eigenwertproblem" [tr. Quantization as an Eigenvalue Problem] on wave mechanics and presented what is now known as the Schrödinger equation. In this paper, he gave a "derivation" of the wave equation for time-independent systems and showed that it gave the correct energy eigenvalues for a hydrogen-like atom. This paper has been universally celebrated as one of the most important achievements of the twentieth century and created a revolution in most areas of quantum mechanics and indeed of all physics and chemistry.

Schrodinger's Equation

Following up on de Broglie's ideas, physicist Peter Debye made an offhand comment that if particles behaved as waves, they should satisfy some sort of wave equation. Inspired by Debye's remark, **Schrödinger** decided to find a proper 3-dimensional wave equation for the electron. He was guided by William R. Hamilton's analogy between mechanics and optics, encoded in the observation that the zero-wavelength limit of optics resembles a mechanical system — the trajectories of light rays become sharp tracks that obey Fermat's principle, an analog of the principle of least action.

By that time, Arnold Sommerfeld had refined the Bohr model with relativistic corrections. Schrödinger used the relativistic energy momentum relation to find what is now known as the Klein–Gordon equation in a Coulomb potential.

He found the standing waves of this relativistic equation, but the relativistic corrections disagreed with Sommerfeld's formula. Discouraged, he put away his calculations and secluded himself in an isolated mountain cabin in December 1925.

While at the cabin, Schrödinger decided that his earlier non-relativistic calculations were novel enough to publish, and decided to leave off the problem of relativistic corrections for the future. Despite the difficulties in solving the differential equation for hydrogen (he had sought help from his friend the mathematician Hermann Weyl) Schrödinger showed that his non-relativistic version of the wave equation produced the correct spectral energies of hydrogen in a paper published in 1926. In the equation, Schrödinger computed the hydrogen spectral series by treating a hydrogen atom's electron as a wave $\Psi(x, t)$, moving in a potential well V, created by the proton. This computation accurately reproduced the energy levels of the Bohr model.

This 1926 paper was enthusiastically endorsed by Einstein, who saw the matter-waves as an intuitive depiction of nature.

Matter wave mechanics

Typically, waves are periodic disturbances that propagate in a medium. More generally, they can be periodic disturbances in something more abstract. For example, electromagnetic waves are periodic disturbances in an abstract "Electromagnetic Field" and matter waves as we shall see in this part of the course, are periodic variations of probability amplitudes in space and time.

We may exploit this idea to write down a "wave equation" obeyed by the amplitudes. The main reason for doing this is that the simple periodic functions namely sine and cosine are not the only possibilities when it comes to describing periodic functions.

We use the simple sine and cosine periodic functions to derive a differential equation for the amplitude. Then we assert that the same equation is going to hold for more complicated types of periodic functions whose form may be hard to guess. The form of these waves have to be found by solving the differential equation for the wave called the "wave equation".

General wave form

A typical wave: $\psi(x,t) = A\sin\left(2\pi\left(\frac{x}{\lambda} - \frac{t}{T}\right)\right)$

Amplitude Maximum amplitude Wavelength Period

Spatial periodicity: $\psi(x+\lambda, t) = \psi(x,t)$ and **Temporal periodicity:** $\psi(x, t+T) = \psi(x,t)$

This simple wave is not only periodic in space and time separately, it also moves in a fixed direction.

Suppose I shift my position of observation of the wave from x to $x + \Delta x$ at time t:

Amplitude changes from $\boldsymbol{\psi(x,t)}$ to $\boldsymbol{\psi(x+\Delta x, t)}$

I ask what is the shortest time I have to wait at this new location before this amplitude becomes the same as the original amplitude $\boldsymbol{\psi(x,t)}$?

If I wait for a time $\boldsymbol{\Delta t}$ at this new location, the amplitude becomes $\boldsymbol{\psi(x+\Delta x, t+\Delta t)}$. But I want this to be the same as $\boldsymbol{\psi(x,t)}$.

Hence $\boldsymbol{\sin\left(2\pi\left(\frac{x+\Delta x}{\lambda} - \frac{t+\Delta t}{T}\right)\right) = \sin\left(2\pi\left(\frac{x}{\lambda} - \frac{t}{T}\right)\right)}$ or v = $\frac{\Delta x}{\Delta t} = \frac{\lambda}{T} > 0$ is the speed of the wave and it moves in the positive x direction.

Governing equation for wave

It may seem odd that we want to derive an equation for $\psi(x,t)$ when we already have an answer for it as shown in the previous slide. It is somewhat like wanting to find the quadratic equation for which the roots are 3 and 4. If you already know the roots why do need the equation? Because there are situations where the equation is more general than the special roots from which the equation was generated. Just as a quadratic equation as a concept allows for complex roots as well, our use of the simple roots 3 and 4 to arrive at a general form of the quadratic equation is really useful.

To do this let us differentiate $\psi(x,t)$ twice with respect to x keeping the time t. The notation for differentiating with respect to x while keeping t fixed is $\frac{\partial}{\partial x}$. It is basically the same as $\frac{d}{dx}$ but since t is also a variable, extra effort is made to remind everyone that t is being held fixed.

$$\frac{\partial^2}{\partial x^2}\psi(x,t) = -\left(\frac{2\pi}{\lambda}\right)^2 A\sin(2\,\pi\left(\frac{x}{\lambda} - \frac{t}{T}\right))$$

Similarly,

$$\frac{\partial^2}{\partial t^2}\psi(x,t) = -\left(\frac{2\pi}{T}\right)^2 A\sin(2\,\pi\left(\frac{x}{\lambda} - \frac{t}{T}\right))$$

Since $\lambda = \mathrm{v}\,T$ this leads to the classical wave equation,

$$\frac{\partial^2}{\partial x^2}\psi(x,t) = \frac{1}{\mathrm{v}^2}\frac{\partial^2}{\partial t^2}\psi(x,t)$$

Solution of wave equation

Just as the quadratic equation has many unusual solutions, this wave equation has many more solutions than the simple special form of a periodic travelling wave from which it was generated.

In fact, it could describe standing waves which are two waves travelling in opposite directions

$$\psi(x,t) = A \sin\left(2\pi \left(\frac{x}{\lambda} - \frac{t}{T}\right)\right) + A \sin\left(2\pi \left(\frac{x}{\lambda} + \frac{t}{T}\right)\right)$$

It could even describe waves that are travelling in the positive x direction but are not periodic

$$\psi(x,t) = A\, \mathrm{e}^{-\left(\frac{x}{\lambda} - \frac{t}{T}\right)^2}$$

Indeed, the most general solution to this classical wave equation may be written as,

$$\psi(x,t) = u(x - \mathrm{v}\, t) + w(x + \mathrm{v}\, t)$$

where u and w can be any functions of their respective arguments.

Matter wave mechanics

In a similar vein, Schrodinger wanted to derive such a wave equation for matter waves obeying the de Broglie relation.

He also said that the amplitude $\psi(x,t)$ could be complex since only the square of its modulus has physical meaning – as the probability per unit length of finding the particle at position x at time t.

Another reason for this choice of a complex amplitude is that free particles not acted upon by forces – simplest situation in Newtonian particle mechanics – should have a matter wave description corresponding to the simplest situation in wave theory - namely sinusoidal waves with fixed wavelength and period. But a choice we had studied earlier $\psi(x,t) = A\, sin(\, 2\, \pi \left(\frac{x}{\lambda} \; - \frac{t}{T}\right))$ is not suitable since even though it meets all the required criteria, the probability of finding the particle at some point varies periodically from point to point and from one time to the next. This implies a certain sequence of points in space at which the probability density is maximum are more special than others which is not acceptable. So he suggested,

$$\psi(x,t) = A\, e^{2\pi i\left(\frac{x}{\lambda} \, - \frac{t}{T}\right)}$$

This is simple and periodic in both space and time and corresponds to a wave moving in the positive x-direction and most importantly the absolute square of the amplitude which is the probability per unit length of finding the particle at x and t is independent of position and time which ensures that no point in space is more special than others.

$$|\psi(x,t)|^2 = |A|^2$$

Wave-particle duality

$$Wave\ property = \frac{h}{Particle\ property} \begin{cases} \lambda = \dfrac{h}{p} \\ \mathrm{T} = \dfrac{h}{E} \end{cases}$$

$$\mathrm{E} = \mathrm{h}\,\nu$$

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

Substituting this into Schrodinger's matter wave we get,

$$\psi(x,t) = A\,\mathrm{e}^{\frac{2\pi i}{h}(p\,x - E\,t)}$$

Differentiating twice with respect to *x*,

$$\frac{\partial^2}{\partial x^2}\psi(x,t) = p^2\left(\frac{2\pi i}{h}\right)^2 A\,\mathrm{e}^{\frac{2\pi i}{h}(p\,x - E\,t)}$$

Differentiating once with respect to *t*,

$$\frac{\partial}{\partial t}\psi(x,t) = -E\,\frac{2\pi i}{h} A\,\mathrm{e}^{\frac{2\pi i}{h}(p\,x - E\,t)}$$

Matter wave mechanics: Schrodinger Equation

Keeping in mind that for a nonrelativistic particle, $E = \frac{p^2}{2m}$ and comparing the earlier two equations allows us to write (where $\hbar = \frac{h}{2\pi}$ is sometimes called the Planck Dirac constant),

$$\underbrace{i\hbar\frac{\partial}{\partial t}}_{E}\psi(x,t) = \underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}}_{\frac{p^2}{2m}}\psi(x,t)$$

The above was for a free particle. Schrodinger saw immediately that the right hand side has kinetic energy and the left hand side has total energy - they are equal for a free particle. For a particle acted upon by a force he added the potential energy to the right hand side to obtain his celebrated **Schrodinger equation**,

$$\underbrace{i\hbar\frac{\partial}{\partial t}}_{E}\psi(x,t) = \underbrace{\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right)}_{\frac{p^2}{2m}+V(x,t)}\psi(x,t)$$

Forthcoming topics….

- Postulates of quantum mechanics
- The ‘Copenhagen interpretation’ of the wave function in QM
- Measurement in QM. The nature of the observer and the observed
- Counter intuitive phenomena:

  – quantum tunneling and zero point motion