

Heisenberg's Uncertainty Principle \Rightarrow

The particles exhibiting both particle and wave nature. So it will not be possible to accurately determine both the position and velocity at the same time.

fundamental limit to the precision with which certain pairs of complementary properties of a particle.

"It is impossible to determine the exact position and momentum of a particle simultaneously".

Mathematically, it is expressed as

The product of uncertainty position and uncertainty momentum of Particle is greater than or equal to $\frac{h}{2\pi}$.

$$\Delta x \cdot \Delta p \geq \frac{h}{2\pi} = \frac{\hbar}{2}$$

where Δx is the uncertainty in the Particle's Position.

Δp is the uncertainty in the Particle's Momentum.

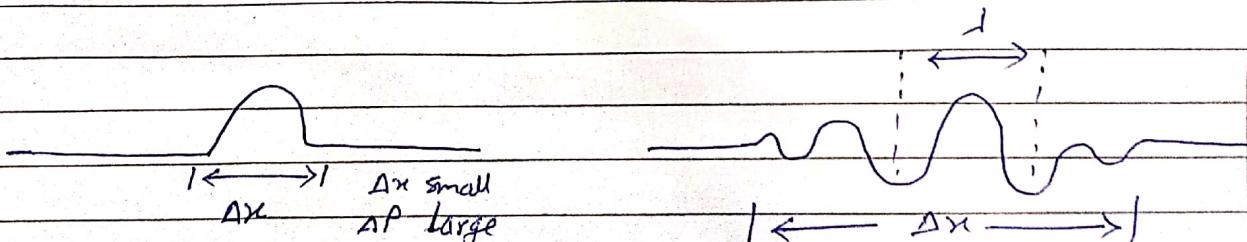
h is the Planck Constant

\hbar is the reduced Planck Constant (1.054×10^{-34} Joule-Sec)

(ii) Relation between uncertainty ~~position~~ Energy (ΔE) and uncertainty ~~momentum~~ time (Δt) of Particle is also greater than $\frac{h}{2\pi}$

$$\Delta E \Delta t \geq \frac{h}{2\pi}$$

(iii) if $\Delta \theta$ and ΔJ are uncertainty angular position and angular momentum then $\Delta \theta \Delta J \geq \frac{h}{2\pi}$



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⇒ Calculate the Uncertainty in the Position of a dust particle with mass equal to 1mg if uncertainty in its velocity is 5.5×10^{-20} m/s

Given: $m = 1\text{mg} = 10^{-6}\text{kg}$, $\Delta V = 5.5 \times 10^{-20}\text{m/s}$

From the Uncertainty Principle, we have

$$\Delta x \times \Delta p \geq \frac{h}{2\pi}$$

$$\Delta V = 5.5 \times 10^{-20}\text{m/s}$$

$$\text{So } \Delta x = \frac{h}{2\pi \times m \Delta V} = \frac{6.63 \times 10^{-34}}{2 \times 3.14 \times 10^{-6} \times 5.5 \times 10^{-20}} \\ = \frac{6.63 \times 10^{-34}}{34.54 \times 10^{-26}}$$

$$\Delta x = 19.2 \text{ A}^\circ$$

Wavefunction and its Physical Significance \Rightarrow

The quantity in quantum mechanics undergoes periodic changes and gives information about the particle within the wave packet. It is called Wave function ψ .

The wavefunction ψ itself has no physical significance but the square of its absolute magnitude $|\psi|^2$ gives the probability of finding the particle at that time.

(a) Normalization of Wave Function \Rightarrow

If the wave function ψ of any system is such that it gives the value of given integral a finite quantity say N.

$$\int_{-\infty}^{\infty} \psi \psi^* dx = \int_{-\infty}^{\infty} |\psi|^2 dx = N \text{ (Integral)}$$

(ψ^* is complex conjugate)

then ψ is called normalization of wave function.

(b) Orthogonal Wave Function \Rightarrow

If the wave function ψ of any system is

when the value of the integral is equal to zero ($N=0$), the wave function ψ is known as orthogonal wave function.

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 0$$

Schrodinger Wave Generation

Schrodinger's equation:-

Schrodinger's equation which is the fundamental equation of quantum mechanics is a wave equation in the variable ψ .

① Time Independent Schrodinger Wave Equation :-

Consider a system of stationary wave to be associated with particle and the position coordinate of the particle (x, y, z) and ψ is the periodic displacement of any instant time 't'.

* The general wave equation in 3-D in differential form is:

$$\boxed{\nabla^2 \psi = \frac{1}{v^2} \frac{\partial^2 \psi}{\partial t^2}} \quad - \textcircled{1}$$

where v = velocity of wave, and

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \text{Laplacian Operator.}$$

The wave function may be written as

$$\psi = \psi_0 e^{-i\omega t}$$

Differentiate above eq with respect to time, we get

$$\frac{\partial \psi}{\partial t} = -i\omega \psi_0 e^{-i\omega t}$$

$$\text{Again Differentiating eq } \frac{\partial^2 \psi}{\partial t^2} = +i^2 \omega^2 \psi_0 e^{-i\omega t}$$

$$\boxed{\frac{\partial^2 \psi}{\partial t^2} = -\omega^2 \psi}$$

Putting these value in eq $\textcircled{1}$

$$\boxed{\nabla^2 \psi / \frac{\partial^2 \psi}{\partial t^2} = -\frac{\partial^2 \psi}{\partial t^2} / \frac{\partial^2 \psi}{\partial t^2} = -\frac{\omega^2}{v^2} \psi} \quad - \textcircled{1}$$

$$\text{But } \omega = 2\pi v = \frac{2\pi v}{1} \Rightarrow \frac{\omega}{v} = \frac{2\pi}{1}$$

eq (1) becomes

$$\nabla^2 \psi = -\frac{4\pi^2}{h^2} \psi$$

from de-Broglie's Wavelength, $\lambda = \frac{h}{mv}$

$$\text{then } \nabla^2 \psi = -\frac{4\pi^2 m v^2}{h^2} \psi \quad - (3)$$

If E and V are the total and potential energies of a particle and E_K is kinetic energy, then

$$E_K = E - V \text{ or } \frac{1}{2}mv^2 = E - V \text{ or } m^2v^2 = 2m(E - V)$$

Now eq (3) becomes

$$\nabla^2 \psi = -\frac{4\pi^2}{h^2} m [E - V] \psi$$

$$\text{since } h = \frac{h}{2\pi}$$

$$\therefore \boxed{\nabla^2 \psi + \frac{2m[E - V]\psi}{h^2} = 0}$$

for free Particle ($V=0$)

$$\boxed{\nabla^2 \psi + \frac{2m}{h^2} E \psi = 0}$$

Time Dependent

Schrodinger Wave equation \Rightarrow

We have wave function is $\psi = \psi_0 e^{-i\omega t}$
on differentiating with respect to time, we get

$$\frac{\partial \psi}{\partial t} = -i\omega \psi_0 e^{-i\omega t} \quad \text{--- (i)}$$

$$\text{or } \frac{\partial \psi}{\partial t} = -i(2\pi\nu)\psi \quad \text{--- (ii)}$$

$$\text{But } E = h\nu \Rightarrow \nu = E/h$$

Putting ν value in eq (ii)

$$\frac{\partial \psi}{\partial t} = -i(2\pi) \left(\frac{E}{h}\right) \psi$$

{ Since $\hbar = \frac{h}{2\pi}$

$$\frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} E \psi$$

$$\text{and } E \psi = \frac{-\hbar}{i} \frac{\partial \psi}{\partial t}$$

$$\text{or } \boxed{E \psi = i\hbar \frac{\partial \psi}{\partial t}} \quad \text{--- (iii)}$$

Now time independent Schrodinger wave equation is

$$\nabla^2 \psi + \frac{2m}{\hbar^2} (E - V) \psi = 0$$

$$\text{or } \boxed{\nabla^2 \psi + \frac{2m}{\hbar^2} [E \psi - V \psi] = 0}$$

Now using eq (ii). we get

$$\nabla^2 \psi + \frac{2m}{\hbar^2} \left[i\hbar \frac{\partial \psi}{\partial t} - V \psi \right] = 0$$

$$\nabla^2 \psi - \frac{2mV\psi}{\hbar^2} = -\frac{2m}{\hbar^2} i\hbar \cdot \frac{\partial \psi}{\partial t}$$

$$\text{or } \left(-\frac{\hbar^2}{2m} \nabla^2 + V \right) \Psi = i\hbar \frac{\partial \Psi}{\partial t}$$

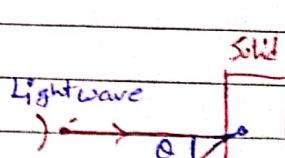
This is required time dependent Schrodinger wave equation.

$$-\frac{\hbar^2}{2m} \nabla^2 + V = H \rightarrow \text{is known as Hamiltonian operator}$$

$$i\hbar \frac{\partial \Psi}{\partial t} = E \rightarrow \text{energy operator}$$

Then

$$H\Psi = E\Psi$$



\Rightarrow Wave Particle Duality \Rightarrow (de Broglie Principle)
 (Light and electron) Wave Particle Duality help us to understand the $\hat{ }$ particle and wave nature.

- * One can understand wave particle duality via the behaviour of light or electron.
- * Diffraction and interference of light explain that it behaves as a waves.
- * The photoelectric influence explains that it consists of particles.

In the Photoelectric effect, Light waves behave as Particles.

The phenomenon is wave particle duality.

The nature of the particle dominates in the case of large objects while wave and particle nature are shown by smaller objects.

Suggest

In 1924, de Broglie Postulated the existence of matter waves. He suggested that since waves exhibits particle like behaviour then particles should be expected to show wave like properties.

The Hypothesis of de Broglie was the existence of a wave-particle duality principle. The momentum of a photon is given by

$$P = \frac{\hbar}{\lambda}$$

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Where λ is the wavelength of the light wave. Then, de Broglie hypothesized that the wavelength of a particle can be expressed as

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

where p is the momentum of the particle and λ is known as the de Broglie wavelength of the matter wave.

Q To calculate the de Broglie wavelength of a particle. Consider an electron traveling at a velocity of 10^7 cm/sec = 10^5 m/s

Solution ⇒ The momentum is given by $p = mv = 9.11 \times 10^{-31} \times 10^5 = 9.11 \times 10^{-26}$

Then, the de Broglie wavelength is

$$\lambda = \frac{h}{p} = \frac{6.625 \times 10^{-34}}{9.11 \times 10^{-26}} = 7.27 \times 10^{-9} \text{ m}$$

$$\lambda = 72.7 \text{ } \text{\AA}$$

Q What is the de Broglie wavelength (in \AA) of an electron at 100 eV? What is the wavelength for electron at 12 KeV?

Solution ⇒ We have

$$v = \sqrt{2E/m}, \quad \lambda = \frac{h}{mv} = \frac{h}{\sqrt{2Em}} = \frac{6.63 \times 10^{-34}}{[2 \times 9.1 \times 10^{-31}]^{\frac{1}{2}}} E^{-\frac{1}{2}} \quad (1)$$

i) for 100 eV

from above eq (1) $\lambda = \frac{4.9 \times 10^{-19}}{(1.6 \times 10^{-19})^{\frac{1}{2}}} \cdot (100)^{-\frac{1}{2}} = 1.23 \times 10^{-9} [100]^{-\frac{1}{2}}$
 $= 1.23 \times 10^{-10} \text{ m} = 1.23 \text{ } \text{\AA}$

ii) for 12 KeV

from above eq (1) $\lambda = \frac{4.9 \times 10^{-19}}{(1.6 \times 10^{-19})^{\frac{1}{2}}} [1.2 \times 10^4]^{-\frac{1}{2}} = 1.23 \times 10^{-9} [1.2 \times 10^4]^{-\frac{1}{2}}$
 $= 1.12 \times 10^{-11} \text{ m} = 0.112 \text{ } \text{\AA}$

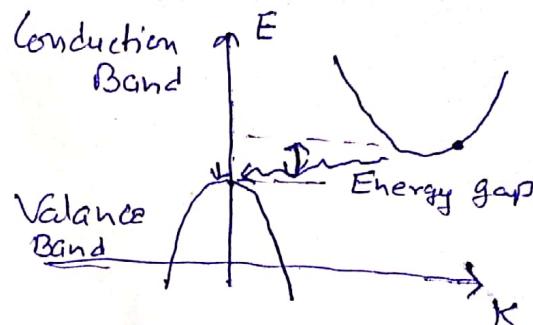
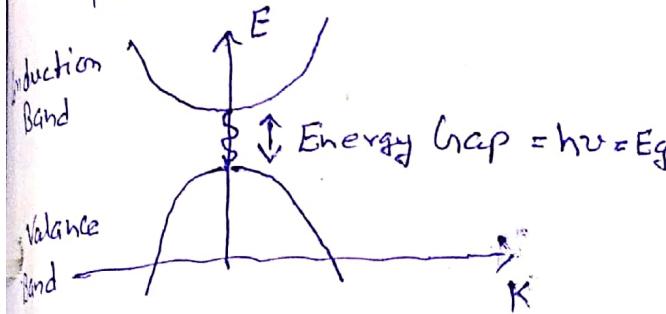
Direct Gap and Indirect Gap Semiconductors \Rightarrow

The energy of an electron is given by $E = \frac{P^2}{2m} = \frac{\hbar^2 K^2}{2m}$

where P is momentum, m is mass of an electron, \hbar is plank's constant and K is propagation constant.

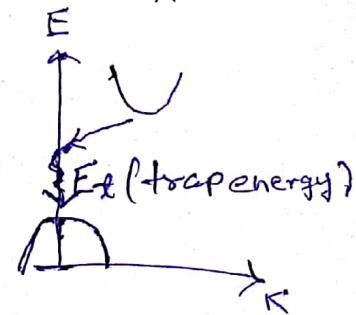
Thus $E \propto K^2$ which is an equation of Parabola.

The graph of E vs K is shown below.



Example:-

The band structure of GaAs has a minimum in the Conduction band and a maximum in the Valence band for the same K value ($K=0$),



On the other hand, Si has its Valence band Maximum at a difference value of K than its Conduction band Minimum. Thus an electron making a smallest-energy transition from the Induction band to the Valence band in GaAs can do so without a change in K value.

On the other hand, a transition from the minimum point in the Si Conduction band to the maximum point of the Valence band requires some change in K .

Direct band gap

direct band-gap Semiconductor
one in which the maximum
level of the Valence
band aligns with Minimum
level of the Conduction
band with respect to momentum.

A direct recombination takes place with the release of energy equal to the energy difference b/w the recombining particles

* Efficiency factor of a DBG Semiconductor is higher.

* IBS for making optical Sources.

Ex. Gallium Arsenide (GaAs).

Indirect band gap

* An Indirect band-gap Semiconductor is one in which the Maximum energy level of the Valence band and the Minimum energy level of the Conduction band are misaligned with respect to momentum.

* first the momentum is conserved by release of energy and only after the both the momenta align themselves, a recombination occurs accompanied with the release of energy.

* The Probability of a radiative recombination is comparatively low.

* efficiency factor is lower.

Example - Silicon and Germanium

Effective Mass

Inside crystal, electrons are not completely free rather they interact with the periodic potential of the lattice, due to which their wave particle motion cannot be expected to be the same as for electrons in free space.

Thus for estimating the charge carriers in a solid we must use altered values of particle mass (Known as effective mass).

The calculation of effective mass must take appropriate averages over the various energy bands.

The effective mass of an electron in a band with a given (E, k) relationship can be calculated as:

The electron momentum is

$$P = m v = h k$$

$$\text{Then } E = \frac{1}{2} m v^2 = \frac{1}{2} \frac{P^2}{m} = \frac{h^2}{2m} k^2 \quad \left\{ E \propto k^2 \right.$$

This shows that the electron energy is parabolic with wave vector k . The electron mass is inversely related to the

Curvature $\frac{d^2 E}{dk^2}$ as:

$$\boxed{\frac{d^2 E}{dk^2} = \frac{h^2}{m}}$$

Considering the influence of the lattice, the effective mass of an electron can be written as:

$$\boxed{m^* = \frac{h^2}{\frac{d^2 E}{dk^2}}}$$

Thus the curvature of the band determines the electron effective mass.