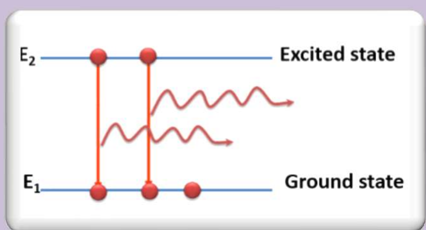
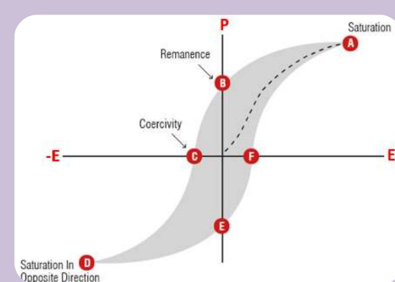
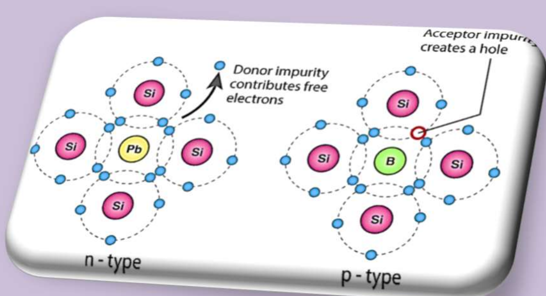
Engineering Physics

$$H\Psi = E\Psi$$







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Unit - I: Quantum Mechanics

Difference between classical and quantum mechanics

Classical Mechanics	Quantum Mechanics
Classical mechanics describes the motion of macroscopic objects. Example: From projectiles to parts of machinery, and astronomical objects, such as spacecraft, planets, stars and galaxies.	Quantum Mechanics describes the motion of microscopic objects. Example: Atoms, protons, electrons
The measurements in classical mechanics are definite. Hence, we may predict exact momentum, position and velocity.	The measurements performed in quantum mechanics are uncertain.
Classical mechanics treats particles and waves differently.	Every object has a particle and wave nature associated to it.
Changes of all physical quantities occur continuously in space and time. The laws determining these changes are deterministic.	On the elementary level, all the changes in nature are discontinuous consisting of quantized steps. The occurrence of these quantum transitions are governed by probability laws.

Limitations of classical mechanics

Classical mechanics failed to explain the following phenomena:

- Certain experimental results such as black body radiation spectrum, Photoelectric effect, Compton scattering, Spectrum of hydrogen emissions were not explained by classical theory.
- It could not explain the non-relativistic motion of atoms, electrons, protons etc.
- It could not explain the stability of atoms
- It could not explain the origin of discrete spectra of atoms as in classical mechanics, the energy changes are considered as continuous.
- It could not explain the observed variation of specific heat capacity of solids.

The inadequacy of classical mechanics led to the introduction of quantum mechanics.

List of Experiments that Evidence Particle and Wave Nature

Experiments that evidence Particle Nature: Black-body Radiation, emission and absorption of line spectra, Compton Scattering of X-rays, Photoelectric effect etc.,

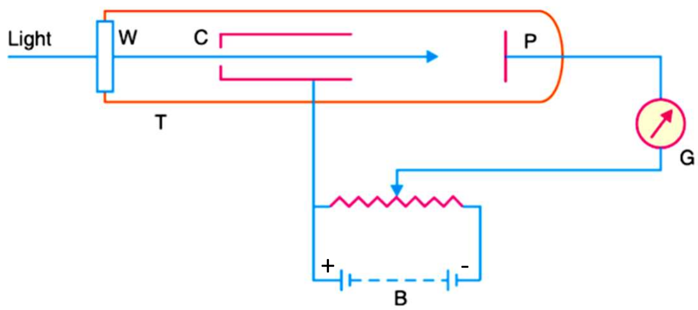
Experiments that evidence Wave Nature: Thomas Young's Double slit experiment, Davisson-Germer experiment, Diffraction and Interference experiments etc.,

Photoelectric effect

When light or electromagnetic radiation (such as X-rays, Ultraviolet rays) falls on a metal surface, it emits electrons. The process of emission of electrons from the metal surface when illuminated by light of suitable wavelength is called Photoelectric effect. The electrons emitted are known as photoelectrons.

In alkali metals such as Lithium (Li), Sodium (Na), Pottasium (K), Rubidium (Rb), Cesium (Cs), and Francium (Fr), photoelectric emission occurs even in visible light because they are soft and highly reactive metals at standard temperature and pressure and readily lose their outermost electron to form cations with charge +1. However, Zinc and cadmium are sensitive to only UV light as their threshold frequency is about 10^{15} Hz.

Experimental investigations on the photoelectric effect



The apparatus shown above consists of an evacuated glass tube T with a quartz window W. P is a photo-electrically sensitive plate. C is a hollow cylinder and it has a small hole that permits the incident light to fall on the plate P. P is connected to the negative end and C is connected to the positive terminal of a battery B. When the electromagnetic radiation falls on the plate P, the photoelectrons are ejected out of the plate P. These photoelectrons are attracted by the positively charged cylinder C. Hence, a photoelectric current flow from P to C in the bulb and from C to P outside the bulb. The photoelectric current flows between P and C can be measured from the deflection produced in the galvanometer G. It is found that the strength of the photoelectric current increases as the potential of C is more and more positive with respect to P. The deflection in the galvanometer decreases when the potential of C is negative with respect to P.

Laws of photoelectric emission:

The results obtained from the above experiment can be summarized as follows

(i) For every metal, there is a particular minimum frequency of the incident light, below which there is no photoelectric emission, whatever is the intensity of the radiation. This minimum energy which can cause photoelectric emission is called the threshold frequency.

(ii) The strength of the photoelectric current is directly proportional to the intensity of the incident light, provided that the frequency is greater than the threshold frequency.

(iii) The velocity and hence the energy of the emitted photoelectrons are independent of the intensity of the light and depends only on the frequency of the incident light and nature of the metal.

(iv) Photoelectric emission is an instantaneous process. The time lag if any between the incident radiation and emission of the electrons is not more than 3 x 10^{-9} s.

Einstein's Photoelectric Equation

According to Einstein, a light of frequency υ consists of a shower of corpuscles or bundles of photons each of energy hυ. When a light of frequency υ is incident on a metal, the energy of the incident photon hυ is completed transferred to a free electron (unpaired electron in the outermost orbital) in the metal. A part of the energy acquired by the electron is used to pull out the electron from the surface of the metal and the rest of it is utilized in imparting kinetic energy to the emitted electron.

Let φ be the energy spent in extracting the electron from the metal often known as photoelectric work function and $\frac{1}{2}\, mv_{max}^2$ is the maximum kinetic energy acquired by the photoelectron.

i.e $$hv = \varphi + \frac{1}{2}\, mv_{max}^2 \qquad \text{........(1)}$$

This relation is known as Einstein's Photoelectric equation.

Suppose, if υ_0 is the threshold frequency which just ejects an electron from the metal without any velocity, then $\varphi = hv_0$

Therefore, $$hv = hv_0 + \frac{1}{2}\, mv_{max}^2 \qquad \text{........(2)}$$

or $$\frac{1}{2}\, mv_{max}^2 = h(v - v_0) \qquad \text{........(3)}$$

The equation (3) suggests that the energy of the emitted photoelectrons is independent of the intensity of the incident radiation but increases with the frequency.

This photoelectric effect experiment is working on the basis of stopping potential. The stopping potential is the necessary retarding potential difference between the photosensitive plate and C in order to stop the most energetic photoelectron emitted.

From the Einstein's photoelectric equation, the K.E acquired by the photoelectron is given by,

$$\frac{1}{2} mv_{max}^2 = hv - \varphi$$

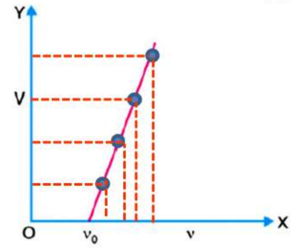
Let V_s be the retarding potential difference that is applied between the emitter and a collecting electrode.

$$eV_s = \frac{1}{2} mv_{max}^2 = hv - \varphi \qquad \text{........(4)}$$

or $$V = \frac{h}{e} v - \frac{\varphi}{e} \qquad \text{........(5)}$$

The work function φ is constant for a given metal and h and e are also constants

The stopping potential (V) is determined for different frequencies of the incident light. The value of $\left(\frac{h}{e}\right)$ can be calculated from the slope of the graph, which is plotted between stopping potential along the Y-axis and the frequency of light along the -axis as shown. The intercept on the X-axis gives the threshold frequency ν_0 for the given emitter. From this, photoelectric work function $\varphi = h\nu_0$ can be calculated.



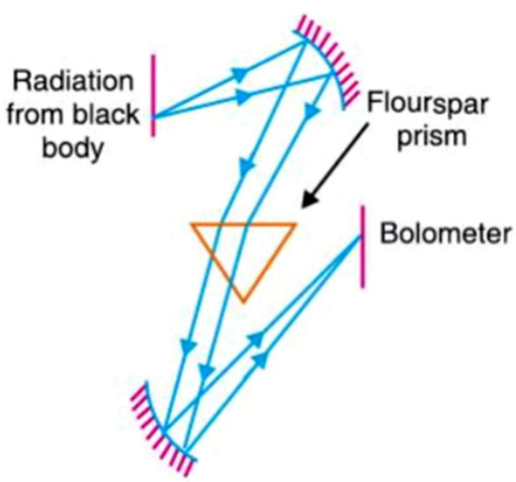
Black body radiation

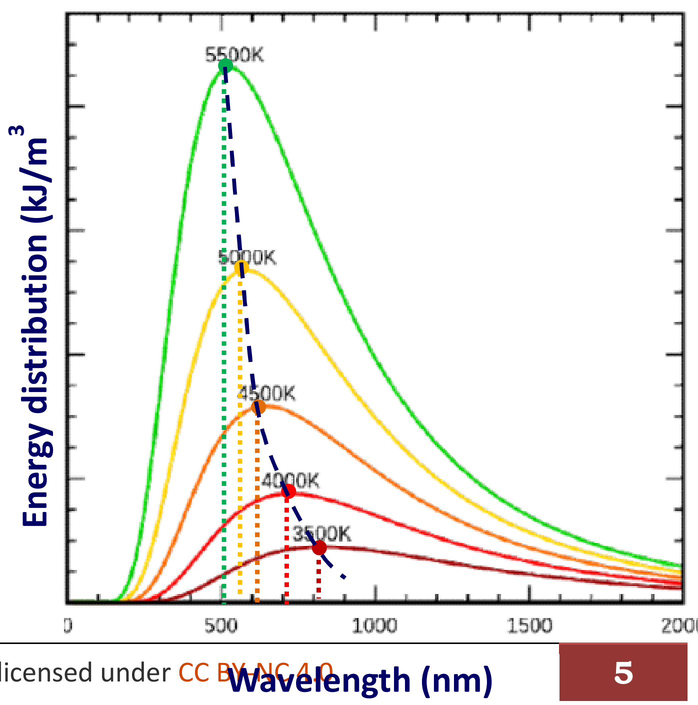
All normal (baryonic) matter emits electromagnetic radiation when it has a temperature above absolute zero. The radiation represents a conversion of a body's internal energy into electromagnetic energy, and is therefore called thermal radiation. It is a spontaneous process of radiative distribution of entropy.

Conversely all normal matter absorbs electromagnetic radiation to some degree. *An object that absorbs all radiation falling on it at all wavelengths is called a* ***black body****. When a black body is at a uniform temperature, its emission has a characteristic frequency distribution that depends on the temperature. Its emission is called* ***black-body radiation***.

The distribution of energy in the black body radiation spectrum

The radiation emitted by a black body at a fixed temperature is analyzed by means of a suitable spectroscopic arrangement by Lummer and Pringsheim as shown in Figure. The radiation emitted by the black body for different wavelengths can be achieved by rotating the prism. The changes in energy E_λ for different wavelengths $\lambda$is measured by galvanometer which is connected to bolometer. The distribution of energy in various parts of the spectrum of black body at different temperatures were analyzed. Then the graphs were plotted for E_λ versus λ and the results are summarized as follows.





(i) At any given temperature, initially E_λ increases with λ and attains a maximum value corresponding to a particular wavelength λ_m and then decreases for longer wavelengths.

(ii) The value of E_λ for any λ increases as temperature increases.

(ii) The wavelength corresponding to the maximum energy shifts to a shorter wavelength side as the temperature increases. This confirms Wien's displacement law $\lambda_m T$=constant.

(iv) Total energy emitted per unit area of the source per second at a given temperature is $\rho = \int_0^\infty E_\lambda d\lambda$. Total energy emitted is represented by the total area between the curve for that temperature and the λ-axis. This area is found to be proportional to the fourth power of the absolute temperature. This verifies Stefan's law. $i.e\ E = \sigma T^4$.

According to the Max Planck's, the energy density of radiation emitted (E) by the black body between the wavelengths λ and λ+dλ should be

$$E_{\lambda\rightarrow\lambda+d\lambda} = \frac{8\pi hc}{\lambda^5\left(e^{\frac{hc}{\lambda kT}} - 1\right)} d\lambda$$

To arrive at this equation, Planck assumed that

(i) A black body radiation chamber is filled up not only with radiation, but also with simple harmonic oscillators or resonators and they can vibrate with all possible frequencies.

(ii) The oscillators do not radiate or absorb energy continuously. According to him, the oscillator of frequency ν can only radiate or absorb energy in units or quanta of magnitude hν where, h is a Planck's constant.

(iii) The emission of radiation corresponds to a decrease and absorption to an increase in the energy and amplitude of an oscillator.

Laws for Explaining the Energy Distribution from a Black-Body

Different laws were proposed for explaining the energy distribution with respect to wavelength. They are as follows:

1. Stefan-Boltzmann's Law

According to this law, the radiant energy (E) of a body is directly proportional to the fourth power of the temperature (T) of the body.

$$i.e.\quad E \propto T^4$$

or

$$E = \sigma\, T^4$$

Where σ is Stefan constant and is given by $\sigma = \frac{2\pi^5 {K_B}^4}{15\, h^3 c^2}$

2. Wien's Displacement Law

This law states that the product of the wavelength (λ_m) corresponding to maximum energy and the absolute temperature (T) is a constant.

$$\lambda_m T = constant$$

This law shows that as the temperature increases, the wavelength corresponding to the maximum energy decreases.

Wien also deduced an expression for the energy distribution of a Black body. According to him,

$$E_\lambda = \frac{8\pi hc}{\lambda^5 \left(e^{\frac{hc}{\lambda kT}}\right)}$$

This law holds good only for shorter wavelengths and not for longer wavelengths.

3. Rayleigh-Jean's Law

According to this law, the energy distribution is directly proportional to the absolute temperature and is inversely proportional to the fourth power of the wavelength.

It is governed by the equation

$$E_\lambda = \frac{8\pi kT}{\lambda^4}$$

This law holds good only for longer wavelength regions and not for shorter wavelengths.

It is found that both Wien's Law and Rayleigh-Jeans Law do not agree with the experimental results completely. Hence, Max Planck proposed the following equation based on quantum mechanical hypothesis which can be used to explain the energy distribution of a black body in both longer wavelength regions and shorter wavelength regions.

$$E_\lambda = \frac{8\pi hc}{\lambda^5 \left(e^{\frac{hc}{\lambda kT}} - 1\right)}$$

Derivation of Planck's Law of Radiation (For Reference Only)

Classical Mechanics considered that the energy changes of radiators take place continuously. However, this theory failed to explain the experimental observations of distributions of energy in the spectrum of a black body. Planck suggested quantum theory of radiation as follows

(i) A black body radiation chamber is filled up not only with radiation, but also with simple harmonic oscillators or resonators and they can vibrate with all possible frequencies.

(ii) The oscillators do not radiate or absorb energy continuously. According to him, the oscillator of frequency ν can only radiate or absorb energy in units or quanta of magnitude hν where, h is a Planck's constant. The emission of radiation corresponds to a decrease and absorption to an increase in the energy and amplitude of an oscillator.

Let N be the total number of Planck's oscillators and E be their total energy.

Then, average energy per oscillator $\bar{\varepsilon} = \frac{E}{N}$ ....(1)

Total number of oscillators $N = N_0 + N_0 e^{-\varepsilon/kT} + N_0 e^{-2\varepsilon/kT} + \cdots + N_0 e^{-r\varepsilon/kT}$

Here N_0 = number of oscillators having 0 energy.

$N_0 e^{-\varepsilon/kT}$ = number of oscillators having energy ε.

$N_0 e^{-2\varepsilon/kT}$ = number of oscillators having energy 2ε.

$N_0 e^{-r\varepsilon/kT}$ = number of oscillators having energy rε and so on.

Taking $\frac{\varepsilon}{kT} = x$

then $N = N_0 + N_0 e^{-x} + N_0 e^{-2x} + \cdots + N_0 e^{-rx}$

$\therefore N = \frac{N_0}{(1-e^{-x})}$ ....(2)

Total energy of the Planck's oscillator is

$E = 0 \times N_0 + \varepsilon \times N_0 e^{-x} + 2\varepsilon \times N_0 e^{-2x} + \cdots + r\varepsilon \times N_0 e^{-rx}$ ....(3)

$Ee^{-x} = \varepsilon \times N_0 e^{-2x} + 2\varepsilon \times N_0 e^{-3x} + \cdots + r\varepsilon \times N_0 e^{-(r+1)x}$ ....(4)

Subtracting equation (4) from (3), we get

$E(1 - e^{-x}) = \varepsilon \times N_0 e^{-x} + \varepsilon \times N_0 e^{-2x} + \varepsilon \times N_0 e^{-3x} + \cdots$

$\therefore E(1 - e^{-x}) = \frac{\varepsilon N_0 e^{-x}}{(1-e^{-x})}$

or $E = \frac{\varepsilon N_0 e^{-x}}{(1-e^{-x})^2}$ ....(5)

$\therefore$ The average energy of the oscillator $\bar{\varepsilon} = \frac{E}{N} = \frac{\varepsilon N_0 e^{-x}}{(1-e^{-x})^2} \times \frac{(1-e^{-x})}{N_0}$

$$\bar{\varepsilon} = \frac{\varepsilon}{(e^x - 1)}$$

According to Planck's hypothesis, $\varepsilon = h\nu$, further $\nu = c/\lambda$

$\therefore \varepsilon = \frac{hc}{\lambda}$ and $x = \frac{\varepsilon}{kT} = \frac{hc}{\lambda kT}$

$\therefore \bar{\varepsilon} = \frac{\left(\frac{hc}{\lambda}\right)}{\left(e^{\frac{hc}{\lambda kT}} - 1\right)}$ ....(6)

Number of oscillators per unit volume in the wavelength range λ and $\lambda + d\lambda = 8\pi\lambda^{-4} d\lambda$

Hence the energy density of radiation between the wavelength λ and $\lambda + d\lambda = \bar{\varepsilon} \times$ number of oscillators per unit volume

$$E_{\lambda \to \lambda + d\lambda} = \frac{\left(\frac{hc}{\lambda}\right)}{\left(e^{\frac{hc}{\lambda kT}} - 1\right)} \times 8\pi\lambda^{-4} d\lambda$$

$E_{\lambda \to \lambda + d\lambda} = \frac{8\pi hc\lambda^{-5}}{\left(e^{\frac{hc}{\lambda kT}} - 1\right)} d\lambda$ ....(7)

Equation (7) represents Planck's radiation law in terms of wavelength. This formula satisfies both Wien's and Rayleigh Jean's law. When λ is small, the equation (7) satisfies the Wien's formula, while λ is large, equation (7) satisfies Rayleigh Jean's formula.

Wave Particle Duality

Wave–particle duality is the quantum mechanical concept that every particle or quantum entity may be partly described in terms not only of particles, but also of waves. It expresses the inadequacy of the classical concepts "particle" or "wave" to fully describe the behaviour of quantum-scale objects.

De Broglie's Wave

According to De Broglie, a moving particle has a wave nature associated with it. He proposed that the wavelength λ associated with any moving particle of momentum p (mass m and velocity v) is given by

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

Here, h is a Planck's constant. The waves associated with matter particles are called matter waves or de broglie waves.

De Broglie wave length

De Broglie derived an expression for the wavelength of matter waves that applies to material particles as well as photons. The momentum of a particle of mass m and velocity v is p=mv and its De Broglie wavelength is accordingly,

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

De Broglie wavelength in terms of K.E.

If E_K is the kinetic energy of the material particle, then $p = \sqrt{2mE_k}$

∴ De Broglie wavelength $\lambda = \frac{h}{\sqrt{2mE_k}}$

If a charged particle carrying a charge q and is accelerated through a potential difference V volts, then the kinetic energy $E_k = qV$

∴ The De Broglie wavelength for a charged particle can be written as $\lambda = \frac{h}{\sqrt{2mqV}}$

In the case of thermal neutrons, their kinetic energy $E_k = KT$

Where K is the Boltzmann's constant

and T is the temperature at which the neutrons are enclosed in the chamber.

∴ The De Broglie wavelength of a material particle at temperature T is $\lambda = \frac{h}{\sqrt{2mE_k}} = \frac{h}{\sqrt{2mKT}}$

Properties of Matter waves or De Broglie waves

- Matter waves are neither electromagnetic nor sound waves as they are independent of charge and pressure. Matter waves are a new kind of waves and are produced by motion of the particles.
- De Broglie waves do not require a physical medium for propagation, as they are a fundamental quantum property of particles themselves. They can propagate in a vacuum or

any other medium, but the characteristics of the wave may change depending on the medium and interactions with it.

- For the smaller velocity of the particle, the wavelength associated with the matter wave is longer. Thus, De Broglie waves cannot be harmonic waves.
- For lighter particles, the wavelength associated with matter waves is longer.
- The velocity of the matter waves depends on the velocity of the material particle and it is not a constant.
- The group velocity of matter waves is equal to the velocity of the particle, and its phase velocity is greater than the group velocity (De Broglie hypothesis).
- Matter waves exhibit diffraction phenomenon as any other waves.

Group Velocity (υ_g) (For Reference Only)

The velocity with which the wave packet propagates is called the group velocity.

$$\upsilon_g = \frac{dE}{dP} = \frac{d\left(\frac{P^2}{2m}\right)}{dP} = \frac{P}{m} = \upsilon$$

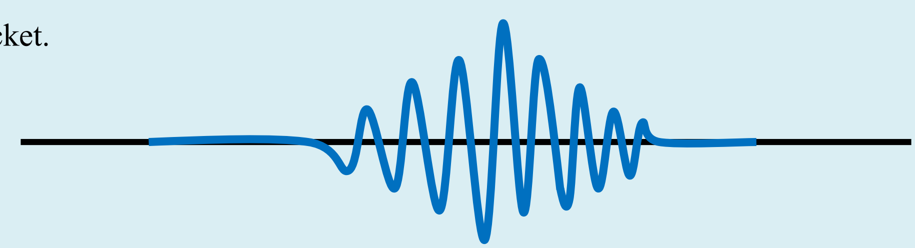
Phase velocity (υ_p)

The velocity with which the plane of equal phase travels through a medium is known as the phase velocity. It thus represents the velocity of propagation of the wavefront.

$$\upsilon_P = \frac{\omega}{k} = \frac{E}{P} = \frac{mc^2}{m\upsilon} = \frac{c^2}{\upsilon}$$

Wave packet

- Wave packet consists of a group of harmonic waves. Each wave has a slightly different wavelength. The superimposition of a very large number of such harmonics of slightly different wavelengths produces a single wave packet.
- The waves interfere constructively over a small region of space and cancel each other everywhere except in that small region as shown in the Figure.
- The position of the particle is then approximately determined by the position of the wave packet.



Wavefunction

- We know that the light and sound waves are characterized by certain quantities that vary with position and time.
- We cannot use the same way for characterizing the De Broglie waves.
- Since the microparticles exhibit wave properties, the wave function Ψ has been introduced.
- Ψ describes the wave as a function of position and time i.e Ψ(x,t). However, Ψ is not an observable quantity and has no physical significance.
- Hence, the square of the magnitude of wavefunction $|\psi|^2$ evaluated in a particular region is used instead of Ψ. $|\psi|^2$ represents the probability of finding the particle in that region will give rise to the probability of finding a particle in a given space.

Suppose, if P is the probability of finding the particle in an infinitesimal volume dV (=*dx,dy,dz*) at a time t, then we may write,

$$P \propto |\psi(x,y,z,t)|^2 \, dV$$

$|\psi(x,y,z,t)|^2$ is called the probability density and $\psi(x,y,z,t)$ is the probability amplitude.

Since the particle is certainly somewhere in the space, the maximum probability of finding the particle in space is always 1.

$$P = \int_{-\infty}^{+\infty} |\psi|^2 \, dV = 1$$

or

$$P = \int_{-\infty}^{+\infty} \psi\psi^* \, dV = 1$$

Where ψ^* is the complex conjugate of ψ

Suppose in such cases if $\int_{-\infty}^{+\infty} \psi\psi^* \, dV \neq 1$, the wave function ψ cannot be a solution.

In such cases, we need a certain multiplicative factor (A) in order to satisfy the relation. Hence, we introduce $A\psi$ instead of Ψ.

Therefore, the above equation becomes $P = A^2 \int_{-\infty}^{+\infty} \psi\psi^* \, dV = 1$

Well-Behaved wavefunctions

- An acceptable wavefunction must be normalized
- The wavefunction $\psi(x,y,z,t)$ must be finite everywhere.
  Even if $x \to \infty$ or $-\infty$, $y \to \infty$ or $-\infty$, $z \to \infty$ or $-\infty$, $\psi(x,y,z,t)$ should not be infinite.
- If $\psi(x,y,z,t)$ is infinite, then this would violate uncertainty principle.

- $\psi(x, y, z, t)$ must be a single-valued function.
- $\psi(x, y, z, t)$ must be a continuous one. Also, the space derivatives of $\psi(x, y, z, t)$ should be continuous across the boundary.

  The wave function satisfying the above conditions are known as well-behaved wave functions.

Heisenberg's Uncertainty Principle

It is impossible to determine precisely and simultaneously the values of two physical quantities which describes the motion of an atomic system. Such pairs of variables are called "Canonically Conjugate Variables".

Example 1: According to this principle, the position and momentum of a particle cannot be determined simultaneously to any desired degree of accuracy.

Taking Δx as the error or uncertainty in determining its position and Δp the error or uncertainty in determining the momentum of a particle at the same instant.

then $\Delta P . \Delta x \geq \frac{\hbar}{2}$

The product of these two quantities is approximately of the order of Planck's constant h.

If Δx is small, ΔP will be large and vice versa. If one quantity is measured accurately, the other quantity becomes less accurate.

Example 2: Similar to position and momentum, the energy of a particle and time cannot be determined simultaneously and precisely.

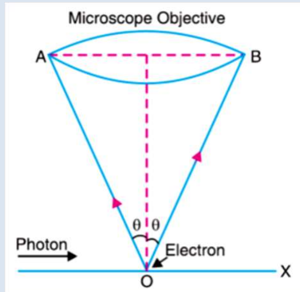
$$\Delta E . \Delta t \geq \frac{\hbar}{2}$$

Where ΔE is the error or uncertainty in determining its energy and Δt the error or uncertainty in determining the time.

Verification of Heisenberg's Uncertainty Principle (For Reference Only)

(i) Determination of Position and momentum of an electron using γ-ray microscope

Let us consider measuring the position and linear momentum of an electron which is disturbed by the photons incident on it. The position and momentum of an electron are measured with the help of very high resolving power electron microscope. The incoming photons will interact with the electron through Compton effect. To be able to see this electron in the microscope, at least one scattered photon must enter into the lens and the scattered photon should enter the microscope within the angle 2θ.



Uncertainty in position measurement

Let Δx be the distance between two points which can be just resolved by the microscope. Therefore, the resolving power of the microscope can be written as

$$\Delta x = \frac{\lambda}{2sin\theta} \qquad \text{.......................(1)}$$

This is the range in which the electron would be visible when disturbed by the photon. Hence, Δx is the error or uncertainty in the position measurement of the electron.

Uncertainty in momentum measurement

According to de Broglie, the momentum imparted by the photon to the electron during the impact is of the order of $\frac{h}{\lambda}$

The component of momentum along $OA = -\frac{h}{\lambda}\, sin\theta$

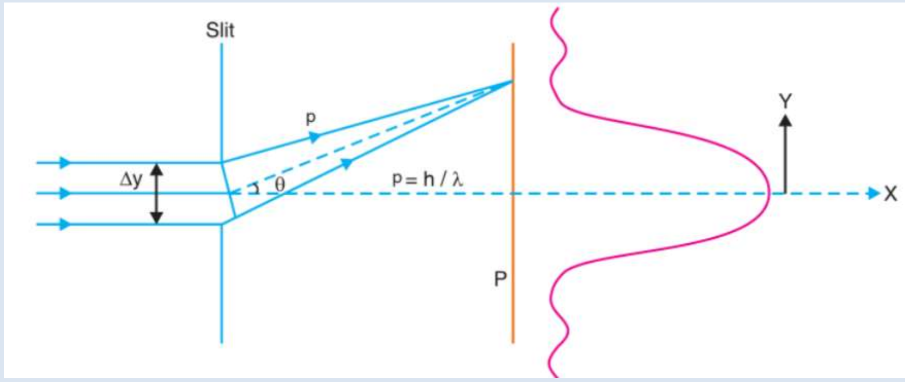
The component of momentum along $OB = \frac{h}{\lambda}\, sin\theta$

The uncertainty in momentum measurement along x-direction is

$$\Delta P_x = \frac{h}{\lambda}\, sin\theta - \left(-\frac{h}{\lambda}\, sin\theta\right) = \frac{2h}{\lambda}\, sin\theta$$

$$\therefore \Delta x . \Delta P_x = \frac{\lambda}{2sin\theta} \times \frac{2h}{\lambda}\, sin\theta = h$$

(ii) Diffraction of a beam electrons by a slit.



In this experiment a beam of electrons is transmitted through a slit of width Δy and received on a photographic plate P kept at some distance from the slit.

Uncertainty in position measurement

Since a beam of electron crosses the slit, we cannot specify its location in the slit. Hence the position of any electron recorded on the photographic plate is uncertain by an amount equal to the width of the slit Δy.

λ is the wavelength of the electrons and θis the angle of deviation corresponding to the first minimum. From the theory of diffraction, we may write

$$\Delta y = \frac{\lambda}{sin\theta} \qquad \text{.......................(1)}$$

This is the error or uncertainty in the position measurement of the electron along y-axis.

Uncertainty in momentum measurement

As the electrons deviated through an angle -θ to +θfrom the initial path by the slit, the y-component of the momentum of an electron may vary between -psinθ to +psinθ.

Therefore, the uncertainty in the y-component of momentum of the electron

$$\Delta P_y = 2p\, sin\theta = \frac{2h}{\lambda} sin\theta$$

$$\therefore \Delta y . \Delta P_y = \frac{\lambda}{sin\theta} \times \frac{2h}{\lambda}\, sin\theta = 2h$$

A more sophisticated approach would show that $\Delta x . \Delta P_x \geq \hbar/2$

Schrodinger's time-dependent form of wave equation

Schrodinger derived a general expression for describing the state of a dynamical particle of mass *m* and momentum *p* with quantum mechanical concepts. If the speed of a particle is small compared to that of light, its total energy is the sum of kinetic energy and potential energy. According to quantum mechanics, the total energy of a freely moving particle can be written as,

$$E\psi = K.E + P.E = \frac{p^2}{2m}\psi + V\psi \qquad \text{.............(1)}$$

Here the quantity ψ is called wave function that characterizes the de Broglie waves. Let us assume that ψ for a particle moving freely in the +*x* direction is specified by

$$\psi = Ae^{-i\omega\left(t-\frac{x}{v}\right)} \qquad \text{...............(2)}$$

Replacing ω in the above equation by $2\pi\nu$ and $v = \nu\lambda$, then

$$\psi = Ae^{-2\pi i\left(\nu t-\frac{x}{\lambda}\right)}$$

From the energy of the photon $E = h\nu$ and de Broglie wave length $\lambda = {h}/{p}$, the above equation can be written as

$$\psi = Ae^{-\frac{2\pi i}{h}(Et-px)} \qquad \text{...............(3)}$$

or

$\psi = Ae^{-\frac{i}{\hbar}(Et-px)}$ since $\hbar = \frac{h}{2\pi}$

This equation (3) describes the wave equivalent of a free particle of total energy E and momentum *p* moving in the +*x* direction.

Now differentiating equation (3) twice with respect to *x*, we get

$$\frac{\partial^2\psi}{\partial x^2} = -\frac{p^2}{\hbar^2}\psi$$

$$p^2\psi = -\hbar^2\frac{\partial^2\psi}{\partial x^2} \qquad \text{...............(4)}$$

Now, differentiating equation (3) with respect to t once, we get

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

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

or

$$E\psi = i\hbar\frac{\partial\psi}{\partial t} \qquad \text{...............(5)}$$

Substituting equation (4) and (5) in equation (1), we get,

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi \qquad \text{...............(6)}$$

The equation (6) is the time-dependent form of Schrodinger's equation in one dimension.

In three dimensions, the time-dependent form of Schrodinger's equation is

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + V\psi \qquad \text{...............(7)}$$

Where the particle's potential energy is a function of x, y, z and t.

Schrodinger's time-independent form of wave equation: Steady state form

Schrodinger derived a general expression for describing the state of a dynamical particle of mass m and momentum p with quantum mechanical concepts. If the speed of a particle is small compared to that of light, its total energy is the sum of kinetic energy and potential energy. According to quantum mechanics, the total energy of a freely moving particle can be written as,

$$E\psi = K.E + P.E = \frac{P^2}{2m}\psi + V\psi \qquad \text{.............(1)}$$

Here the quantity ψ is called wave function that characterizes the de Broglie waves. Let us assume that ψ for a particle moving freely in the +$x$direction is specified by

$$\psi = Ae^{-i\omega\left(t - \frac{x}{v}\right)} \qquad \text{...............(2)}$$

Replacing ω in the above equation by $2\pi\nu$ and $\upsilon = \nu\lambda$, and further, from the energy of the photon $E = h\nu$ and de Broglie wave length $\lambda = {h}/{p}$, the above equation can be written as

$$\psi = Ae^{-\frac{2\pi}{h}(\mathrm{E}t - px)} \qquad \text{...............(3)}$$

or

$\psi = Ae^{-\frac{i}{\hbar}(\mathrm{E}t - px)}$ since $\hbar = \frac{h}{2\pi}$

This equation (3) describes the wave equivalent of a free particle of total energy E and momentum p moving in the +x direction.

After differentiating the wave function ψ with respect to x and t, Schrodinger obtained time-dependent form of wave function as follows,

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi \qquad \text{............. (4)}$$

But in many situations, the potential energy of a particle does not depend on time explicitly. Hence potential energy V vary with position of the particle only. When this is true, the Schrodinger's equation may be simplified by removing all reference to t.

For deriving the time-independent form, the wave function in equ (3) is modified as,

$$\psi = Ae^{-\frac{i}{\hbar}(\mathrm{E}t-px)} = Ae^{\frac{i}{\hbar}px}.e^{-\frac{i}{\hbar}\mathrm{E}t} = \psi_0 e^{-\frac{i}{\hbar}\mathrm{E}t} \qquad \text{.............. (5)}$$

Now, differentiating the equation (5) with respect to *t,* we get

$$\frac{\partial\psi}{\partial t} = -\frac{i}{\hbar}\mathrm{E}\psi_0 e^{-\frac{i}{\hbar}\mathrm{E}t} \qquad \text{.............. (6)}$$

Now, differentiating the equation (5) twice with respect to *x,* we get

$$\frac{\partial^2\psi}{\partial x^2} = \frac{\partial^2\psi_0}{\partial x^2}e^{-\frac{i}{\hbar}\mathrm{E}t} \qquad \text{.............. (7)}$$

Substituting equations (5)- (7) in equation (4), we have,

$$i\hbar\left(-\frac{i}{\hbar}\mathrm{E}\psi_0\, e^{-\frac{i}{\hbar}\mathrm{E}t}\right) = \frac{-\hbar^2}{2m}\left(\frac{\partial^2\psi_0}{\partial x^2}\right)e^{-\frac{i}{\hbar}\mathrm{E}t} + V\psi_0 e^{-\frac{i}{\hbar}\mathrm{E}t}$$

$$\mathrm{E}\psi_0 = \frac{-\hbar^2}{2m}\left(\frac{\partial^2\psi_0}{\partial x^2}\right) + V\psi_0$$

$$\left(\frac{\partial^2\psi_0}{\partial x^2}\right) + \frac{2m}{\hbar^2}(\mathrm{E}-\mathrm{V})\psi_0 = 0 \qquad \text{.............. (8)}$$

The equation (8) is the time-independent or steady state form of the Schrodinger's wave equation in one dimension.

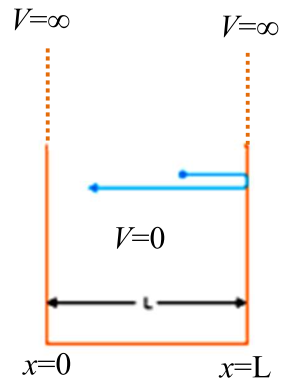
Steady state form of the Schrodinger's in three dimensions is,

$$\left(\frac{\partial^2\psi_0}{\partial x^2} + \frac{\partial^2\psi_0}{\partial y^2} + \frac{\partial^2\psi_0}{\partial z^2}\right) + \frac{2m}{\hbar^2}(\mathrm{E}-\mathrm{V})\psi_0 = 0 \qquad \text{.............. (9)}$$

The particle in a box: Infinite Square well potential

The simplest quantum mechanical problem is that of a particle trapped in a box with infinitely hard walls. Consider a particle is moving inside a box along the x-direction. Since the height of the walls at x=0 and x=L is infinite, no particle can escape from the box. Hence, the particle bounces back and forth between the walls of the box. The particle has a mass m and its position x at any instant is given by $0 < x < \mathrm{L}$.

The potential energy V of the particle is infinite on both sides of the box, and it can be assumed to be zero between x=0 and x=L. The particle cannot exist outside the box and so its wave function ψ outside the box is 0 for $x \leq 0$ and $x \geq \mathrm{L}$. Hence, we need to find the particle's wave function inside the box using Schrodinger's equation by employing the boundary conditions.



The time-independent Schrodinger's equation is

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0 \qquad \text{................(1)}$$

Inside the box, V=0, then the above equation becomes,

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}E\psi = 0$$

The general solution of this equation is

$$\psi = Asin\frac{\sqrt{2mE}}{\hbar}x + Bcos\frac{\sqrt{2mE}}{\hbar}x \qquad \text{..............(2)}$$

Here A and B are the constants. The boundary conditions can be used to evaluate these constants

At $x = 0, \psi = 0$, Hence B=0

At $x = \mathrm{L}, \psi = 0,$

$$Asin\frac{\sqrt{2mE}}{\hbar}L = 0 \qquad \text{..............(3)}$$

In this case ψ will be zero only when the quantity $\frac{\sqrt{2mE}}{\hbar}L = n\pi$, where n=1,2,3 .....

This result comes about because the sines of the angles $\pi, 2\pi, 3\pi$ ... . are all zero

It is clear from equation (3) that the energy of a particle can have only certain values, which are the Eigen values. These Eigen values can be found by the formula

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \qquad \text{n=1,2,3 .....} \qquad \text{..............(4)}$$

The wave functions of a particle in a box of whose energies E_n are,

$$\psi_n = A\ sin\frac{\sqrt{2mE_n}}{\hbar}x \qquad \text{..............(5)}$$

Substituting equation (4) in equation (5) we get,

$$\psi_n = A\sin\frac{n\pi x}{L} \qquad \text{.............(6)}$$

The probability of finding the particle inside the box can be found by taking the normalized wave function,

$$\int_0^L \psi * \psi \, dx = \int_0^L |\psi_n|^2 \, dx = A^2 \int_0^L sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

or

$$A^2 \int_0^L \left(\frac{1 - cos2\left(\frac{n\pi x}{L}\right)}{2}\right) dx = 1$$

$$\frac{A^2}{2}\int_0^L dx - \frac{A^2}{2}\int_0^L cos2\left(\frac{n\pi x}{L}\right) dx = 1$$

$$\frac{A^2}{2}\left[x - \frac{sin2\left(\frac{n\pi x}{L}\right)}{2}\right]_0^L = 1$$

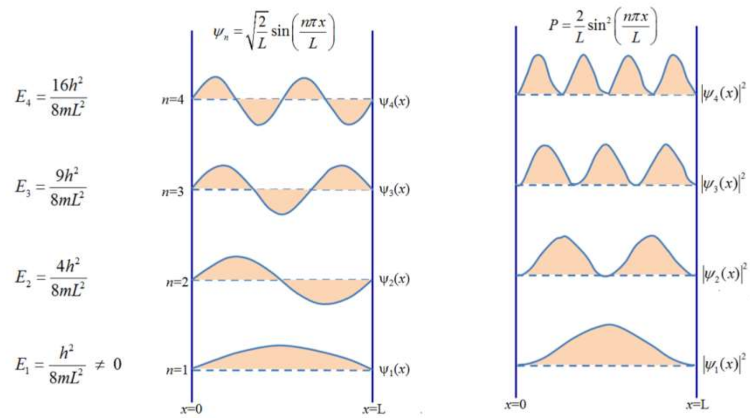
$$\frac{A^2}{2}L = 1$$

$$\therefore \qquad A = \sqrt{\frac{2}{L}}$$

$\therefore$ The normalized wavefunctions of the particles

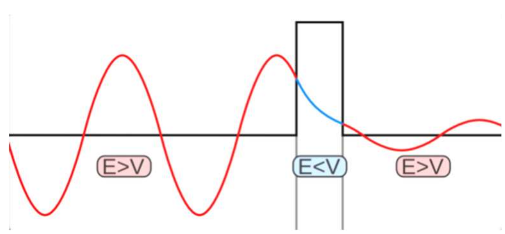
$$\psi_n = \sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L} \qquad \text{.............(7)}$$

The normalized wavefunctions of the particles are plotted in the Figure.



Quantum Tunneling effect

The quantum tunneling effect is a quantum phenomenon that describes the particles moving through a potential barrier even when their kinetic energy is less than the potential energy of the barrier. In classical mechanics, when a particle has insufficient energy, it would not be able to overcome a potential barrier. In the quantum world, however, particles can often behave like waves. On encountering a barrier, a quantum wave will not end abruptly; rather, its amplitude will decrease exponentially. If the barrier is thin enough, then the amplitude may be non-zero on the other side. This would imply that there is a finite probability that some of the particles will tunnel through the barrier.

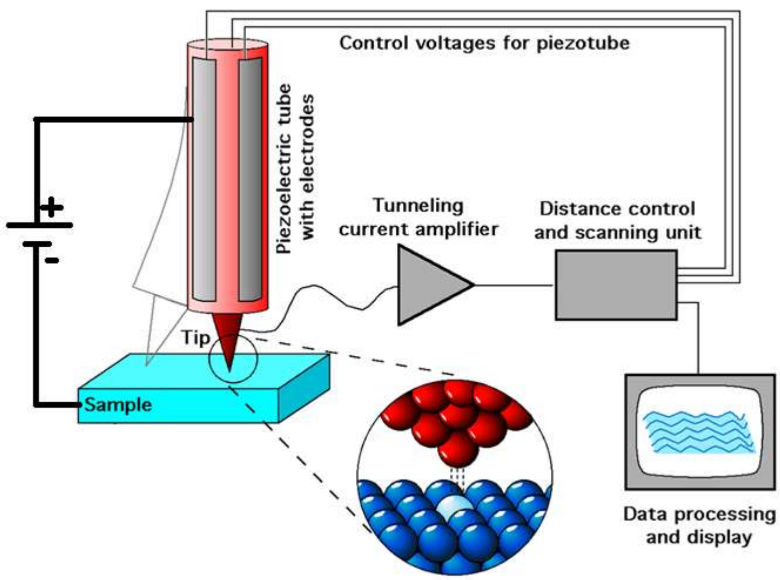


Tunneling current

The tunneling current is defined as the ratio of the current density emerging from the other side barrier divided by the current density incident on the barrier. If this transmission coefficient across the barrier is a non-zero value, then there is a finite likelihood of a particle tunneling through the barrier.

Scanning tunneling Microscope

A Scanning Tunneling Microscope (STM) is based on the concept of quantum tunneling. it is used to study the surfaces (position of atoms and electron density distribution) on an atomic scale size. It consists of a very sharp conducting probe (metal tip) and is brought very near to the surface to be examined. When a bias or voltage difference is applied between the tip and the metal surface, electrons can tunnel across the gap between them if the gap is small enough. As the gap gets wider or narrower, the tunneling current gets smaller or larger, respectively. The resulting tunneling current is a function of tip position, applied voltage, and the local density of states (LDOS) of the sample.



This technique usually employs two modes of measurements such as constant height and constant current.

In constant current mode, the current control system adjusts the height of the tip by supplying a voltage to the piezoelectric height control mechanism. This leads to a height variation, and thus, the image comes from the tip topography across the sample, giving a constant charge density surface. Hence, the atomic position can be measured in this mode.

In constant height mode, the voltage and height are both held constant while the current changes to keep the voltage from changing. This leads to an image made of current changes over the surface. Hence the electron density of the atoms can be measured in the mode.

Low-Dimensional Quantum structures

When one or more of the dimensions of a bulk material are reduced sufficiently, novel electrical, mechanical, chemical, magnetic, and optical properties can be introduced. The resulting structure is then called a low-dimensional structure (or system). The confinement of particles, usually electrons or holes, to a low - dimensional structure leads to a dramatic change in their behaviour and to the manifestation of size effects that usually fall into the category of quantum-size effects.

The low dimensional materials exhibit new physicochemical properties not shown by the corresponding large-scale structures of the same composition. Nanostructures constitute a bridge between molecules and bulk materials. Suitable control of the properties and responses of nanostructures can lead to new devices and technologies.

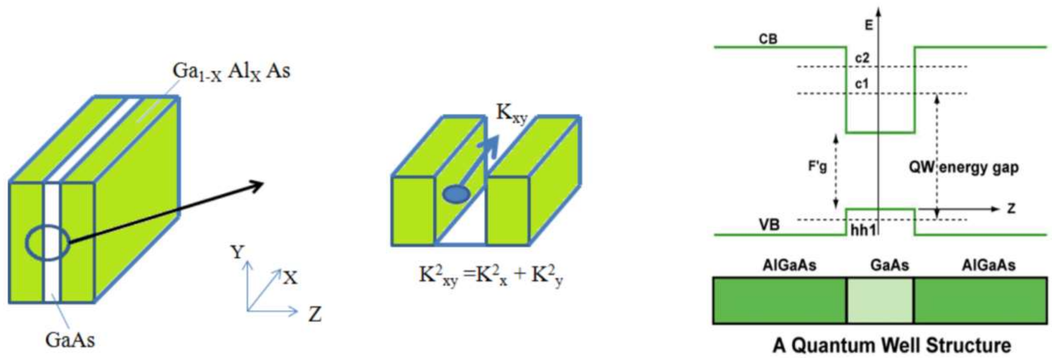
Classification of Low-dimensional Materials

Low-dimensional structures are usually classified according to the number of reduced dimensions they have. More precisely, the dimensionality refers to the number of degrees of freedom in the particle momentum. Accordingly, depending on the dimensionality, the following classification is made:

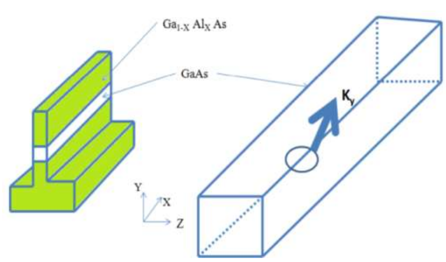
Three-dimensional (3D) structure or bulk structure: No quantization of the particle motion occurs, i.e., the particle is free. Electron in conduction band and holes in valence band are free to move in all three dimensions of space. The size of the particle varies from mm to few cms.

Two-dimensional (2D) structure: Quantization of the particle motion occurs in one direction, while the particle is free to move in the other two directions. Examples: Thin films and quantum wells. The thickness of the 2D structures typically varies from 1 - 1000 nm. Quantum wells are formed in semiconductors by having a material, like gallium arsenide sandwiched between two layers of material with wider band gap like aluminium arsenide using molecular beam epitaxy or chemical vapor deposition techniques.

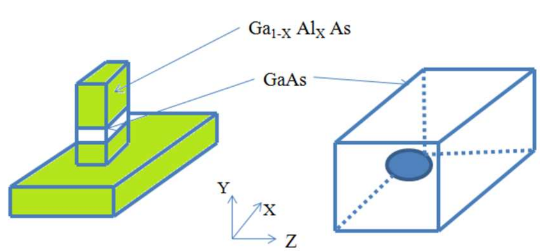
Quantum wells are used to make high electron mobility transistors which are used in low-noise electronics (Hetero structure FET). Quantum well infrared photo detectors are also based on quantum wells, and are used for infrared imaging.



One-dimensional (1D) structure: Quantization occurs in two directions, leading to free movement along only one direction. Examples: Quantum wires, nanowires, nanorods, nanotubes and nanopillars etc. The size (radius) of the nanowire typically varies from 1-100 nm. The most important application of nanowires in nanoelectronics is using them as junctions or as multi-segment nanowires or crossed nanodevices. It is used in energy storage devices.



Zero-dimensional (0D) structure: Quantization occurs in all three directions. Hence, the number of degrees of freedom for the movement of holes and electrons in a quantum dot is zero. Examples: Quantum Dots and nanodots. The size of the quantum dot typically varies from 1-10 nm. Quantum dots are found in commercial applications including bioimaging, solar cells, LEDs, diode lasers, and transistors.



Unit - I (Quantum Mechanics) problems

Problems related to Photoelectric effect

1) In a photoelectric effect experiment, a UV light of wavelength 320 nm falls on a photosensitive plate. If the work function of the metal is 2.1 eV, find its stopping potential (Vs)?

Given data:

Wavelength of the incident light λ= 320 nm or 320 x 10^{-9} m

Work function of the metal $\phi = h\upsilon_0$= 2.1 eV

Solution:

From the Einstein's photoelectric equation, we may write

$$eV_s = h\vartheta - h\vartheta_0 = \frac{hc}{\lambda} - \frac{hc}{\lambda_0}$$

$$eV_s = \frac{6.626 \times 10^{-3} \ J.s \times 3 \times 10^8 \ m/s}{320 \times 10^{-9} \ m} - 2.1 \ eV$$

$$eV_s = 6.2119 \times 10^{-19} J - 2.1 \ eV$$

$$eV_s = \frac{6.2119 \times 10^{-19}}{1.602 \times 10^{-19}} \ eV - 2.1 \ eV$$

$$eV_s = 3.8775 \ eV - 2.1 \ eV = 1.778 \ eV$$

Therefore, the stopping potential $\boxed{V_s == 1.778 \ V}$

----

2) Suppose if it takes 208.4 kJ of energy to remove one mole of electrons from the atoms on the surface of rubidium metal when illuminated by a light of wavelength 254 nm. What is the maximum kinetic energy of the ejected electrons?

Given data:

Wavelength of the incident light λ= 254 nm or 254 x 10^{-9} m

Work function of the metal $\phi = h\upsilon_0$= 208.4 kJ/mole

Solution:

From the Einstein's photoelectric equation, we may write

$$\frac{1}{2}mv_{max}^2 = h\vartheta - h\vartheta_0 = \frac{hc}{\lambda} - \frac{hc}{\lambda_0}$$

$$\frac{1}{2}mv_{max}^2 = \frac{6.626 \times 10^{-34} \times 3 \times 10^8}{254 \times 10^{-9}} - \frac{208.4 \times 10^3}{6.023 \times 10^{23}}$$

$$\frac{1}{2}mv_{max}^2 = 7.8260 \times 10^{-19}J - 3.4601 \times 10^{-19}J$$

$$\frac{1}{2}mv_{max}^2(Joule) = 4.3659 \times 10^{-19}J$$

$$\frac{1}{2}mv_{max}^2(eV) = \frac{4.3659 \times 10^{-19}}{1.602 \times 10^{-19}} \ eV$$

$$\frac{1}{2}mv_{max}^2(eV) = 2.7253 \ eV$$

Therefore the maximum kinetic energy of the ejected electron would be

$\boxed{4.3659 \times 10^{-19}J \text{ or } 2.7253 \ eV}$

----

3) The work function of metal is 1 eV. The light of wavelength 3000 Å is incident on this metal surface. The velocity of emitted photoelectrons will be…..

Given data:

Wavelength of the incident light λ= 3000 Å or 3000 x 10^{-10} m

Work function of the metal ϕ = 1 eV

Solution:

From the Einstein's photoelectric equation, we may write

$$\frac{1}{2}mv_{max}^2 = h\vartheta - h\vartheta_0 = \frac{hc}{\lambda} - \frac{hc}{\lambda_0}$$

$$\frac{1}{2}mv_{max}^2 = \frac{6.626 \times 10^{-34} \times 3 \times 10^8}{3000 \times 10^{-10} \ m} - 1 \times 1.602 \times 10^{-19}$$

$$\frac{1}{2}mv_{max}^2 = 6.626 \times 10^{-19}J - 1.602 \times 10^{-19}$$

$$\frac{1}{2}mv_{max}^2 = 5.024 \times 10^{-19}\,J$$

$$v_{max}^2 = \frac{2 \times 5.024 \times 10^{-19}\,J}{m} = \frac{10.048 \times 10^{-19}\,J}{9.11 \times 10^{-31}}$$

$$v_{max}^2 = 1.1030 \times 10^{12}$$

Therefore, the maximum velocity of the ejected electron is

$$\boxed{v_{max} = 1.0502 \times 10^{6}\,m/s}$$

---

4) The photoelectric work function for a metal surface is 4.125 eV. The cut-off or threshold wavelength of the metal surface will be ……

Given data:

Work function of the metal $\phi = 4.125$ eV

Solution:

we know that the work function of the metal surface,

$$\varphi = h\vartheta_0 = \frac{hc}{\lambda_0}$$

From this

$$\lambda_0 = \frac{hc}{\varphi} = \frac{6.626 \times 10^{-34} \times 3 \times 10^{8}}{4.125 \times 1.602 \times 10^{-19}}$$

$$\lambda_0 = 3.0081 \times 10^{-7}\,m$$

or

The cut-off wavelength of the metal surface would be

$$\boxed{\lambda_0 = 3008 \times 10^{-10}\,m \;\; or\; 3008\ \text{Å}}$$

Problems related to De-Broglie wavelength

1) Find the K.E of the neutron in units of electron volt whose De-broglie wavelength is 1Å. Given that mass of the neutron = $\mathbf{1.674 \times 10^{-27}}$kg. Planck's constant = $\mathbf{6.626 \times 10^{-34}}$J. S

Given data:

Wavelength of the neutron = 1Å = 1×10^{-10}m

Mass of the neutron = 1.674×10^{-27}kg

Planck's constant = 6.626×10^{-3} J. S

Solution:

We know that De-Broglie wavelength in terms of K.E

$$\lambda = \frac{h}{\sqrt{2mE_k}}$$

From this equation, K.E of the neutron can be written as

$$E_k = \frac{h^2}{2m\lambda^2}$$

$$E_{k(Joule)} = \frac{(6.626 \times 10^{-34})^2}{2 \times 1.674 \times 10^{-27} \times (1 \times 10^{-10})^2}$$

$$E_{k(Joule)} = \frac{4.3904 \times 10^{-67}}{3.348 \times 10^{-47}}$$

$$\boxed{E_{k(Joule)} = 1.3114 \times 10^{-20} \text{ J}}$$

$$E_{k(electronVolt)} = \frac{1.3114 \times 10^{-20}}{1.602 \times 10^{-19}}$$

$$\boxed{E_{k(electronVolt)} = 0.0819 \text{ eV}}$$

----

2) Calculate the momentum, energy and mass of a photon of wavelength 10 Å.

Given data:

Wavelength of the Photon = 10 Å = 10 $\times 10^{-10}$m

Solution:

i) According to De-Broglie, the momentum of the photon can be written as

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

$$P = \frac{6.626 \times 10^{-3}}{10 \times 10^{-10}}$$

$$\boxed{P = 6.626 \times 10^{-2} \quad kg\ ms^{-1}}$$

ii) According to De-Broglie, the energy of the photon can be written as

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

$$E_{(Joules)} = \frac{6.626 \times 10^{-34} \times 3 \times 10^{8}}{10 \times 10^{-10}}$$

$$E_{(Joules)} = \frac{1.9878 \ \times 10^{-25}}{10 \times 10^{-1}}$$

$$\boxed{E_{(Joules)} = 1.9878 \ \times 10^{-16}\,\mathrm{J}}$$

$$E_{(electronVolts)} = \frac{1.9878 \ \times 10^{-16}}{1.6 \ \times 10^{-19}}$$

$$\boxed{E_{(electronVolts)} = 1.242 \ \times 10^{3}\mathrm{eV} = 1.242\ \mathrm{keV}}$$

iii) According to De-Broglie, the mass of the photon can be written as

$$m = \frac{h}{\lambda C} = \frac{6.626 \times 10^{-34}}{10 \times 10^{-10} \times 3 \times 10^{8}}$$

$$\boxed{m = 2.2086 \times 10^{-33}\,\text{kg}}$$

---

3) Calculate the De-Broglie wavelength for a beam of electrons whose energy is 45 eV.

Given data:

Energy of a beam of electrons = 45 eV

Solution:

The De-Broglie wavelength of electron is given by

$$\lambda = \frac{h}{\sqrt{2mE_k}}$$

$$\lambda = \frac{6.626 \times 10^{-3}}{\sqrt{2 \times 9.11 \times 10^{-31} \times (45 \times 1.6 \times 10^{-19})}}$$

$$\lambda = \frac{6.626 \times 10^{-34}}{3.6219 \times 10^{-24}}$$

$$\boxed{\lambda = 1.8294 \times 10^{-10} m = 1.8294\ \text{Å}}$$

---

4) Calculate the wavelength associated with an electron subjected to a potential difference of 1.25 kV.

Given data:

Energy of a beam of electrons = 45 eV

Solution:

We know that De-Broglie wavelength in terms of potential difference is

$$\lambda = \frac{h}{\sqrt{2meV}}$$

$$\lambda = \frac{6.626 \times 10^{-34}}{\sqrt{2 \times 9.11 \times 10^{-3} \times 1.602 \times 10^{-19} \times 1.25 \times 10^{3}}}$$

$$\lambda = \frac{6.626 \times 10^{-34}}{1.1901 \times 10^{-2}}$$

$$\boxed{\lambda = 0.3469 \times 10^{-10}\, m \text{ (or) } 0.3469 \text{ Å}}$$

---

5) An electron and photon have same wavelength. If P is the momentum of electron and E is the energy of photon, then calculate P/E in S.I units.

Solution:

From the De-Broglie wave-particle duality, the momentum of the electron and energy of the photon can be written as

Momentum of the electron

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

Energy of the photon

$$E = \frac{hC}{\lambda}$$

The ratio of ${}^{P}/_{E}$ would be

$$^{P}/_{E} = \frac{\left(\frac{h}{\lambda}\right)}{\left(\frac{hC}{\lambda}\right)} = \frac{1}{C}$$

$$^{P}/_{E} = \frac{1}{3 \times 10^{8}}$$

$$\boxed{^{P}/_{E} = 3.33 \times 10^{-9} \mathrm{s/m}}$$

Problems related to Heisenberg's Uncertainty principle

1) Uncertainty in time of an excited atoms is about 10^{-8}s. What are the uncertainties in energy and in frequency of radiation.

Given data:

Uncertainty in time $\Delta t = 10^{-8} s$

Solution:

According to Heisenberg's Uncertainty principle

$$\Delta E \, . \Delta t \approx \frac{h}{4\pi}$$

$$\Delta E \approx \frac{h}{4\pi \, \Delta t}$$

$$\Delta E \approx \frac{6.626 \times 10^{-3}}{4 \times 3.14 \times 10^{-8}}$$

Therefore, the uncertainty in energy,

$$\boxed{\Delta E \approx 0.5275 \times 10^{-26} J}$$

The uncertainty in frequency of radiation can be determined by,

$$\Delta \vartheta \approx \frac{\Delta E}{h} = \frac{0.5275 \times 10^{-26} J}{6.626 \times 10^{-3} \; J.s}$$

$$\Delta\vartheta \approx 0.0796 \times 10^{8} s^{-1}\ or\ Hz$$

$$\boxed{\Delta\vartheta \approx 7.96 \times 10^{6}\ Hz\ or\ 7.96\ MHz}$$

---

2) An electron is confined to a potential well of width 10 nm. Calculate the minimum uncertainty in its velocity.

Given data:

Uncertainty in finding the position of an electron $\Delta x = 10\ nm$

Solution:

According to Heisenberg's Uncertainty principle

$$\Delta P\ .\ \Delta x \approx \frac{h}{4\pi}$$

$Since\ \Delta P = m\Delta v$

$$m\Delta v.\Delta x \approx \frac{h}{4\pi}$$

$$\Delta v \approx \frac{h}{4\pi\ m\ \Delta x}$$

$$\Delta v \approx \frac{6.626 \times 10^{-3}}{4 \times 3.14 \times 9.11 \times 10^{-31} \times 10 \times 10^{-9}}$$

Therefore, the uncertainty in finding its velocity

$$\Delta v \approx 5790.9\ m/s$$

or

$$\boxed{\Delta v \approx 5.7909\ km/s}$$

---

3) An electron has a speed of 800 m/s with an accuracy of 0.004 %. Calculate the uncertainty in finding its position.

Given data:

Speed of the electron $v = 800\ m/s$

The uncertainty in velocity of the electron can be determined as follows,

$$\Delta v \approx v \times 0.004\%$$

$$\Delta v \approx 800 \times \frac{0.004}{100}$$

$$\Delta v \approx 0.032\ m/s$$

Solution:

According to Heisenberg's Uncertainty principle,

$$\Delta x \approx \frac{h}{4\pi\ m\ \Delta v}$$

$$\Delta x \approx \frac{6.626\ \times 10^{-34}}{4 \times 3.14 \times 9.11 \times 10^{-31} \times 0.032}$$

$$\Delta x \approx \frac{6.626\ \times 10^{-34}}{4 \times 3.14 \times 9.11 \times 10^{-31} \times 0.032}$$

Therefore, the uncertainty in finding the position of an electron is

$$\boxed{\Delta x \approx 1.8096\ \times 10^{-3} m}$$

---

4) Find the uncertainty in the position of electrons moving with the velocity of 600 m/s with an accuracy of 0.06%.

Given data:

Velocity of electron $v = 600 \frac{m}{s}$

Therefore, uncertainty in velocity $\Delta v \approx v \times 0.06\%$

$$= 600\frac{m}{s} \times 0.06\% = 600\frac{m}{s} \times \frac{0.06}{100} = 0.36\, m/s$$

Solution:

According to Heisenberg's Uncertainty principle,

$$\Delta x \approx \frac{h}{4\pi\, m\, \Delta v}$$

$$\Delta x \approx \frac{6.626 \times 10^{-34}}{4 \times 3.14 \times 9.11 \times 10^{-31} \times 0.36}$$

Therefore, the uncertainty in finding the position of an electron is

$$\boxed{\Delta x \approx 1.6085 \times 10^{-4} m}$$

----

5) If the kinetic energy of an electron known to be about 1eV, must be measured to within 0.0001 eV, what accuracy can its position be measured simultaneously?

Given data:

K.E of the electron E =1 eV = 1.602 × $10^{-19}\, J$

Therefore, uncertainty in measuring k.E $\Delta E = E \times 0.0001\, eV$

$$= 1 \times 0.0001 = 0.0001\, eV\; or\; 1.602 \times 10^{-2}\;\; J$$

Solution:

The relation between the K.E and position of can electron can be determined as follows,

As we know, $E = \frac{P^2}{2m}$

$$\Delta E = \Delta\left(\frac{P^2}{2m}\right) = \frac{\Delta(P^2)}{2m} = \frac{2P\Delta P}{2m} = \frac{P\Delta P}{m}$$

$$\Delta P = \frac{m}{P}\Delta E$$

According to Heisenberg's Uncertainty Principle,

$$\Delta P\,.\,\Delta x \approx \frac{h}{4\pi}$$

$$\Delta x \approx \frac{h}{4\pi \times \Delta P} = \frac{h}{4\pi \times \frac{m}{P}\Delta E} = \frac{h \times P}{4\pi \times m\,\Delta E} = \frac{h \times \sqrt{2mE_k}}{4\pi \times m\,\Delta E}$$

Substituting the values of E and ΔE in the above equation, we get

$$\Delta x \approx \frac{6.626\ \times 10^{-34} \times \sqrt{2 \times 9.11 \times 10^{-31} \times 1.602 \times 10^{-19}}}{4 \times 3.14 \times 9.11 \times 10^{-31} \times 1.602 \times 10^{-23}}$$

$$\Delta x \approx \frac{3.5792\ \times 10^{-58}}{1.833 \times 10^{-52}}$$

Therefore, the uncertainty in finding the position of an electron is

$$\boxed{\Delta x \approx 1.953\ \times 10^{-6} m \text{ or } 1.953\ \mu m}$$

Problems related to Particle in a Box

1) A particle is moving in one-dimensional infinite potential well of width 25 Å. Calculate the probability of finding the particle within a small interval of 0.05 Å at the center of the box when it is in its state of least energy.

Given data:

Width of the potential well L = 25 Å

The space Interval $dx = 0.05$ Å

For the particle in its lowest energy n=1,

To find the particle at the center of the box $x = L/2$

Solution:

Probability of finding the particle, $P = \int_{-\infty}^{+\infty} |\psi|^2\, dx$

$$P = A^2 \int_0^L Sin^2\left(\frac{n\pi x}{L}\right)\, dx$$

$$P = \frac{2}{L}\int_0^L Sin^2\left(\frac{n\pi x}{L}\right)\, dx$$

Substituting the values of L, *x* and *dx*, we get,

$$-P = \frac{2}{25 \times 10^{-10}}\int_0^L Sin^2\left(\frac{\pi}{2}\right)\, 0.05 \times 10^{-1}$$

$$\boxed{P = 0.004}$$

The probability of finding the particle is $\boxed{\text{0.004 or 0.4 \%.}}$

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2) An electron is confined to a one-dimensional potential well of width 2 Å. Calculate the lowest energy of the electron.

Given data:

Width of the potential well $L = 2$ Å

For the Lowest energy of an electron $n = 1$

Solution:

The energy of an electrons in various energy levels in a one-dimension potential well,

$$E = \frac{n^2h^2}{8mL^2}$$

Substituting the value of L, h, m and *n*, we get,

$$E = \frac{(6.626\ \times 10^{-34})^2}{8 \times 9.11\ \times 10^{-3}\ \times (2 \times 10^{-10})^2}$$

$$E = 1.5075\ \times 10^{-18} J$$

Or

$$E = 9.4225\ eV$$

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3) The lowest energy of a particle in an infinite potential well of width 50 Å is 0.1 eV. Then, what is the mass of the particle?

Given data:

Width of the potential well $L = 50$ Å

Energy of the particle $E = 0.1\, eV = 1.602 \times 10^{-20}\, J$

For the Lowest energy of an electron $n = 1$

Solution:

The energy of an electrons in various energy levels in a one-dimension potential well,

$$E = \frac{n^2 h^2}{8mL^2}$$

From the above equation, the mass of the particle can be written as,

$$m = \frac{n^2 h^2}{8EL^2}$$

Substituting the values of *n, h, E* and *L*, we get,

$$m = \frac{(6.626 \times 10^{-34})^2}{8 \times 1.602 \times 10^{-20} \times (50 \times 10^{-1})^2}$$

Therefore, the mass of the particle is $\boxed{m = 1.37 \times 10^{-31}\, kg}$

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4) A one dimensional box of length 1 Å has three electrons. Calculate the lowest total energy of the system.

Given data:

Width of the potential well $L = 1$ Å

Number of electrons N = 3

Solution:

According to the Pauli's exclusion principle, the first two electrons occupy the state for which *n=1* and the third electron occupy the state for which *n=2*

The total energy of the system, $E = 2\frac{h^2}{8mL^2} + \frac{2^2h^2}{8mL^2} = 6\frac{h^2}{8mL^2}$

Substituting the values of *h, m, and L,* we get,

$$E = \frac{6 \times (6.626 \times 10^{-3})^2}{8 \times 9.11 \times 10^{-3} \times (1 \times 10^{-10})^2}$$

Therefore, the total energy of the system will be

$E = 3.618 \times 10^{-1}\ J$

Or

$E = 226.15\ eV$

Problem related to Quantum Mechanical Tunneling

1) The probability of an electron penetrating a potential barrier of 10.0 eV is equal to 0.8 %. If the width of the potential barrier is 0.6 nm, find the energy of an electron.

Given data:

Width of the potential barrier $l = 0.6\ nm$ or $0.6 \times 10^{-9}\ m$

Potential energy of the barrier $V = 10.0\ eV$ or $1.602 \times 10^{-1}\ J$

The probability of an electron penetrating through the barrier = 0.8 % or 0.008 (This is equivalent to the transmission coefficient of the barrier)

Solution:

The energy of an electron can be determined from the formula,

$$E = V - \frac{\left(\frac{h \ln T}{4\pi\, l}\right)}{2m}$$

For reference:

As we know that $T = e^{-2\alpha l} = e^{-\frac{2l\sqrt{2m(V-E)}}{\hbar}}$

Taking natural log on both sides, we get

$$\ln T = -\frac{2l\sqrt{2m(V-E)}}{\hbar} \quad or \quad -\frac{4\pi l\sqrt{2m(V-E)}}{h}$$

$$\sqrt{2m(V-E)} = -\left(\frac{h\ln T}{4\pi l}\right)$$

$$2m(V-E) = \left(\frac{h\ln T}{4\pi l}\right)^2$$

$$E = V - \frac{\left(\frac{h\ln T}{4\pi\, l}\right)}{2m}$$

$$E = 1.602 \times 10^{-18} - \frac{\left(\frac{6.626\times 10^{-3} \quad \ln(0.008)}{4 \times 3.14 \times 0.6 \times 10^{-9}}\right)}{(2 \times 9.11 \times 10^{-3}\ )}$$

Therefore, the energy of the electron,

$$\boxed{E = 1.5 \times 10^{-1}\ J\ or\ 9.4\ eV}$$

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