DEPARTMENT OF SCIENCE AND HUMANITIES

Course Code/Name : **PH3151 / ENGINEERING PHYSICS**
Regulation : **2021 – R**

Course Objective:

1. To make the students effectively to achieve an understanding of mechanics.
2. To enable the students to gain knowledge of electromagnetic waves and its applications.
3. To introduce the basics of oscillations, optics and lasers.
4. Equipping the students to successfully understand the importance of quantum physics.
5. To motivate the students towards the applications of quantum mechanics.

UNIT V APPLIED QUANTUM MECHANICS

The harmonic oscillator(qualitative)- Barrier penetration and quantum tunneling(qualitative)- Tunneling microscope - Resonant diode - Finite potential wells (qualitative)- Bloch's theorem for particles in a periodic potential –Basics of Kronig-Penney model and origin of energy bands.

After completion of this course, the students should be able to

COs	OUTCOMES	RBT
C103.1	Remember the concepts of Mechanics and understand the Fundamentals of static and dynamics of bodies.	K1
C103.2	Understand the properties of electro Magnetic waves and its practical applications.	K2 & K3
C103.3	Demonstrate a strong foundational knowledge, and understand the principles of sound, Light and optics with experimental examples.	K2
C103.4	Understand and deduce the basic quantum concepts and equations.	K2
C103.5	Understand the fundamentals of quantum applications	K2
Revised Bloom's Taxonomy **K1**- Remembering, **K2**- Understanding, **K3**- Applying, **K4**- Analyzing, **K5**- Evaluating, **K6**- Creating		

CO-PO Mapping

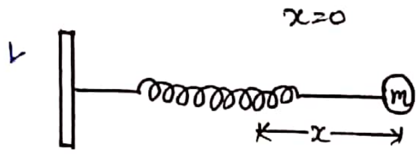
COs	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
C103.1	3	2	1									
C103.2	3	2	1									
C103.3	3	2	1									
C103.4	2											
C103.5	1											
Avg	2.4	2	1									

Harmonic Oscillator:-

In quantum harmonic oscillator the molecular atomic vibrations are quantized and the allowed energies of a quantum harmonic oscillator are discrete and evenly spaced.

Derivation:-

Let us consider a particle of mass 'm' executing simple harmonic motion along the 'x' direction.



When a particle is moved a distance x, a restoring force acts so as to return the particle again to its equilibrium position.

The restoring force $F = -kx$

where $k \rightarrow$ force constant

Schroedinger time independent eqn for a particle moving in one dimension is given by

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0 \quad -(1)$$

The P.E $V = \frac{1}{2}kx^2 \quad -(2)$

$$\left\{ \begin{array}{l} V = -\int F dx \\ V = k\int x dx \\ V = \frac{1}{2}kx^2 \end{array} \right.$$

$\therefore$ Eqn (1) can be written as

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left[E - \frac{1}{2}kx^2\right]\psi = 0 \quad -(3)$$

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\left(\frac{h^2}{4\pi^2}\right)}\left[E - \frac{1}{2}kx^2\right]\psi = 0 \quad \left[\hbar = \frac{h}{2\pi}\right]$$

$$\frac{d^2\psi}{dx^2} + \left[\frac{8\pi^2 mE}{h^2} - \frac{4\pi^2 mkx^2}{h^2}\right]\psi = 0 \quad -(4)$$

Let $\frac{8\pi^2 mE}{h^2} = \alpha$ and $\left[\frac{4\pi^2 mk}{h^2}\right]^{1/2} = \beta$.

$\therefore$ Eqn (4) becomes

$$\frac{d^2\psi}{dx^2} + [\alpha - \beta^2 x^2]\psi = 0 \quad -(5)$$

To simplify the eqn, let us introduce a dimensionless variable

$$y = x\sqrt{\beta} \quad -(6)$$

$$x^2 = \frac{y^2}{\beta^2} \quad -(7)$$

Diff. eqn (6) w.r.t 'x' we get

$$\frac{dy}{dx} = \sqrt{\beta} \quad -(8)$$

we can write

$$\frac{d\psi}{dx} = \frac{d\psi}{dy}\cdot\frac{dy}{dx} \quad -(9)$$

Substituting eqn (8) in eqn (9)

$$\frac{d\psi}{dx} = \frac{d\psi}{dy}\cdot\sqrt{\beta}$$

Diff. we get

$$\frac{d^2\psi}{dx^2} = \frac{d^2\psi}{dy^2}\cdot\sqrt{\beta}\cdot\sqrt{\beta}$$

$$\frac{d^2\psi}{dx^2} = \beta\cdot\frac{d^2\psi}{dx^2} \quad -(10)$$

Substituting eqns (7) & (10) in eqn (5)

$$\beta\frac{d^2\psi}{dx^2} + \left[\alpha - \beta^2\frac{y^2}{\beta}\right]\psi = 0$$

$$\div\beta \Rightarrow \frac{d^2\psi}{dx^2} + \left[\frac{\alpha}{\beta} - y^2\right]\psi = 0 \quad -(11)$$

The Solution of eqn (11) is

$$\boxed{\psi = f(y)\, e^{-y^2/2}} \quad \text{--- (12)}$$

By introducing ψ of eqn (12) in eqn (11) we can write

$$\frac{d^2 f}{dy^2} - 2y\frac{df}{dy} + \left[\frac{\alpha}{\beta} - 1\right] f = 0 \quad \text{--- (13)}$$

Let $\frac{\alpha}{\beta} - 1 = 2n$

$$(13) \Rightarrow \frac{d^2 f}{dy^2} - 2y\frac{df}{dy} + 2nf = 0 \quad \text{--- (14)}$$

This is similar to the Hermite's equation

$$\text{(i.e.)} \boxed{\frac{d^2 H}{dy^2} - 2y\frac{dH}{dy} + 2nH = 0} \quad \text{--- (15)}$$

The Solution of eqn (15) are called Hermite Polynomial.

$$\boxed{\psi_n(y) = N\, H_n(y)\, e^{-y^2/2}} \quad \text{--- (16)}$$

Where $N \rightarrow$ Normalization Constant

Eqn (16) respresents the Eigen function of the harmonic oscillator

Energy Eigen Values:-

We know $\frac{\alpha}{\beta} - 1 = 2n$

$$\frac{\alpha}{\beta} = 2n+1$$

$$\alpha = [2n+1]\beta \quad \text{--- (17)}$$

Substitute $\alpha = \frac{8\pi^2 mE}{h^2}$, $\beta = \left[\frac{4\pi^2 mk}{h^2}\right]^{1/2}$ in eqn (17) we get

$$\frac{8\pi^2 mE}{h^2} = [2n+1]\left[\frac{4\pi^2 mk}{h^2}\right]^{1/2}$$

$$E = \frac{h^2}{8\pi^2 m}(2n+1)\frac{2\pi(mk)^{1/2}}{h}$$

$$E = \frac{h}{4\pi}(2n+1)\frac{(mk)^{1/2}}{m}$$

$$E = 2\left[n+\frac{1}{2}\right]\cdot\frac{h}{4\pi}\left[\frac{k}{m}\right]^{1/2}$$

$$\boxed{E = \left[n+\frac{1}{2}\right]\frac{h}{2\pi}\sqrt{\frac{k}{m}}} \quad \text{--- (18)}$$

The frequency of oscillation is given by

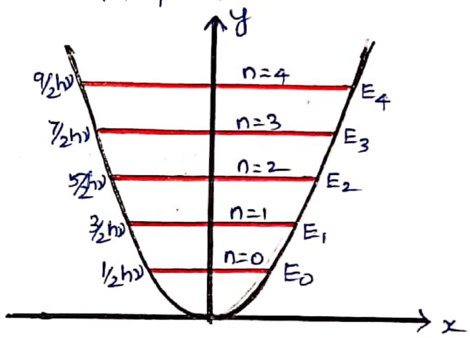
$$\nu = \frac{1}{2\pi}\sqrt{\frac{k}{m}}$$

$\therefore$ Eqn (18) $\Rightarrow E = \left[n+\frac{1}{2}\right]h\nu$

The energy of harmonic oscillator is quantised in steps of $h\nu$

$$\boxed{E_n = \left[n+\frac{1}{2}\right]h\nu} \quad \text{--- (19)}$$

$n = 0, 1, 2, 3 \ldots$



Normalized wave function:-

The normalized wave function of the harmonic oscillator is given by

$$\int_{-\infty}^{+\infty} |\psi_n|^2 dy = 1 \qquad \text{where } n = 0, 1, 2, 3 \ldots$$

The general formula for n^{th} normalised function in terms of Hermite is given by

$$\psi_n = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}}\, e^{-y^2/2} H_n(y)$$

Conclusions:

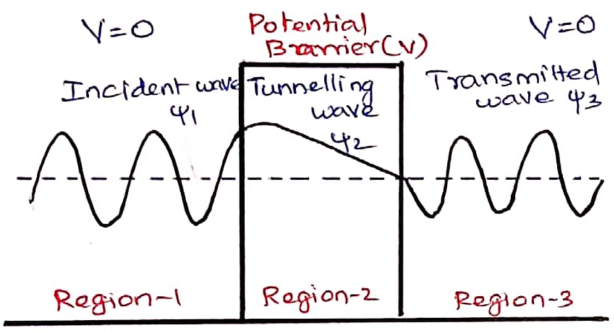
* The Particles executing SHM will have discrete energy values
* The energy values are equidistant
* The minimum energy is not zero.

Barrier Penetration:-

A particle having lesser energy (E) than the barrier potential (V) can easily cross over the potential barrier having a finite width (l) even without climbing over the barrier by tunnelling through the barrier. This process is called tunnelling.

According to classical mechanics the probability of a particle to penetrate the barrier is zero, but according to quantum mechanics it is finite.

Derivation:-



Let us consider a particle with energy E<V incident from left side and tunnell the region 2 of width l and comes out as a transmitted wave in region-3.

The boundary conditions shall be given by for various regions.

For region-1 when $x<0$; $V=0$
For region-2 when $0<x<l$; $V=V$
For region-3 when $x>l$; $V=0$

Let ψ_1, ψ_2, ψ_3 be the wave functions in Regions 1, 2, and 3 respectively.

For Region-1

The Schroedinger's wave eqn is given by

$$\frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2}[E-V]\psi_1 = 0$$

Since $V=0$

$$\frac{d^2\psi_1}{dx^2} + \frac{2mE}{\hbar^2}\psi_1 = 0 \quad \text{--- (1)}$$

For Region-2

$$\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}[E-V]\psi_2 = 0$$

Since $E<V$

$$\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}[V-E]\psi_2 = 0 \quad \text{--- (2)}$$

For Region-3

$$\frac{d^2\psi_3}{dx^2} + \frac{2mE}{\hbar^2}\psi_3 = 0 \quad \text{--- (3)} \quad [\because V=0]$$

Let $\alpha^2 = \frac{2mE}{\hbar^2}$, $\beta^2 = \frac{2m}{\hbar^2}[V-E]$

Eqns (1), (2) & (3) can be written as

$$\frac{d^2\psi_1}{dx^2} + \alpha^2\psi_1 = 0 \quad \text{--- (4)}$$

$$\frac{d^2\psi_2}{dx^2} - \beta^2\psi_2 = 0 \quad \text{--- (5)}$$

$$\frac{d^2\psi_3}{dx^2} + \alpha^2\psi_3 = 0 \quad \text{--- (6)}$$

The solutions for eqns (4), (5) & (6) can be written as

$$\psi_1 = Ae^{i\alpha x} + Be^{-i\alpha x} \quad — (7)$$

$$\psi_2 = Fe^{\beta x} + Ge^{-\beta x} \quad — (8)$$

$$\psi_3 = Ce^{i\alpha x} + De^{-i\alpha x} \quad — (9)$$

Where A, B, C, D, F, G → amplitudes of Corresponding waves.

Let us discuss the behaviour of wave function and the amplitudes in each region as follows.

Region-1

The ~~inci~~ wave function of incident wave in region-1 is given by

$$\boxed{\psi_1(\text{Incident}) = Ae^{i\alpha x}}$$

A → Amplitude of incident wave

The wave function of reflected wave in region-1 is given by

$$\boxed{\psi_1(\text{Reflected}) = Be^{-i\alpha x}}$$

Region-2

The wave function of the transmitted (or) tunnelling wave at Region-2 is given by

$$\boxed{\psi_2 = Fe^{\beta x} + Ge^{-\beta x}}$$

Where

β → The wave number

F → Amplitude of tunnelling wave in Region-2

G → Amplitude of reflected wave at the boundary between Region-1 and Region-2

Region-3

The wave function of the transmitted wave in Region-3 is given

$$\boxed{\psi_3(\text{Transmitted}) = Ce^{i\alpha x}}$$

Where C → Amplitude of Transmitted wave

In Region-3, there is no possibility of refelected wave, therefore the amplitude of reflected wave in region-3 is equal to zero.

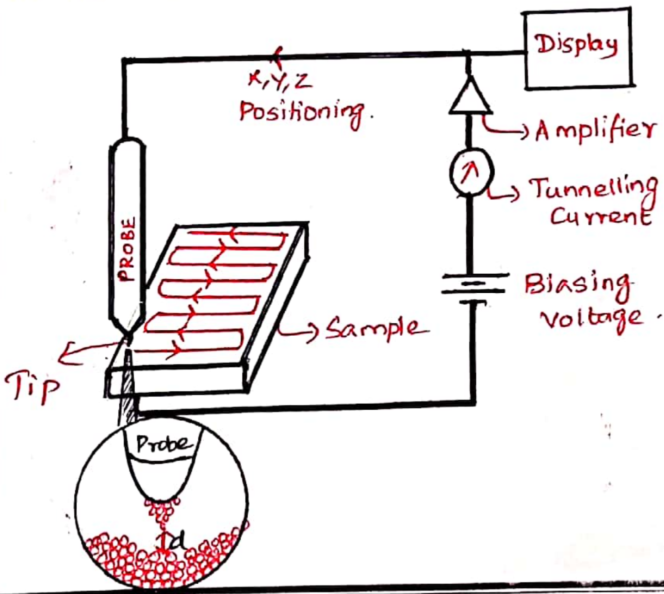
(i.e) D = 0

$$\therefore \boxed{\psi_3(\text{Refected}) = 0}$$

Scanning Tunnelling Microscope:

Principle:

STM has a metal needle that scans a sample by moving back and forth and gathering information about the curvature of the surface. It follows the smallest changes in the contours of a sample.



It has the following Components.

* Piezo electric tube - capable of moving in x, y, z directions.

* Fine needle tip - for scanning the surface of the sample.

Piezo electric materials exhibit an elongation or contraction along their length when an electric field is applied. It control the position and movement of the tip on an atomic scale. The x, y, piezos control the back and forth motion of the tip, while the z piezo allow the tip to approach the surface.

Working:

* The tip is mechanically connected to the scanner and xyz positioning device.

* The distance between the tip and surface is of the order of a few angstroms(Å).

* A bias voltage is applied between the sample and the tip

* When the needle is at positive voltage electron can tunnel through the gap and set up tunnelling current in the needle.

* This current is amplified and measured.

* The sensitivity of STM is so large that electronic corrugation of surface atoms can be detected.

Advantages:

* It can scan, the positions & topography atom by atom (or) even electrons.

* Very accurate measurement shall be obtained

* It is latest technique used in Research Laboratories.

Disadvantages:

* Even a very small sound (or) vibrations will distrub the measurement setup.

* Cost is high

* More complexity.

Applications:

* It is used to produce IC's

* It is used is Biomedical devices.

* Chemical and material sciences research labs are the major areas in which it is used.

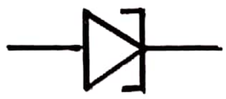
Resonant Tunnelling Diode:-

Resonant tunnelling occurs through a potential profile which consists of two potential barriers, so called double barrier structure which are located very close to each other.

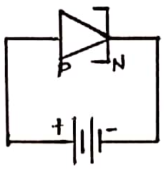
CHENNAI INSTITUTE OF TECHNOLOGY DEPARTMENT OF SCIENCE AND HUMANITIES

Principle:

Resonant tunnelling diode works on the principle of tunnelling effect, in which the charge carriers cross the energy barrier(s) even with lesser energy than the barrier potential, quantum mechanically. The probability of tunnelling increases with the decreasing barrier energy.



SYMBOL

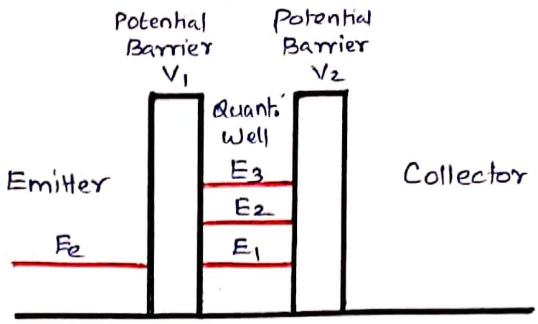


Theory:

A resonant tunnelling diode is formed using P and N-materials with heavy doping. Due to heavy doping, the barrier potential decreases drastically, so that the charge carriers can easily tunnel the junctions.

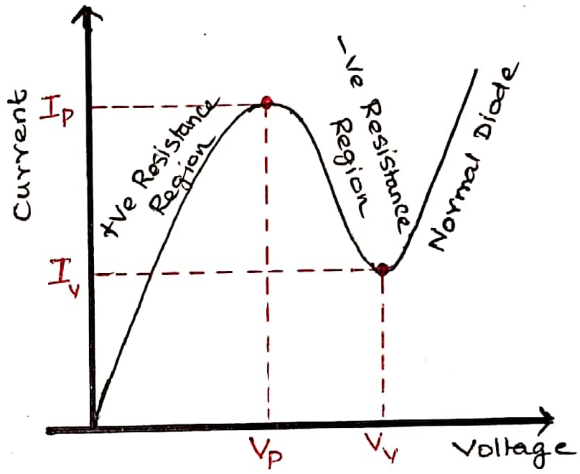
Quantum Well structure:-

A RTD consists of a quantum well structure with discrete energy values E_1, E_2 etc, surrounded by two thin layer of potential barriers (V_1 and V_2) with emitter and collector on either side as shown in the figure.



V-I Characteristics:-

During the forward bias, when voltage is increased, then the current in the diode varies at the different resistance regions as follows.



Positive Resistance Region:-

When voltage is applied, a terahertz wave is emitted and therefore at resonance the energy E_1 becomes equal to the energy E_e in the emitter side.

(ie) At low voltage

$$E_1 \approx E_e.$$

At resonance, the charge carriers tunnel the potential barriers and reaches collector region by the process called resonant tunnelling.

CHENNAI INSTITUTE OF TECHNOLOGY
DEPARTMENT OF SCIENCE AND HUMANITIES

∴ The current increases rapidly due to tunnelling effect and reaches the peak point P.

The current and voltage are called as Peak current (I_p) and Peak voltage (V_p) respectively.

This region is called positive resistance region.

Negative Resistance Region:-

When the voltage is increased further, the terahertz wave dies out and E_1 becomes lesser than E_e

(i.e) At Higher Voltage

$$E_1 < E_e$$

Since the quantum well has discrete energy values, the energy value (E_2) is still larger than the energy value (E_e)

$$(i.e)\ E_2 > E_e.$$

∴ The charge carriers cannot tunnel the barriers and thus the current in the diode decreases and reaches the valley point V.

This minimum current is called valley current and corres-ponding voltage is called Valley Voltage.

This region is called negative resistance region.

Normal Diode:-

When the voltage increased further beyond valley point V, the energy E_2 becomes equal to the energy E_e.

∴ The current again increases and RTD behaves as a normal diode.

The total current is given by

$$I_{Tot} = I_T + I_D + I_E$$

where $I_T \rightarrow$ Tunnelling current
$I_D \rightarrow$ Diode current
$I_E \rightarrow$ Excess current.

Advantages:

* Cost and noise is low
* Fabrication is very simple.
* Operation speed is very high.

Disadvantages:

* Difficult to isolate the input and output.
* It is a low output swing device

Applications:

* It is used as high frequency microwave oscillators.
* It can be used as normal diodes also.
* RTD is used in memory cells, multivalued logic current devices etc.

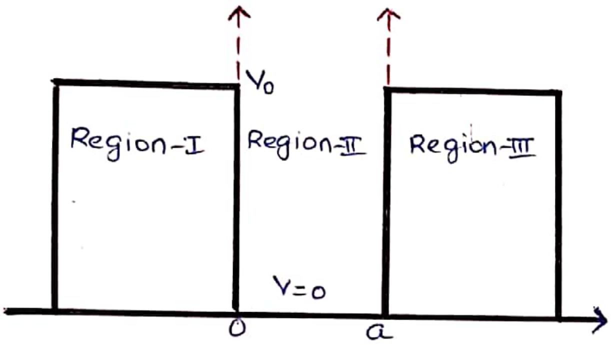
Particle in a finite Potential well

Consider a particle of mass 'm' moving with velocity v along the x-direction between $x=0$ & $x=a$.

Let $E \rightarrow$ Total energy of the particle

$V \rightarrow$ Potential Energy.

The P.E is zero within the box and it is V_0 in outside of the box. (Also $V_0 > E$)



$V(x) = V_0$	$x \leq 0$	Region-I
$V(x) = 0$	$0 < x < a$	Region-II
$V(x) = V_0$	$x \geq a$	Region-III

Classically, the particle with energy $E < V_0$ cannot be present in regions I and III outside the box.

Schroedinger's time independent eqn is given by

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0 \quad — (1)$$

For Region-I

$$\frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2}(E-V_0)\psi_1 = 0 \quad — (2)$$

For Region-II

$$\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}E\psi_2 = 0 \quad \because V=0 \quad — (3)$$

For Region-III

$$\frac{d^2\psi_3}{dx^2} + \frac{2m}{\hbar^2}(E-V_0)\psi_3 = 0 \quad — (4)$$

Let $\frac{2mE}{\hbar^2} = k^2$ and $\frac{2m(E-V_0)}{\hbar^2} = -k'^2$

Then eqns (2), (3), (4) can be written as

$$\frac{d^2\psi_1}{dx^2} - k'^2\psi_1 = 0 \quad — (5)$$

$$\frac{d^2\psi_2}{dx^2} + k^2\psi_2 = 0 \quad — (6)$$

$$\frac{d^2\psi_3}{dx^2} - k'^2\psi_3 = 0 \quad — (7)$$

The solutions of these equations are of the form

$\psi_1 = Ae^{k'x} + Be^{-k'x}$ for $x<0$

$\psi_2 = Fe^{ikx} + Ge^{-ikx}$ for $0<x<a$

$\psi_3 = Ce^{k'x} + De^{-k'x}$ for $x>a$

As $x \rightarrow \pm\infty$ should not become infinite. Hence $B=0$ and $C=0$.

Hence the wave functions in three regions are

$$\psi_1 = Ae^{k'x}$$

$$\psi_2 = Fe^{ikx} + Ge^{-ikx}$$

$$\psi_3 = De^{-k'x}$$

The constants A, D, F and G can be determined by applying the boundary conditions.

CHENNAI INSTITUTE OF TECHNOLOGY DEPARTMENT OF SCIENCE AND HUMANITIES

The wave function ψ_2 is equal to ψ_1 in the ~~region~~ boundary between Region-I and Region-II.

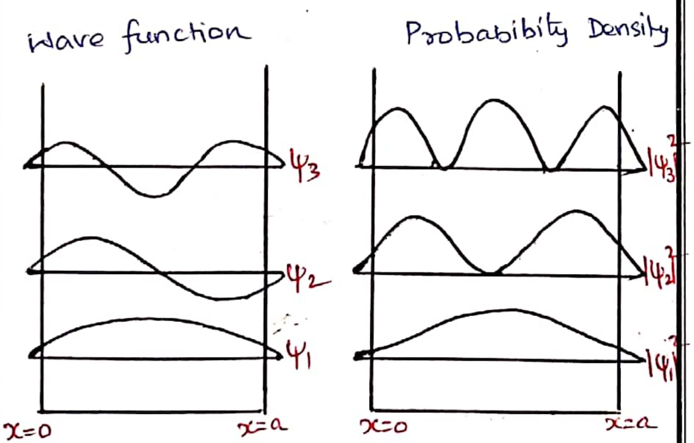
III'y The wave function ψ_2 is equal to ψ_3 in the boundary between Region-II and Region-III

(i.e) At $x=0$

$$\boxed{\begin{gathered}\psi_1 = \psi_2 \\ \frac{d\psi_1}{dx} = \frac{d\psi_2}{dx} \\ \text{At } x=l \\ \psi_2 = \psi_3 \\ \frac{d\psi_2}{dx} = \frac{d\psi_3}{dx}\end{gathered}}$$

* Using these four conditions, the constants, A, F, G, D can be determined.

* The wave functions and probability densities are shown in figure.



* Even the particle energy E is less than the P.E V_0, there is a definite probability that the particle is found outside the box

* The energy of particle is not enough to break through the walls of the box but it can penetrate the walls and leak out.

* The energy levels of the particle are still discrete but there are a finite number of them.

Bloch's Theorem:-

It is a mathematical statement of an electron (Particle) wave function moving in a perfectly periodical potential.

Explanation:-

Let us consider a particle moving in a periodic potential.

The Schroedinger's eqn for this particle is given by

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi(x) = 0 \quad \text{--- (1)}$$

Since the potential energy is periodic $V(x) = V(x+a)$ --- (2)

$a \rightarrow$ Periodicity of the potential

The solution of eqn (1) is given by

$$\boxed{\psi(x) = e^{ikx} u_k(x)} \quad \text{--- (3)}$$

where $\boxed{u_k(x) = u_k(x+a)}$ --- (4)

Here e^{ikx} represents the plane wave

$u_k(x)$ represents the periodic function.

Eqn (3) is called Bloch theorem, and eqn (4) is called Bloch function.

Proof:

By use of eqn(2) we can write the wave function (eqn(3)) as follows

$$\psi(x+a) = e^{ik(x+a)} u_k(x+a)$$

$$\psi(x+a) = e^{ika} \cdot e^{ikx} u_k(x+a)$$

Since $u_k(x+a) = u_k(x)$ we can write

$$\psi(x+a) = e^{ikx} \cdot e^{ika} u_k(x)$$

Since $\psi(x) = e^{ikx} u_k(x)$

$$\psi(x+a) = e^{ika} \psi(x) \quad —(5)$$

$$\psi(x+a) = Q\,\psi(x)$$

Where $Q = e^{ika}$

If ψ is a single-value function

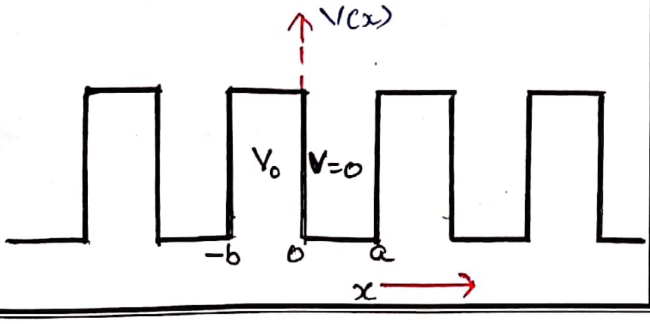
$$\psi(x) = \psi(x+a)$$

Hence Bloch theorem is proved.

The Kronig-Penny Model:-

* It is a simplest example for 1D periodic potential.

* The P.E of an electron has the form of a periodic array of square wells.



Here we have two regions,

Region-(i)

In this region, between the limits $0<x<a$, the P.E is zero and hence the electron is assumed to be a free particle.

The Schroedinger's eqn is given by

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E-0]\psi = 0$$

$$\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0 \quad —(1)$$

where $\alpha^2 = \frac{2mE}{\hbar^2}$

Region-(ii)

In this region between the limits $-b<x<0$, the P.E of the electron is V_0.

The schroedinger's eqn is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E-V_0]\psi = 0$$

$$\frac{d^2\psi}{dx^2} - \beta^2\psi = 0 \quad —(2)$$

where $\beta^2 = \frac{2m}{\hbar^2}(V_0-E)$

For both region the appropriate solution suggested by Bloch's is of the form

$$\psi(x) = e^{ikx} u_k(x) \quad —(3)$$

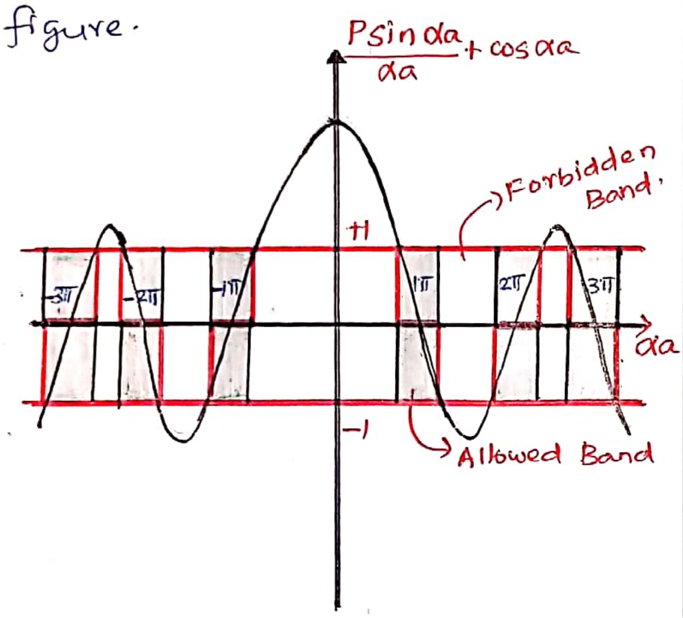
Differentiating eqn (3) and Substituting it in eqns (1), (2) and then solving we get

$$\boxed{P\frac{\sin\alpha a}{\alpha a} + \cos\alpha a = \cos ka} \quad \text{--- (4)}$$

Where $P = \frac{mV_0ba}{\hbar^2}$ → Scattering power.

It is the measure of the strength with which the electrons are attracted by the +ve ions.

A plot is made between the LHS of eqn (4) and αa for a value of $P = \frac{3\pi}{2}$ as shown in figure.



Conclusions:

* The width of allowed energy band increases with the increase in αa.
* When P increases, the binding energy of the $\bar{e}$s is also increased. ∴ The electron will not able to move freely and hence the width of the allowed energy band is decreased.
* When P is decreased, the binding energy decreased, so that the width of allowed band increased.
* Thus by varying P from zero to infinity we get the energy spectra of all ranges.