PHYS-3301

Lecture 6

Sep. 10, 2024

Chapter. 4
Wave & Particles II

"Matter" behaving as "Waves"

Outline:

- A Double-Slit Experiment (watch "video")
- Properties of Matter Waves
- The Free-Particle Schrödinger Equation
- **Uncertainty Principle**
- **The Bohr Model of the Atom**
- **Mathematical Basis of the Uncertainty Principle – The Fourier Transform**

The Free-Particle Schrodinger Wave Equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

$\psi(x,t)$ **Probability Wave Function**

$\psi^*(x,t)\psi(x,t) = |\psi(x,t)|^2$ **Probability Density**

$\psi(x,t)$ **a complex function**

4.3 The Free-Particle Schrödinger Eq.

******* Probability Density**

--- Probability of detecting the particle ~ (wave's Amplitude)^2

[Q] What does this mean if wave has 2 parts;

E & B or real & imaginary part of ψ(x,t)?

$\psi(x,t) \equiv \psi_1(x,t) + i\psi_2(x,t)$

$\psi^*(x,t) \equiv \psi_1(x,t) - i\psi_2(x,t)$

Complex Conjugate

$i \equiv \sqrt{-1}$

$i^2 = -1$

Probability Density = ?

$\psi(x,t) \equiv \psi_1(x,t) + i\psi_2(x,t)$

$\psi^*(x,t) \equiv \psi_1(x,t) - i\psi_2(x,t)$

$i = \sqrt{-1}$

Probability Density

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

$= \psi_1\psi_1 - ii\psi_2\psi_2 - i\psi_1\psi_2 + i\psi_2\psi_1 =$

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

$|\psi(x,t)|^2 = \psi_1^2(x,t) + \psi_2^2(x,t)$

probability of finding the particle in certain region!!

per unit length
per unit volume

Probability density = |ψ(x,t)|^2

The Plane Wave

$$\Psi(x, t) = Ae^{i(kx-\omega t)}$$

$$\Psi(x, t) = \begin{cases} Ae^{i(kx-\omega t)} \\ A\cos(kx-\omega t) + iA\sin(kx-\omega t) \\ \Psi_1(x, t) + i\Psi_2(x, t) \end{cases}$$

Is the Plane Wave a solution of the Schrodinger Equation?

$$\Psi(x, t) = Ae^{i(kx-\omega t)}$$

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Taking the partial derivatives on both sides..

$$-\frac{\hbar^2}{2m}(ik)^2 Ae^{i(kx-\omega t)} = i\hbar(-i\omega)Ae^{i(kx-\omega t)}$$

Is the Plane Wave a solution of the Schrodinger Equation?

$$\Psi(x,\ t) = Ae^{i(kx-\omega t)}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,\ t)}{\partial x^2} = i\hbar\frac{\partial\Psi(x,\ t)}{\partial t}$$

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$$\frac{\hbar^2k^2}{2m} = \hbar\omega$$

Is the Plane Wave a solution of the Schrodinger Equation?

$$\Psi(x,\ t) = Ae^{i(kx-\omega t)}$$

Let's see how the Schrödinger wave eq. relates to the classical physics of particle?

$$\frac{\hbar^2k^2}{2m} = \hbar\omega$$

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

YES

So. Our answer is "YES".

It's a solution of Schrödinger eq.

Is the Plane Wave a solution of the Schrodinger Equation?

$$\Psi(x,\ t) = Ae^{i(kx-\omega t)}$$

$$\frac{\hbar^2k^2}{2m} = \hbar\omega$$

Mean:
Particle's KE = Total E
True, classically!!
since a free particle has no PE

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

YES

$$E = \frac{(mv)^2}{2m} = \frac{mv^2}{2}$$

Is the Plane Wave a solution of the Schrodinger Equation?

$$\Psi(x,\ t) = Ae^{i(kx-\omega t)}$$

The Schrödinger equation is related to a classical accounting of energy!!

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YES

The Magnitude of a Plane Wave

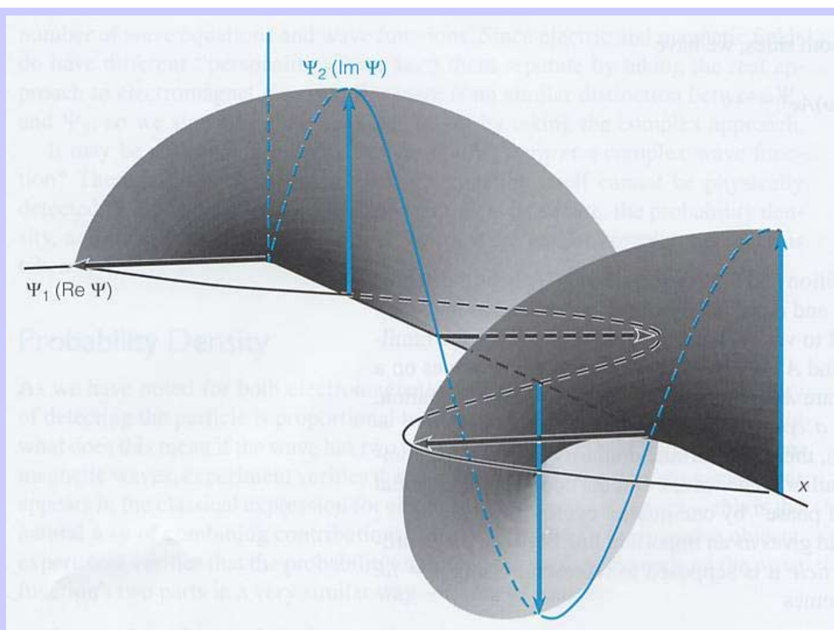
$$\Psi(x, t) = Ae^{i(kx - \omega t)}$$

$$|\Psi(x, t)|^2 = \Psi^*(x, t)\Psi(x, t) = [Ae^{-i(kx-\omega t)}]\,[Ae^{+i(kx-\omega t)}] = A^2$$

$$|\Psi(x, t)| = A$$

Constant in space and time!

Constant Probability Density



The Schrödinger equation is based upon energy. The simplest solution is a plane wave, a complex exponential with two sinusoidal parts. The wave's magnitude and the probability density vary neither in time nor in position.

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x, t)}{\partial x^2} = i\hbar\frac{\partial\Psi(x, t)}{\partial t}$$

$$\frac{\hbar^2 k^2}{2m} = \hbar\omega \qquad \frac{p^2}{2m} = E$$

Kinetic energy

$$\Psi(x, t) = Ae^{i(kx - \omega t)}$$

Plane wave

$$|\Psi(x, t)|^2 = \Psi^*(x, t)\Psi(x, t) = [Ae^{-i(kx-\omega t)}]\,[Ae^{+i(kx-\omega t)}] = A^2$$

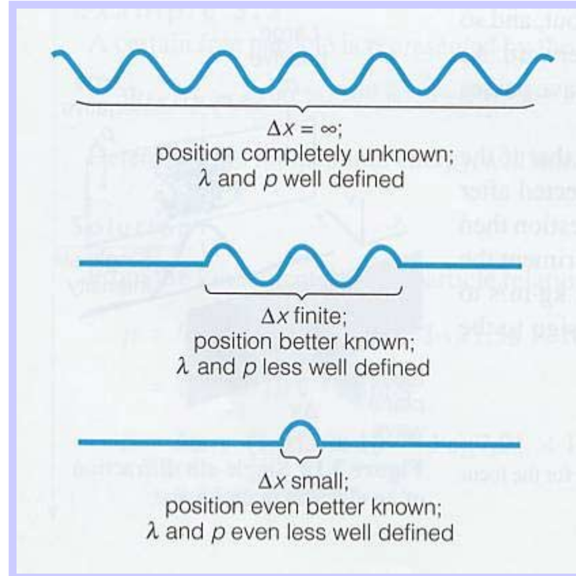
$$|\Psi(x, t)| = A$$

= constant (x,t)

Uncertainty Principle

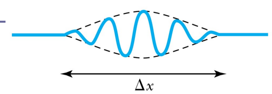
If a phenomenon has a wave nature, it is theoretically impossible to know precisely the position along an axis and the component of momentum along that axis *simultaneously*; Δx and Δp_x cannot be simultaneously zero. Rather, there is a strict theoretical lower limit on their product:

$$\Delta p_x \Delta x \geq \frac{\hbar}{2} \quad \text{(3-9)}$$



$$\Delta p_x \, \Delta x \geq \frac{\hbar}{2}$$

Wave Packet Envelope



$$\Psi(x,t) = \Psi_1(x,t) + \Psi_2(x,t) = 2A\cos\left(\frac{\Delta k}{2}x - \frac{\Delta\omega}{2}t\right)\cos(k_{av}x - \omega_{av}t)$$

- The superposition of two waves yields a wave number (k) and angular frequency (ω) of the wave packet envelope.

$$\frac{\Delta k}{2}x - \frac{\Delta\omega}{2}t$$

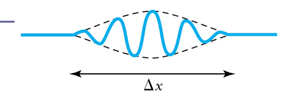
- We can identify a localized region $\Delta x = x_2 - x_1$ where x_1 & x_2 represent two consecutive points where the envelope is zero. This must be different by a phase of π for the values x_1 & x_2 , because $x_2 - x_1$ represent only one half of the wavelength of the envelope confining the wave.

- The range of wave numbers and angular frequencies that produce the wave packet have the following relations:

$$(1/2)\,\Delta\kappa\, x_2 - (1/2)\,\Delta\kappa\, x_1 = \pi \longrightarrow \Delta k \, \Delta x = 2\pi$$

- Similarly, $\Delta\omega \, \Delta t = 2\pi$

Wave Packet Envelope



- The superposition of two waves yields a wave number (k) and angular frequency (ω) of the wave packet envelope.

$$\frac{\Delta k}{2}x - \frac{\Delta\omega}{2}t$$

- The range of wave numbers and angular frequencies that produce the wave packet have the following relations:

$$\Delta k \, \Delta x = 2\pi \qquad \Delta\omega \, \Delta t = 2\pi$$

- A **Gaussian wave packet** has similar relations:

$$\Delta k \Delta x = \frac{1}{2} \qquad \Delta\omega \, \Delta t = \frac{1}{2}$$

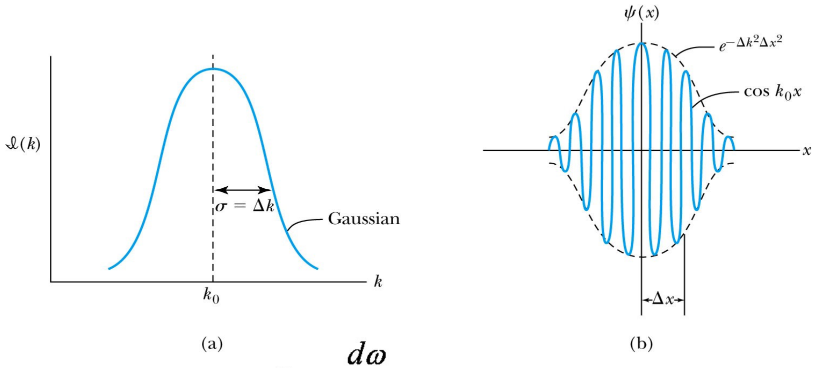
- The localization of the wave packet over a small region to describe a particle requires a large range of wave numbers. Conversely, a small range of wave numbers cannot produce a wave packet localized within a small distance.

Gaussian Function

Gaussian wave packets are often used to represent the position of particles, because the associated integrals are relatively easy to evaluate.

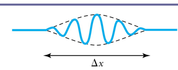
- A Gaussian wave packet describes the envelope of a pulse wave.

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



- The group velocity is $u_{gr} = \dfrac{d\omega}{dk}$

$$u_{gr} = \frac{\Delta\omega}{\Delta k}$$



Uncertainty Principle

- It is impossible to measure simultaneously, with no uncertainty, the precise values of *k* and *x* for the same particle. The wave number *k* may be rewritten as

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

- For the case of a Gaussian wave packet we have

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

Thus for a single particle we have Heisenberg's **uncertainty principle**:

$$\Delta p_x \; \Delta x \geq \frac{\hbar}{2}$$

Energy Uncertainty

- If we are uncertain as to the exact position of a particle, for example an electron somewhere inside an atom, the particle can't have zero kinetic energy.

$$K_{\min} = \frac{p_{\min}{}^2}{2m} \geq \frac{(\Delta p)^2}{2m} \geq \frac{\hbar^2}{2m\ell^2}$$

- The energy uncertainty of a Gaussian wave packet is

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

combined with the angular frequency relation

$$\Delta\omega \; \Delta t = \frac{\Delta E}{\hbar} \Delta t = \frac{1}{2}$$

- Energy-Time Uncertainty Principle: $\Delta E \; \Delta t \geq \dfrac{\hbar}{2}$.

Gaussian Wave form

$$\Delta x \Delta p_x = \frac{1}{2}\hbar$$

= minimum uncertainty