Define waves and particles:

Particles:

1. It is very easy to understand particles, since it can be **seen physically**
2. It has a well-defined **mass** and occupies a **particular position**
3. If its position changes it leads to its **velocity**
4. The mass and velocity give its **momentum** and hence **energy**
5. There the characteristics of particles are
   - **Mass**
   - **Velocity**
   - **Momentum**
   - **Energy**

Waves:

1. Waves are nothing but spreading of disturbances
2. They cannot occupy a particular position
3. The characteristics of waves are
   - Wave length
   - Frequency
   - Amplitude
   - Phase
   - Intensity

Explain the concept of dual nature of light (or) What are matter waves: Obtain the wavelength of matter waves. (or) Show that wavelength "λ" associated with the electron of mass "m" and K.E "E" is given by $\lambda = \frac{h}{\sqrt{2mE}}$ (or) Discuss the de Broglie's Hypothesis of duality of material particle.

Like radiations (ie., visible light, X-rays, UV rays) **material particles also exhibits dual nature**(ie., both particle and wave nature). This concept is given by the French Scientist who is called de Broglie, according to him when a material particle of mass "m", moving with velocity "v" will be associated with some sort of waves. Those waves are called as **de Broglie waves**

The wavelength associated with the wave can be calculated in the following way.

According to Planck's Quantum theory, the energy of the photon is given by

$E=h\nu$ ------ (1)

The Einstein's mass-energy relation is given by

$E=mc^2$ ------- (2)

From eq (1) & (2)

$h\nu = mc^2$

but $c = \nu\lambda$, $\nu = \frac{c}{\lambda}$

$$h \times \frac{c}{\lambda} = mc^2$$

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

The above equation is showing the wavelength of light, but for a material particle (like electron, proton, or neutron, etc) the wavelength associated with it when it is moving with a velocity "v" is given by

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

If the particle is electron , e^- is accelerated by means of the potential "V", then

$$eV = \frac{1}{2} mv^2$$

(Electrical energy) (K.E of the electron)

$$v = \sqrt{\frac{2eV}{m}}$$

$$\lambda = \frac{h}{m\sqrt{\frac{2eV}{m}}} = \frac{h}{\sqrt{2eVm}}$$

If the particle is e^-

$$\lambda = \frac{6.624 \times 10^{-34}}{\sqrt{2 \times 1.602 \times 10^{-19} \times V \times 9.11 \times 10^{-31}}} = \frac{12.27}{\sqrt{V}} \text{Å}$$

Give the Properties of de Broglies waves

We know that the wavelength of the de Broglies waves,

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

from the above we can tell that,

1. If the mass(m) of the particle is less the wavelength(λ) is more
2. If the velocity (v) of the particle is less the wavelength(λ) is more
3. If the particle is at rest (v=0), the wavelength of the particle is "∞"
4. Both charged and uncharged particles can capable of acting as waves when they are in motion.
5. The velocity of de Broglie's waves is more than the light waves.
6. The de Broglie's waves are not electromagnetic waves; they are the guiding waves or called pilot waves.
7. The wave nature of matter introduces the uncertainty in the predicting of the position of the particle

Explain Heisenberg's Uncertainty Principle:

According to classical theory, each and every point has a fixed position and momentum in a given region, both position and momentum can be predicted simultaneously accurately at any time, but it is not true, if they are measured simultaneously **error occurs**, therefore according to Heisenberg's Uncertainty principle, **both position and momentum cannot be calculated simultaneously, accurately,** if they are measured simultaneously, then error occurs ,if

The error in position is **Δx**

The error in momentum is **Δp**

Then $\boxed{\Delta x.\ \Delta p = \frac{h}{2\pi}}$

As a result, we can say that, it is impossible to conduct an experiment which is capable of demonstrating both particle and wave nature. Similarly, the two more parameter, energy and time cannot be measured accurately simultaneously

Then $\boxed{\mathbf{\Delta E.\ \Delta t} = \frac{h}{2\pi}}$

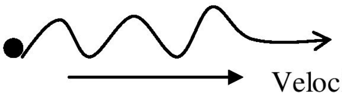
Derive Schrödinger's Time Independent Wave equation:

According to de Broglie hypothesis, the particle in motion always associated with waves. To describe the motion of such a particle which acts as waves , Schrödinger derived a equation known as Schrödinger's equation .

Let us consider a particle of mass "m" moving with velocity "v" along the x-direction. The displacement of the wave associated with the particle is given by means of the Classical wave equation is

$$y = A \sin \frac{2\pi x}{\lambda}$$

A-Amplitude



For the de Broglie's waves

$$\mathbf{\Psi = A \sin} \frac{2\pi x}{\lambda}$$

$$\frac{\partial \psi}{\partial x} = A \left(\frac{2\pi}{\lambda}\right) \cos \frac{2\pi x}{\lambda}$$

$$\frac{\partial^2 \psi}{\partial x^2} = -A \left(\frac{2\pi}{\lambda}\right)\left(\frac{2\pi}{\lambda}\right) \text{Sin } \frac{2\pi x}{\lambda}$$

$$\frac{\partial^2 \psi}{\partial x^2} = -\left(\frac{4\pi^2}{\lambda^2}\right) \Psi$$

$$\frac{1}{\lambda^2} = -\frac{\partial^2 \psi}{\partial x^2} \frac{1}{4\pi^2 \psi} \text{ ------------(1)}$$

This equation is meant for "de broglie's waves"

W.K.T

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

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

but, $K.E = \frac{1}{2}mv^2 = \frac{1}{2}mv^2 \text{ x } \frac{m}{m} = \frac{p^2}{2m}$

$$K.E = \frac{h^2}{2m\lambda^2},$$

if we substitute the value for $\frac{1}{\lambda^2}$ in equation 1 gives,

$$K.E = -\frac{h^2}{2m}\frac{1}{4\pi^2\psi}\left(\frac{\partial^2\psi}{\partial x^2}\right)\psi$$

$$K.E = -\frac{h^2}{8\pi^2 m\psi}\left(\frac{\partial^2\psi}{\partial x^2}\right)$$

But E + V = K.E

K.E = E-V

$$E - V = -\frac{h^2}{8\pi^2 m\psi}\left(\frac{\partial^2\psi}{\partial x^2}\right)$$

$$E - V + \frac{h^2}{8\pi^2 m\psi}\left(\frac{\partial^2\psi}{\partial x^2}\right) = 0$$

Divide throughout by $\frac{h^2}{8\pi^2 m\psi}$

$$\boxed{\left(\frac{\partial^2\psi}{\partial x^2}\right) + \frac{8\pi^2 m}{h^2}\,\mathbf{(E\text{-}V)}\;\psi\; \mathbf{=0}}$$

Known as **Schrödinger's 1-Dim wave equation**

For 3-dim

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{8\pi^2 m}{h^2}\,(E\text{-}V) = 0$$

<u>Significance of Ψ :</u>

1. Ψ itself does not possess any physical meaning.
2. But the Quantity which we are getting by using "Ψ" will give very important information about the presence of the particle in a particular region called "Probability Density".
3. Since "Ψ" is a Complex Quantity, "P" the probability density can be calculated in the following manner.
   $\Psi = (a+ib)$, $\Psi^* = (a-ib)$
   $\Psi \text{x } \Psi^* = \left|\Psi\right| = P$
4. If we want to know the presence of a particle in a particular region, then

$$\int_{-\infty}^{+\infty} \Psi^2 \, dx = 1$$ (shows the presence of the particle) ---------------(1)

if

$$\int_{-\infty}^{+\infty} \Psi^2 \, dx = 1$$ (shows the absence of the particle) __________ (2)

The process which shown in eq(1) is known as "<u>Normalization process</u>" and the wave function which is obeying eq(1) is known as "<u>Normalized</u>

<u>Particle in a 1-dimentional potential box:</u>

Let us consider a particle of mass "m" is confined to move in a 1-dim potential box of length "a" & can capable of moving only along X-direction. It can capable of moving only inside the box since, the walls are given infinite potential, while reaching the walls it feels infinite potential and inside the box it possess purely kinetic energy that is its potential energy v=0

Therefore

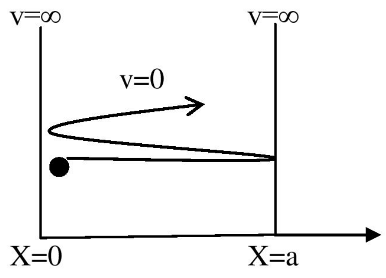
V= 0 $0 < x < a$ (Inside the potential box)

V= ∞ $0 \geq x \leq a$ (at the walls of the potential box)

In order to calculate the energy possessed by the electron and its wave function when it moves inside the potential box, let us consider Schrödinger's Time independent equation.

$$\left(\frac{\partial^2 \psi}{\partial x^2}\right) + \frac{8\pi^2 m(E-V)}{h^2} \psi = 0$$

$$\left(\frac{\partial^2 \psi}{\partial x^2}\right) + \frac{8\pi^2 mE}{h^2} \psi = 0$$ **(inside the box V=0)**



$$\left(\frac{\partial^2 \psi}{\partial x^2}\right) + k^2 \psi = 0$$ **---------------------- (1)**

$$k^2 = \frac{8\pi^2 mE}{h^2}$$

$$E = \frac{k^2 h^2}{8\pi^2 m}$$ **("k" value is unknown)**

<u>Calculation of "k":</u>

In order to find the value of "k", consider the solution of the above equation (1) will be of the form,

ψ = A sin kx + B cos kx

In order to calculate the arbitrary constants A, B and k, let us apply the boundary conditions,

The first boundary condition, that is when x =0, $\psi = 0$

0= A sin k(0) + B cos k(0)

$$\boxed{B = 0}$$

While applying the second boundary condition that is When $x = a$, $\psi = 0$

$0 = A \sin k(a) + (0) \cos k(a)$

$A \sin ka = 0$ (This equation will be satisfied when i) $A=0$ (But we cannot consider , since already $B= 0$, if A is also equal to "0", no solution for the equation.)

Therefore let us consider $\mathbf{\sin ka = 0}$, this is posible only if $\mathbf{ka = n\pi}$

So $\mathbf{k = \frac{n\pi}{a}}$

$$E_n = \frac{n^2h^2}{8ma^2}$$

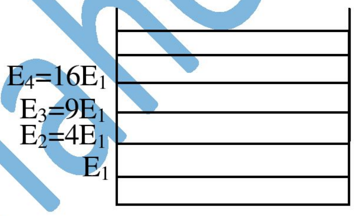
$n = 1,2,3,\ldots\ldots\ldots$

$n = 1$

$E_1 = \frac{1^2h^2}{8ma^2} = \frac{h^2}{8ma^2}$ called Zero point energy

$E_2 = \frac{2^2h^2}{8ma^2} = 4\frac{h^2}{8ma^2} = 4E_1$ called 1st excited energy

$E_3 = \frac{3^2h^2}{8ma^2} = 4\frac{h^2}{8ma^2} = 9E_1$ called 2nd excited energy



$E_1, E_2, E_3\ldots\ldots$.. called Eigen values.

Explain about the merits and demerits of Classical Free electron theory

1. The free electrons of a metal are having like the molecules of a gas in a container.
2. The free electrons are free to move in all possible directions about the whole volume of metals but in a particular direction, the resultant velocity of the free electron is zero.
3. In the absence of an electric field, the free electrons move in random directions making elastic collisions with no loss of energy.
4. When an external field is applied, the free electrons are slowly drifting towards the positive potential.
5. Since the electrons are assumed to be a perfect gas they obey classical kinetic theory of gasses.
6. Classical free electrons in the metal obey Maxwell- Boltzmann statistics.
7. The drift velocity 'v_d' is the average velocity acquired by the free electron of a metal in a particular direction by the application of the electric field.
8. Relaxation time 't' is defined as the time taken by the free electron to reach its equilibrium position from its disturbed position in the presence of electric field.
9. The collision time 't_c' is the average time taken by a free electron between two successive collisions.
10. For an isotropic solid, like a metal $t = t_c$.

$\sigma = \frac{ne^2\lambda}{\sqrt{3KTm}}$ $\rho = \frac{\sqrt{3KTm}}{ne^2\lambda}$

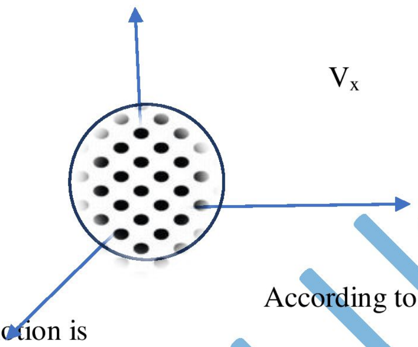
Advantages of classical free electron theory

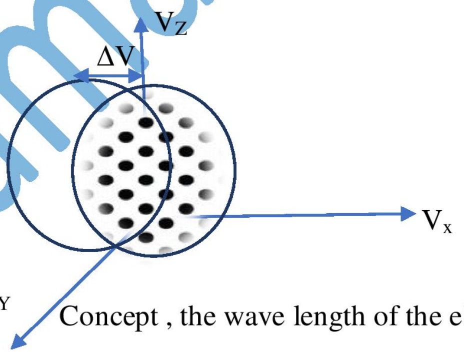
- It explains the electrical conductivity and thermal conductivity of metals.
- It explains the Wiedemann - Franz law.
- It verifies Ohm's law.
- It is used to explain the optical properties of metals.

Drawbacks of classical free electron theory

- It fails to explain the electric specific heat and the specific heat capacity of metals.
- It fails to explain superconducting properties of metals.
- It fails to explain new phenomena like photo-electric effect, Compton effect, Black body radiation, etc.
- It fails to explain electrical conductivity of semiconductors or insulators.
- The classical free electronmodel predicts the incorrect temperature dependence of σ.
- It fails to give a correct mathematical expression for thermal conductivity.
- Ferromagnetism could not be explained by this theory.
- Susceptibility has greater theoretical value than the experimental value.

Quantum Free electron Theory :





According to de Broglie Concept , the wave length of the electron when it is motion is

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

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

$$p = \frac{h}{\lambda} X \frac{2\pi}{2\pi}$$

$$mv = p = \hbar \times k$$

$$mv = \hbar \times k$$

$$v = \frac{\hbar}{m} \times k$$

Differentiate on both sides

$$\frac{dv}{dt} = \frac{\hbar}{m} \times \frac{dk}{dt}$$

$$a = \frac{\hbar}{m} \times \frac{dk}{dt}$$

Since we are applying the electric field , the force excreted by the electric field on the electrons is

$$F = eE$$

$$m \times a = e \times E$$

$$\cancel{m} \times \frac{\hbar}{\cancel{m}} \times \frac{dk}{dt} = e \times E$$

$$dk = \frac{eE}{\hbar} \times dt$$

$$\int_0^t dk = \frac{eE}{\hbar} \int_0^t dt$$

$$\underbrace{[k(t) - k(0)]} = \frac{eE}{\hbar} [t - 0]$$

$$\Delta k = \frac{eE}{\hbar} \tau_F$$

But we know that

$$\Delta v = \frac{\hbar}{m} \times \Delta k$$

$$\Delta k = \frac{\Delta v \times m}{\hbar}$$

$$\frac{\Delta v \times m}{\cancel{\hbar}} = \frac{eE}{\cancel{\hbar}} \tau_F$$

$$\Delta v = \frac{eE}{m} \tau_F$$

$$J = ne \, \Delta v$$

$$J = ne \frac{eE}{m} \tau_F$$

$$J = \frac{ne^2E}{m} \tau_F$$

$$\sigma = \frac{J}{E} = \frac{n_{eff} e^2}{m^*} \tau_F$$

Merits of Quantum Free electron theory

1. It successfully explains the electrical and thermal conductivity of the material
2. Thermionic emission can be explained by this theory
3. Thermal conductivity of metals can be successfully explained by this theory
4. Specific heat capacity and magnetic susceptibility of the metals can be explained by this theory

Demerits of Quantum free electron theory

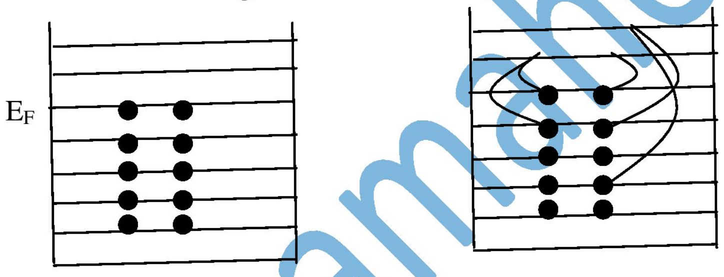
1. Unable to explain the metallic properties exhibited by some crystals
2. Unable to explain why metallic crystals prefer only certain atomic arrangements only

What is Fermi-level? Derive an expression Fermi-Dirac distribution for electrons in a metal. Discuss the variation with temperature

In the case of metals, the free electrons moves randomly just like gaseous molecules, called free-electron gas and they obey Fermi-dirac distribution. The fermi-dirac distribution describes the behavior of electrons on the basis of pauli's exclusion principle and quantum theory.

According to Pauli's exclusion principle, maximum of two electrons can occupy a particular energy level. Therefore at absolute zero, two electrons occupy the first energy level, the next two electrons will occupy the next level and so on, and the **highest occupied state is called Fermi level (E_f).** Therefore we can say that the Fermi level is the energy level which separates both filled and unfilled states & it always lies in between the filled and unfilled states.

As the temperature increases the electrons on the filled state will be excited to unfilled states. At low temperature the electrons in and near to Fermi level will be excited, as the temperature increases the electrons excited to Fermi-level will also be increasing.



T=0K **T >400K**

The probability of occupation of an electron in a particular energy level at a given temperature is

$$F(E) = \frac{1}{1+e^{\frac{E-E_F}{K_B T}}}$$

F(E) is called Fermi - Dirac probability distribution function.

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<u>Variation of F(E) with temperature</u>.

Case:1 (Temperature T=0)

For E < E$_F$, $\frac{E-E_F}{K_BT} \longrightarrow \frac{-(E-E_F)}{K_B(0)} \longrightarrow$ **- ∞**

$$F(E) = \frac{1}{1+e^{-\infty}} = \frac{1}{1+\frac{1}{e^{\infty}}}, \boxed{F(E) = 1}$$

From the above we can tell that the energy levels below E$_F$ is completely filled.

For E >E$_F$, $\frac{E-E_F}{K_BT} \longrightarrow \frac{(E-E_F)}{K_B(0)} \longrightarrow +\infty$

$$\frac{1}{1+e^{\infty}} = \frac{1}{\infty} = 0, \boxed{F(E) = 0}$$

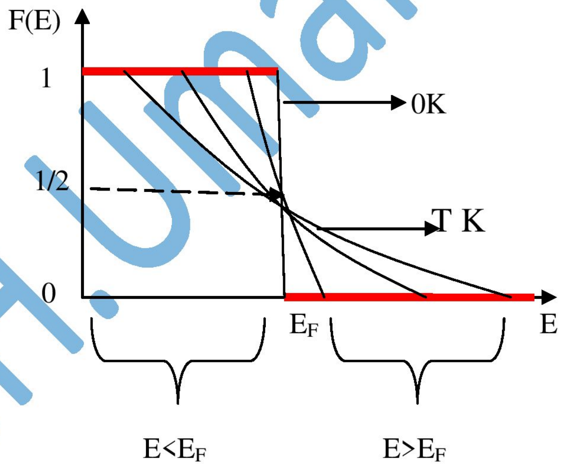
From the above we can tell that the energy levels above E$_F$ is completely empty.

<u>When T >0K , E =E$_f$</u>

$$\frac{E-E_F}{K_BT} \longrightarrow 0$$

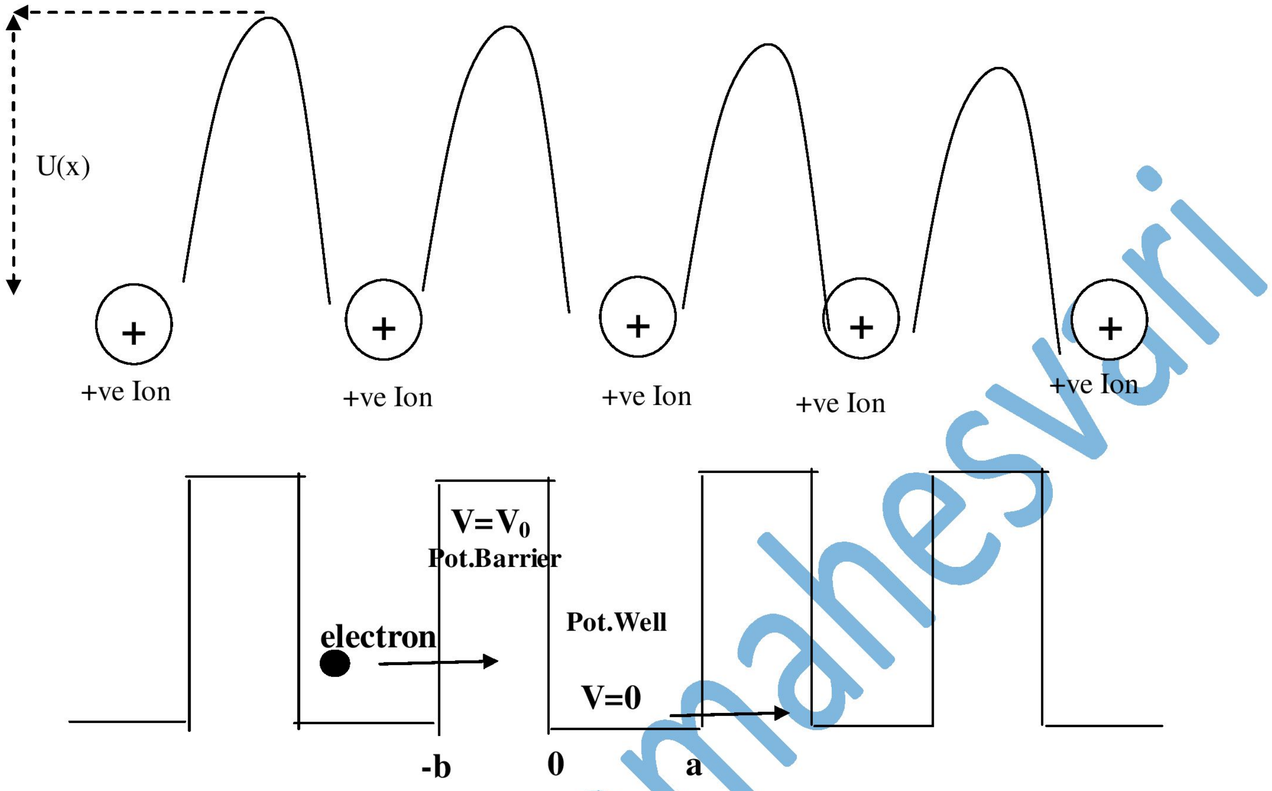
$$F(E) = \frac{1}{1+e^{0}}, \boxed{F(E) = \frac{1}{2}}$$

From the above we can tell that the "E$_F$" always lies between the filled and unfilled states.



Explain about Kronig Penny Model

According to free electron theory. The potential inside the metal is uniform but according to Kronig- Penny Model, the potential inside the metal is a periodic potential. The periodic potential is created by the positive ions. So the electron must move in a variable potential which is created inside the metal, the potential energy variation in a 1-domentional metallic lattice is given below



When an electron reaches the site of the positive ion, it experience minimum potential energy (V=0)and in between two ions the potential is maximum (V-V_0), so while moving through this periodic potential , the electron behaviour is totally different .

Potential Barrier width = V_0
Potential Well width = a

While moving in this periodic potential , the energy possessed by the electron will be calculated by the Schrodinger's time independent wave equation

$$\left(\frac{\partial^2\psi}{\partial x^2}\right) + \frac{8\pi^2 mE}{h^2}\psi = 0 \qquad \textbf{(inside the box V=0)} \qquad \text{---------------(1)}$$

$$\left(\frac{\partial^2\psi}{\partial x^2}\right) + \alpha^2\psi = 0 \qquad \textbf{(inside the box V=0)} \qquad \text{---------------(2)}$$

$$\alpha^2 = \frac{8\pi^2 mE}{h^2}$$

(α is the measure of Kinetic energy of an electron while moving inside the well)

$$\frac{\partial^2 \Psi}{\partial x^2}+\frac{8\pi m((E-V_0)}{h^2}\Psi = 0 \quad \text{---------------(3)}$$

$$\frac{\partial^2 \Psi}{\partial x^2}+\beta^2\Psi = 0 \quad \text{---------------(4)}$$

$$\beta^2 = \frac{8\pi m((E-V_0)}{h^2}$$ is the measure of potential barrier strength

On solving the eqn,1 & eqn. 2

The solution which we are getting will be of the form

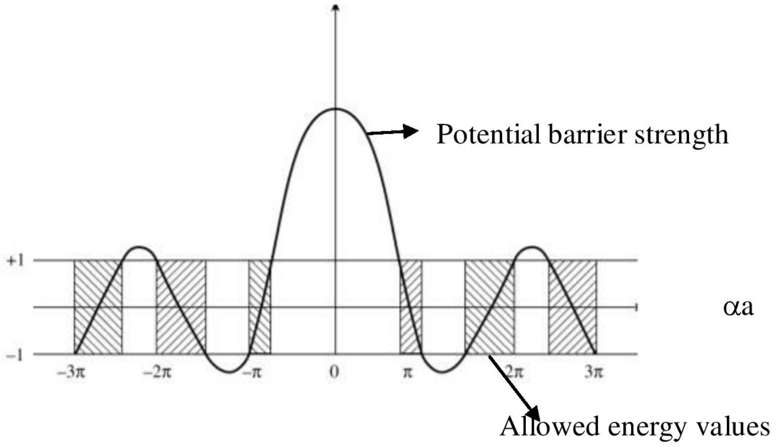
$$\frac{mV_0\,ab}{n^2}\;\frac{\sin\alpha a}{\alpha}+cos\alpha a = \cos ka$$

$$P = \frac{mV_0\,ab}{\hbar^2}$$

$$\boxed{P\;\frac{\sin\alpha a}{\alpha}+cos\alpha a = \cos ka}$$

From the above it is clear that as P value increases the allowed energy value (α) decreases

$$P\;\frac{\sin\alpha a}{\alpha}+cos\alpha a = \cos ka$$



In the above graph barrier strength is taken along Y-axis (V_0) and the allowed energy values of the electron is taken along X-axis (α), as the barrier strength decreases (continuous line), allowed energy value increases (Shadowed region)

If **$P\rightarrow\infty$,** that is the barrier strength is infinite , the electron will be well trapped in the potential well and posses energy which is equal to

$$E_n = \frac{n^2h^2}{8ma^2}$$

E-K Relation

According to Kronig -Penny model, the electron inside the solid posses only a certain energy calues known as allowed energy band and the un allowed energy values known as forbidden gap

W.K.T

$$P\ \frac{\sin \alpha a}{\alpha} + cos\alpha a = \cos ka$$

If P→0 (if the barrier is not present , then)

$$cos\alpha a = \cos ka$$

$\alpha a = ka$

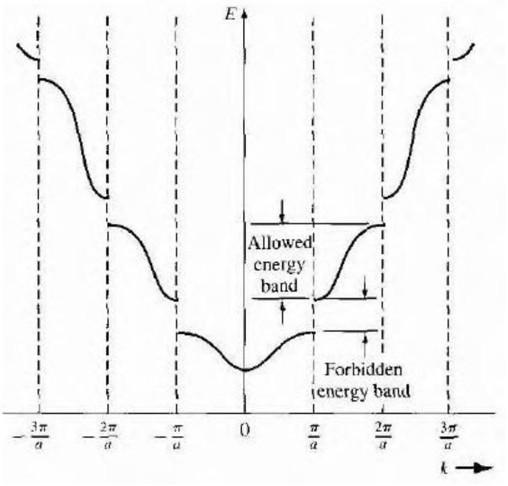
$\alpha = k$

$\alpha^2 = k^2$

W.K.T $\boldsymbol{\alpha^2 = \frac{8\pi^2 mE}{h^2}} = k^2$

$$E = \frac{k^2\ h^2}{8\pi^2 m}$$

As we draw a graph between the allowed energy values "E" & K called propagation vector , then



The allowed energy values are represented by continuous line , the gap in between them is called forbidden gap The first allowed energy values extend from k=$\frac{\pi}{a}$ to $\frac{-\pi}{a}$ known as **1st Brillouine zone**

The second allowed energy values extends from k=$\frac{\pi}{a}\ to\ \frac{2\pi}{a}\ and\ \frac{-\pi}{a}\ to\ \frac{-2\pi}{a}$ known as **2nd Brillouine zone** and so on……..

The gap in between them is known as **forbidden gap**

Band theory of Solids

The concentration in of the atoms in the gaseous medium is low compare to the concentration of the atoms in the solid medium. The interaction between the two atoms in the solid phase is more compare to the gaseous phase, since the interatomic distance is very low, due to the interaction , the allowed energy values and the unallowed energy values of the atoms in the solid over alp and produce energy bands known as valence band and the conduction band .

Valence band: The energy band that consists of valence electrons energy levels, is known as the valence band. The valence band is present below the conduction band and the electrons of this band are loosely bound to the nucleus of the atom.

Conduction band: The energy band that consists of free electrons energy levels, is known as the conduction band. For electrons to be free, external energy must be applied such that the valence electrons get pushed to the conduction band and become free.

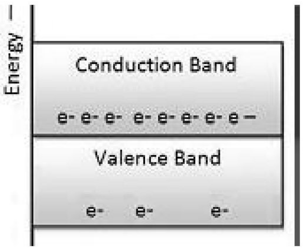
Forbidden band: The energy gap between the valence band and the conduction band is known as the forbidden band which is also known as the forbidden gap.

The electrical conductivity of a solid is determined from the forbidden gap and also the classification of the materials as conductors, semiconductors, and insulators.

Conductors:

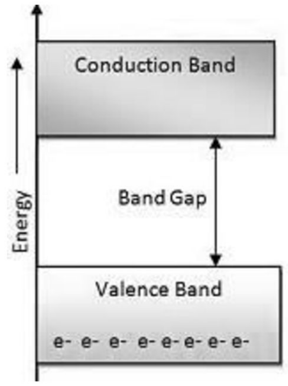
In case of metallic conductors, conduction band overlaps on the electrons in the valence band.

In the below diagram the conduction and valence bands overlap each other. Hence, electrons can easily move from the valence to the conduction band. This makes a large number of electrons available for conduction. Also, the resistivity of such solids is low or the conductivity is high.



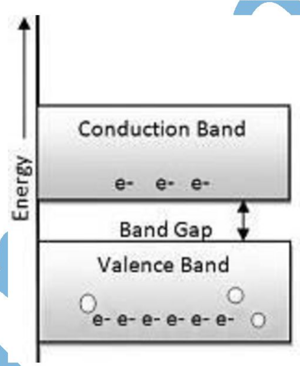
Insulators

In insulators, there is a large gap between both these bands. Hence, the electrons in the valence band remain bound and no free electrons are available in the conduction band, the energy gap (Eg) is very large (>3 eV). Due to this large gap, electrons cannot be excited to move from the valence to the conduction band by thermal excitation. Hence, there are no free electrons in the conduction band and no conductivity. These are insulators.



Semiconductors

Semiconductors have a small gap between both these bands. The energy gap is small (< 3 eV). Since the gap is small, some electrons acquire enough energy even at room temperature and enter the conduction band. These electrons can move in the conduction band increasing the conductivity of the solid. These are semiconductors. The resistivity of semiconductors is lower than that of insulators but higher than that of metals.



Concept of the hole

- When valence electron goes to conduction band positively charged empty state is created.
- If a valence electron gets a small amount of energy, it can occupy this empty state.
- Movement of valence electron movement of +vely charged empty state in opposite direction.
- The charge carrier in the form of +vely charged empty state is called the hole.