Q. 1. What do you mean by Bloch theorem and Bloch functions ?

Ans. The Schrodinger equation for an electron moving in one dimensional periodic potential is

$$\frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}[E-V(x)]\,\psi = 0 \qquad ...(i)$$

Where V(*x*) is the potential at a distance *x* from the origin and assumed to vary periodically in space with an interval equal to the lattice constant '*a*'.

i.e.,

$$V(x) = V(x+a)$$

The solution of Schrodinger equation is of the form

$$\psi = U_k(x)\exp(\pm ikx) \qquad ...(ii)$$

where

$$U_k(x) = U_k(x+a)$$

i.e., the solutions are plane waves modulated by the function $u_k(x)$ which has the same periodicity as the lattice. This theorem is called Bloch theorem. Thus *Bloch Theorem is a mathematical statement regarding the form of the one electron wave functions for a perfectly periodic potential.*

The functions of the type (eq. ii) are called Bloch functions having the property

$$\psi_k(x+a) = \exp(ikx)\,\psi(x)$$

Q. 2. What is the cause of failure of free electron theory ?

Ans. The failure of free electron theory is the over-simplified assumption that the electrons move in a region of zero or constant potential in the metals, their motion is only restrained by the surface of the metal. But this is not the case. The potential experienced by electrons is very complicated and to a reasonable approximation, we can assume that electrons move in the periodic potential of the ion cores with periodicity of the lattice.

Q. 3. What is the basic assumption in Kronig Penney model ? *(H. P. U. 2003, 2009)*

Ans. Kronig and Penney studied the behaviour of electron in a periodic potential with the assumption that the potential energy of an electron in a linear array of positive nuclei has the form of a periodic array of square wells.

Q. 4. What do you mean by effective mass electron ?

Ans. In general mass is the ratio of force applied to the acceleration produced is *(H.P.U. 2008)*

$$m = \frac{F}{a}$$

But in *k* space, the mass of the electron comes out to be

$$m^* = \frac{\hbar^2}{(d^2E/dk^2)}$$

where E is the energy of the electron and m^* is called *effective mass*. m^* can have positive or negative value even it can become infinite.

Q. 5. **What are the conclusions drawn from Kronig Penney model ?**

Ans. Following conclusions are drawn :

(i) The energy spectrum of electrons consists of a number of allowed energy bands separated by forbidden bands.

(ii) The width of allowed energy band increases with increasing energy values *i.e.*, with the increasing values of αa .

(iii) With increasing P *i.e.*, with increasing binding energy of electrons, the width of particular allowed band decreases. For $P \to \infty$ the allowed energy region becomes infinitely narrow and the energy spectrum is a line spectrum. In the other extreme case $P \to 0$, we simply have the free electron model of energy spectrum.

Q. 6. **Define forbidden energy gap.**

Ans. From Kronig Penney model, we find that the energy spectrum of electrons consists of a number of allowed energy bands separated by forbidden regions. Such forbidden regions are called forbidden gaps.

Q. 7. **What do you mean by valence band, conduction band and foridden band ?**

Ans. *Valence band* : The higher energy band occupied by the valence electrons is called valence band.

Conduction band : The empty band is called conduction band.

Forbidden band : The separation between conduction band and valence band is called forbidden band.

Q. 8. **What is the value of band gap in a good conductor ?**

Ans. In a good conductor, there is no band gap because the conduction band and valence band overlap each other.

Q. 9. **What is energy gap in insulator ?**

Ans. In an insulator the conduction band and valence band are separated by a wide gap *e.g.*, for diamond, the energy gap is 7 eV.

Q. 10. **What is the value of band gap in semiconductors ?** PU 2012

Ans. In Si the energy gap is 1.1 eV and in Ge it is 0.7 eV.

$$\boxed{\frac{P}{\alpha a}\sin\alpha a + \cos\alpha a = \cos ka} \quad \text{--- (12)}$$

This eqn is Kronig-Penney Model.

$$\boxed{P = \frac{mV_0 ba}{\hbar^2}}$$

P = Power of potential

a = Interatomic distance

Case I : $\{P \rightarrow \infty\}$

Dividing 'P' throughout eqn (12),

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

Applying $P \rightarrow \infty$,

$$\left[\frac{1}{\infty} : 0\right]$$

$$\sin\alpha a = 0$$

$$\alpha a = n\pi \Rightarrow \alpha = \frac{n\pi}{a} \Rightarrow \alpha^2 = \frac{n^2\pi^2}{a^2} \quad \text{--- (a)}$$

But, from eqn (3) $\rightarrow \alpha^2 = \frac{2m}{\hbar^2}(E)$ --- (b)

$$\therefore \frac{n^2\pi^2}{a^2} = \frac{2m(E)}{\hbar^2}$$

$$\Rightarrow \boxed{E = \frac{n^2h^2}{8ma^2}} \text{ ---} \qquad \left[\because \hbar = \frac{h}{2\pi}\right]$$

n = order $= 1, 2, 3, 4 \cdots$

m = mass of $e^{\ominus}$

a = Intermediate Distance

This case $\{P \to \infty\}$ represent the nature of insulator.

Case – II → {P → 0} put in Kronig-Penny equation (12)

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

$$\Rightarrow \alpha a = ka$$

$$\Rightarrow \alpha = k$$

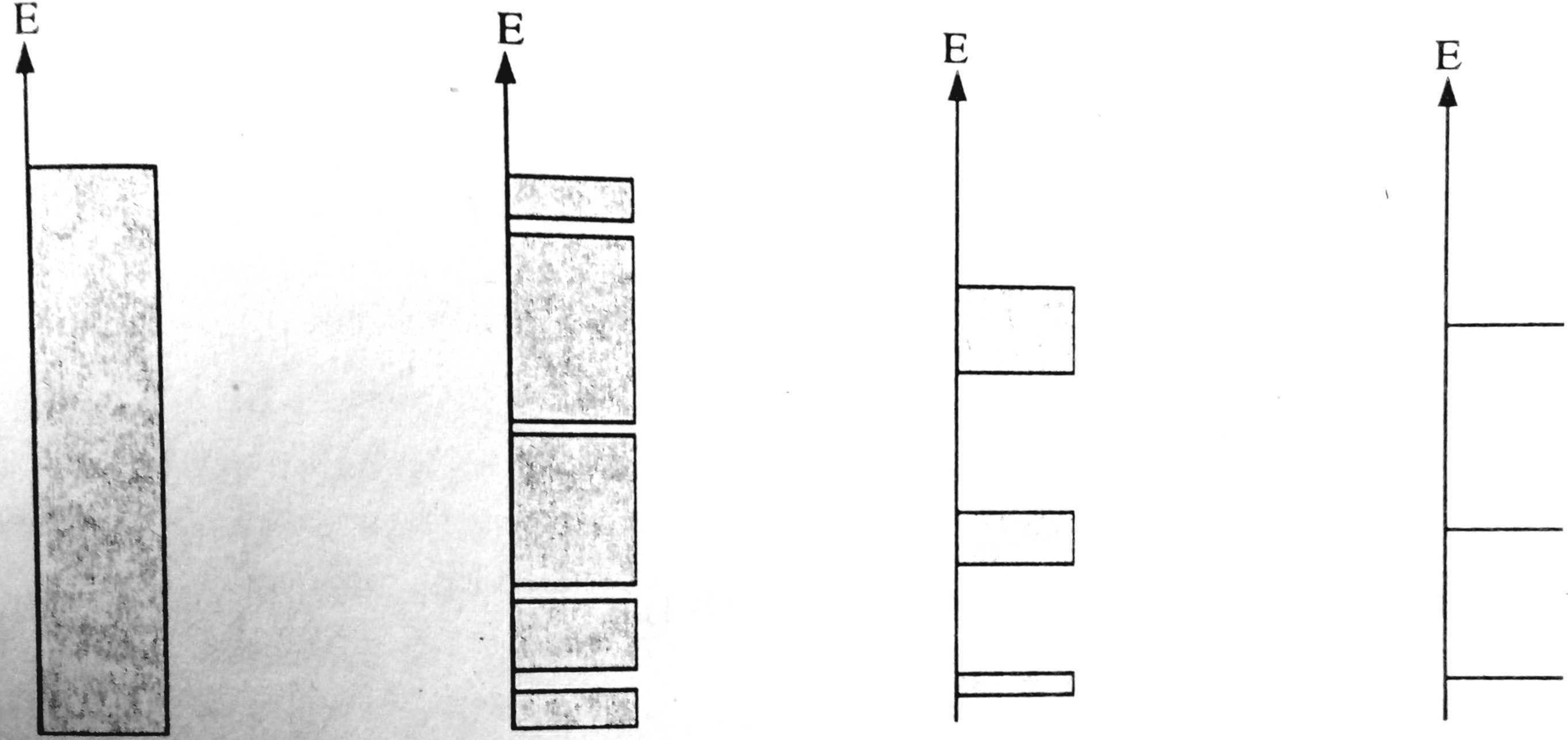
$$\Rightarrow \alpha^2 = k^2 \quad \text{—— (C)}$$

from eqn (3) → $\alpha^2 = \frac{2mE}{\hbar^2}$ $\Rightarrow E = \frac{\alpha^2\hbar^2}{2m}$

$$E = \frac{\hbar^2 k^2}{2m} \quad [\text{Put } \alpha^2 = k^2 \text{ from (C)}]$$

$$\boxed{E = \frac{p^2}{2m}} \quad \text{where } p = \hbar k$$

P → 0 represents the K.E of electrons & Thus indicates Nature of conductor.



P = 0
Free electron model
(a)

P small
Nearly free electron model
(b)

P large
Tight binding model
(c)

P = ∞
Free atom model
(d)

Example 2. *Using the Kronig Penney model, show that the energy of electron becomes* $E = \frac{\hbar^2 k^2}{2m}$ *if the electron is a free electron.*

Solution. For a free electron, $V_0 = 0$.

Therefore $$P = \frac{mV_0 ab}{\hbar^2} = 0$$

$\therefore$ from equation

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

We have $$\cos \alpha a = \cos ka \quad \text{i.e.,} \quad \alpha a = ka$$

or $$\alpha = k \qquad \text{...(1)}$$

But $$\alpha^2 = \frac{2mE}{\hbar^2} \quad \text{or} \quad E = \frac{\alpha^2 \hbar^2}{2m}$$

Therefore, form eqn. (1).

$$E = \frac{k^2 \hbar^2}{2m}.$$