

# **Semiconductor Physics(18PYB103J)**

## ***Module I – Lecture 2 & 3***



## Lecture 2 & 3 Topics

- **Density of states**
- **Energy band in solids**
- **Kronig- Penney model**

# Density of States

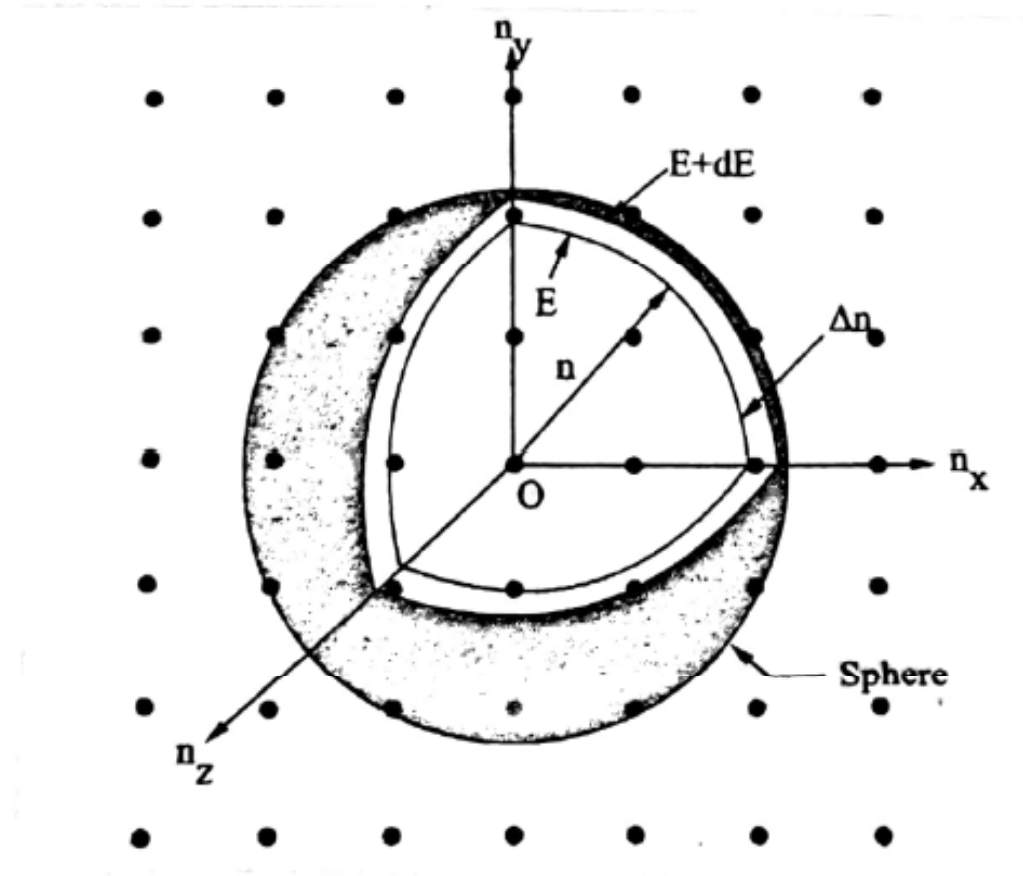
The density of states is defined as the number of available electron states per unit volume in an energy interval  $E$  and  $E + dE$ .

Let us consider a metal piece of side ' $l$ '. To find the density of states, construct a sphere of radius ' $n$ ' in the space as shown in diagram. The sphere is further divided into many shells corresponding to quantum numbers  $n_x$ ,  $n_y$  and  $n_z$ .

We consider two energy levels having values ' $E$ ' and  $E + dE$ , correspond to the quantum numbers  $n$  and  $n + dn$ .

$$\left. \begin{array}{l} \text{The no. of states within sphere} \\ \text{of radius } n \end{array} \right\} = \frac{4}{3} \pi n^3 \rightarrow (1)$$

We take only  $\frac{1}{8}$  of volume of sphere. because the quantum numbers are positive values.



The no. of states within  
the sphere of radius 'n' }  $= \frac{1}{8} \left[ \frac{4}{3} \pi n^3 \right] \rightarrow (2)$

The no. of states within  
the sphere of radius 'n' and  $n+dn$  }  $= \frac{1}{8} \left[ \frac{4}{3} \pi (n+dn)^3 \right] \rightarrow (3)$

The no. of states between the  
shells of radius n and  $n+dn$  }  $= \frac{1}{8} \frac{4}{3} \pi \left[ (n+dn)^3 - n^3 \right]$

$$= \frac{\pi}{6} \left[ n^3 + 3n^2 dn + 3n dn^2 + dn^3 - n^3 \right]$$

$$= \frac{\pi}{6} \left[ 3n^2 dn \right]$$



$$\text{No of states} = \frac{\pi}{2} (n) (ndh) \rightarrow (4)$$

The energy of the electron moving in a cubical metal piece of side 'l' is given by,

$$E = \frac{h^2 h^2}{8ml^2}$$

$$h^2 = \frac{8ml^2}{h^2} E \rightarrow (5)$$

$$h = \left( \frac{8ml^2}{h^2} \right)^{1/2} E^{1/2} \rightarrow (6)$$

...

Differentiating eqn (5) w.r.t  $E$

$$2n \, dn = \frac{8ml^2}{h^2} dE$$

$$n \, dn = \frac{1}{2} \left( \frac{8ml^2}{h^2} \right) dE \quad \rightarrow (7)$$

Substitute eqn (6) and (7) in eqn (4) we get,

$$\text{No of states} = \frac{\pi}{2} \left( \frac{8ml^2}{h^2} \right)^{1/2} E^{1/2} \frac{1}{2} \left( \frac{8ml^2}{h^2} \right) dE$$

$$\frac{\text{No of states}}{l^3} = \frac{\pi}{4} \left( \frac{8m}{h^2} \right)^{3/2} E^{1/2} dE$$

$$\text{Density of states } Z(E) dE = \frac{\pi}{4} \left( \frac{8m}{h^2} \right)^{3/2} E^{1/2} dE$$

Acc. to Pauli's exclusion principle,

$$Z(E) dE = 2 \times \frac{\pi}{4} \left( \frac{8m}{h^2} \right)^{3/2} E^{1/2} dE$$

$$Z(E) dE = \frac{\pi}{2} \left( \frac{8m}{h^2} \right)^{3/2} E^{1/2} dE \quad \rightarrow (8)$$



Carrier Concentration in metals:  $N(E) dE$

The number of electrons in the filled energy states between the energy intervals  $E$  and  $E+dE$  is given by,

$$N(E) dE = Z(E) dE \cdot F(E)$$

$$N(E) dE = \frac{\pi}{2} \left( \frac{8m}{h^2} \right)^{3/2} E^{1/2} dE \cdot F(E)$$

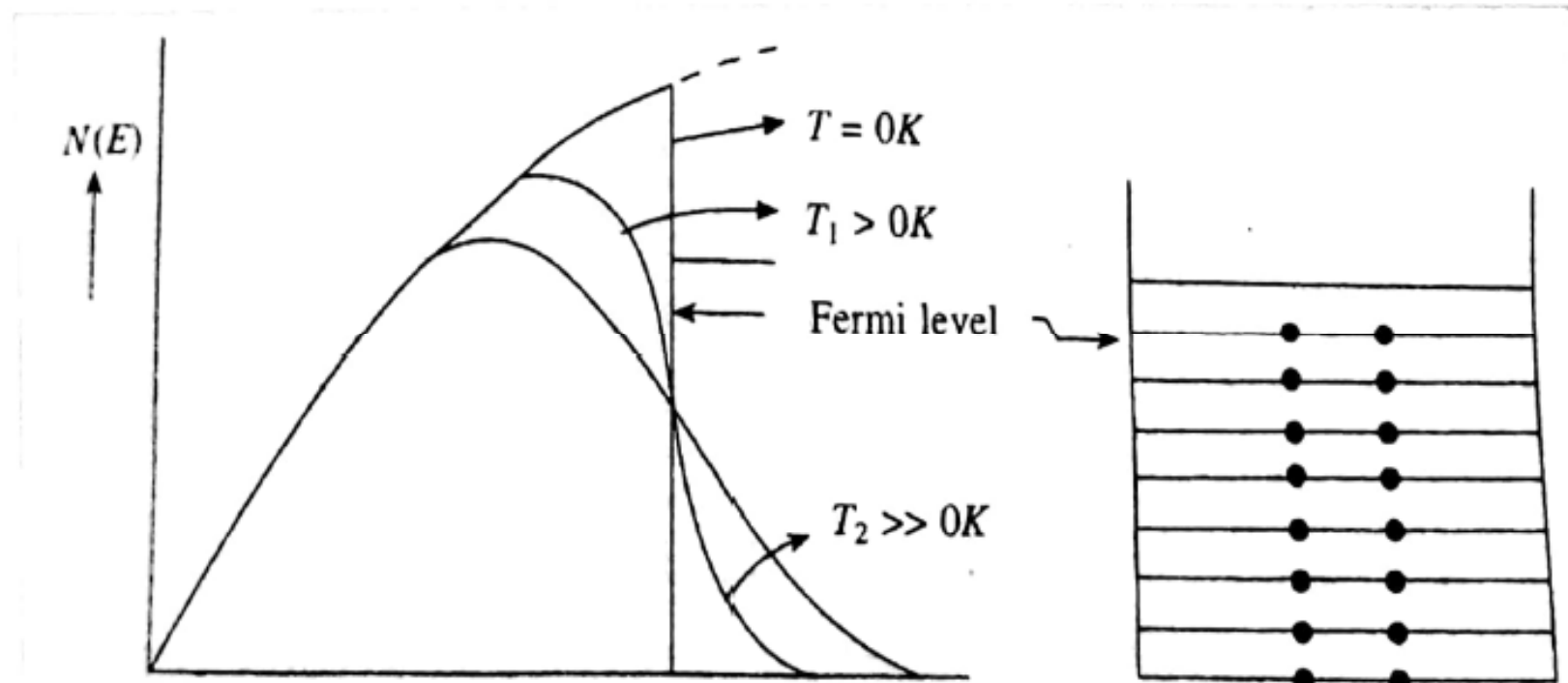
The Fermi energy of electrons at  $T=0K$ :

When  $T=0K$  ;  $F(E) = 1$

$$\therefore \int_0^N dN = \int_0^{E_{F_0}} \frac{\pi}{2} \left( \frac{8m}{h^2} \right)^{3/2} E^{1/2} dE$$

$$N = \frac{\pi}{3h^3} (8m)^{3/2} E_{F_0}^{3/2}$$

$$E_{F_0} = \frac{h^2}{8m} \left( \frac{3N}{\pi} \right)^{2/3}$$



# Band Theory of Solids

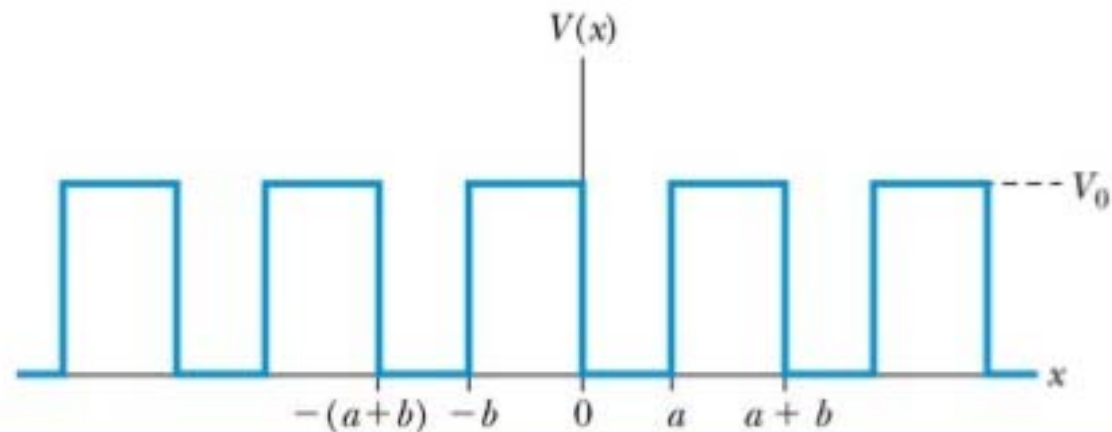
- Band/Zone theory was developed by Bloch in the year 1928.
- Free electrons move in a periodic potential provided by the lattice.
- It explains semi conductivity based on bands

# Band Theory of Solids

- **Band theory**, in solid-state physics, theoretical model describing the states of electrons, in solid materials, that can have values of energy only within certain specific ranges.
- The behaviour of an electron in a solid (and hence its energy) is related to the behaviour of all other particles around it.
- This is in direct contrast to the behaviour of an electron in free space where it may have any specified energy.
- The ranges of allowed energies of electrons in a solid are called allowed bands.
- Certain ranges of energies between two such allowed bands are called forbidden bands—i.e., electrons within the solid may not possess these energies.
- The band theory accounts for many of the electrical and thermal properties of solids and forms the basis of the technology of solid-state electronics.

# Kronig-Penney Model

- Kronig and Penney assumed that an electron experiences an infinite one-dimensional array of finite potential wells.
- Each potential well models attraction to an atom in the lattice, so the size of the wells must correspond roughly to the lattice spacing.

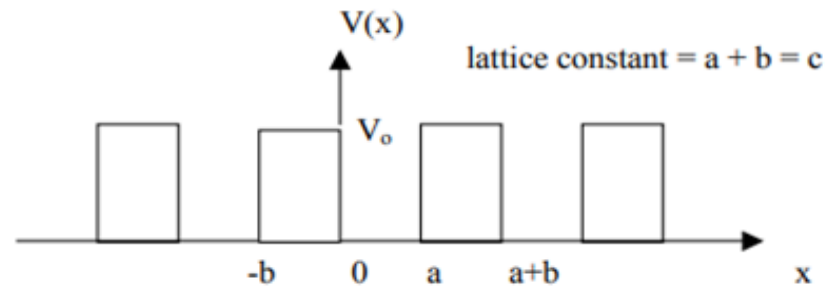


# Kronig-Penney Model

- The Kronig-Penney model is a simplified model for an electron in a one-dimensional periodic potential. The possible states that the electron can occupy are determined by the Schrödinger equation,

Consider the following idealized crystal potential:

We assume  $E < V_0$



for  $0 \leq x \leq a$ :

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

and

$$\psi = A \sin \alpha x + B \cos \alpha x \quad \frac{d\psi}{dx} = A \alpha \cos \alpha x - B \alpha \sin \alpha x \quad \alpha = \frac{\sqrt{2mE}}{\hbar}$$

and for  $-b \leq x \leq 0$ :

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



$$\psi = A \sin \alpha x + B \cos \alpha x \qquad \frac{d\psi}{dx} = A \alpha \cos \alpha x - B \alpha \sin \alpha x \qquad \alpha = \frac{\sqrt{2mE}}{\hbar}$$

and for  $-b \leq x \leq 0$ :

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

Solution is periodic, barrier of limited thickness - solution does not continue decaying to zero. There is tunneling between wells.

$$\psi = C \sinh(\gamma x) + D \cosh(\gamma x) \qquad \frac{d\psi}{dx} = C \gamma \cosh(\gamma x) + D \gamma \sinh(\gamma x)$$

$$\gamma = \frac{\sqrt{2m(V_o - E)}}{\hbar}$$

$\psi$  must be continuous at  $x = 0$ , so  $B = D$ .

Also,  $\frac{d\psi}{dx}$  must be continuous at  $x = 0$ , so  $A\alpha = C\gamma$  or  $C = (\alpha/\gamma)A$

From Bloch's theorem (Periodic potential)

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

and

$$\psi(a) = e^{jk(a+b)}\psi(-b)$$

$$\left.\frac{d\psi}{dx}\right|_a = e^{jk(a+b)} \left.\frac{d\psi}{dx}\right|_{-b}$$

Therefore

$$A \sin \alpha a + B \cos \alpha a = e^{jk(a+b)} (A \sinh(-\gamma b) + B \cosh(-\gamma b))$$

$$A \left[ \sin(\alpha c) + \frac{\alpha}{\gamma} e^{jk(a+b)} \sinh(\gamma b) \right] + B \left[ \cos(\alpha c) - e^{jk(a+b)} \cosh(\gamma b) \right] = 0$$

(42)

and

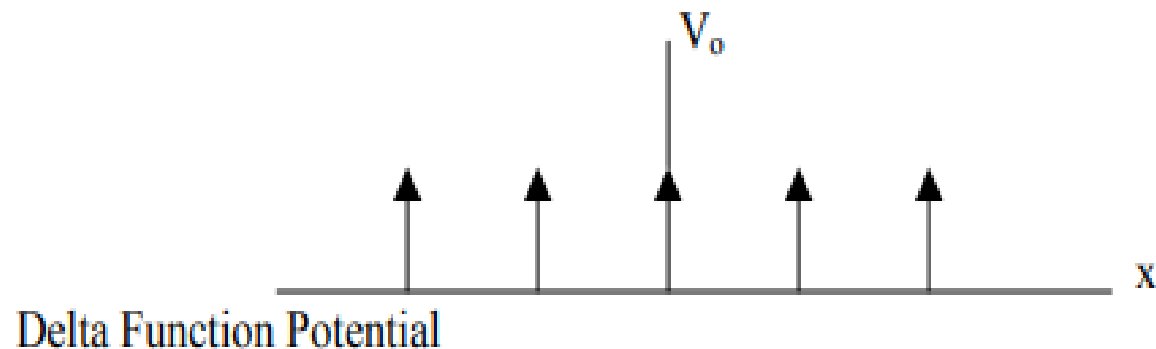
$$A\alpha \left[ \cos(\alpha c) - e^{jk(a+b)} \cosh(\gamma b) \right] + B \left[ -\alpha \sin(\alpha c) + \gamma e^{jk(a+b)} \sinh(\gamma b) \right] = 0$$

(43)

Equations (42) and (43) have a non-trivial solution (i.e. a solution other than  $A=B=0$  only if

$$\frac{\gamma^2 - \alpha^2}{2\alpha\gamma} \sin(\alpha x) \sinh(\gamma b) + \cos(\alpha x) \cosh(\gamma b) = \cos(k(b + c)) \quad (44)$$

At this point it is convenient to consider the special case in which  $b \rightarrow 0$  and  $V_0 \rightarrow \infty$  (makes things a little simpler – no problem for  $E > V_0$  transition) while the product  $V_0 b$  remains constant.



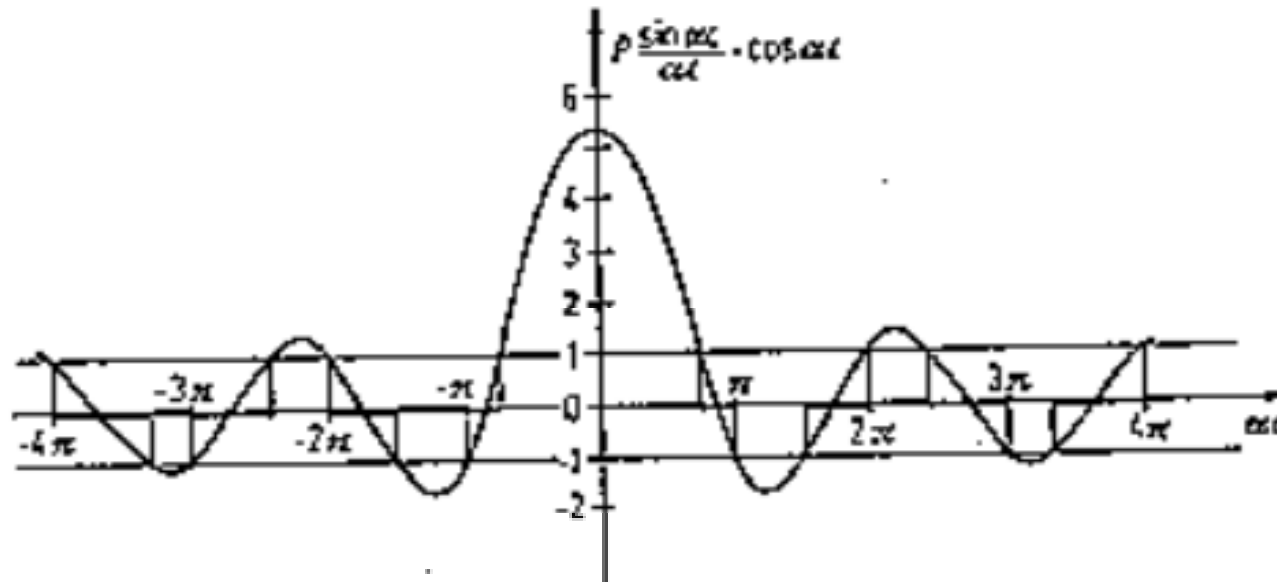
Letting  $P = (mV_0bc)/\hbar^2$ , (44) becomes

$$\frac{P}{\alpha c} \sin(\alpha c) + \cos(\alpha c) = \cos(kc)$$

(term 1)

(term 2)

This can be solved graphically. Solutions for  $P = 3\pi/2$  (corresponding to a high barrier) are shown below. We plot (1) and (2) as function of  $\alpha c$ .

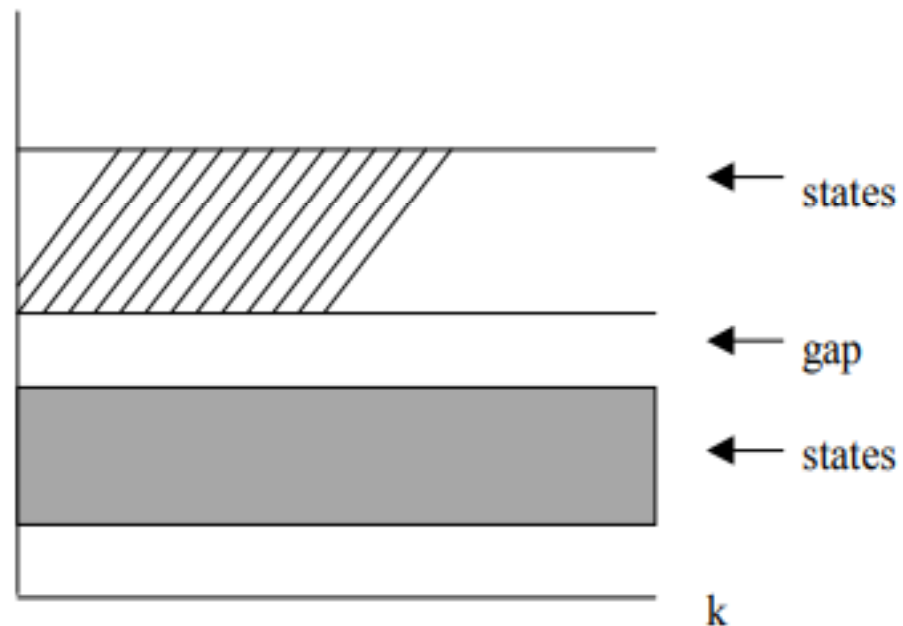


We can only have a Solution for this when

$$\frac{P}{\alpha c} \sin(\alpha c) + \cos(\alpha c) \leq 1$$

and as  $\cos(kc) \leq 1$  always we have a valid solution for ranges of  $\alpha c$  which implies a valid solution for particular energy regions.

E

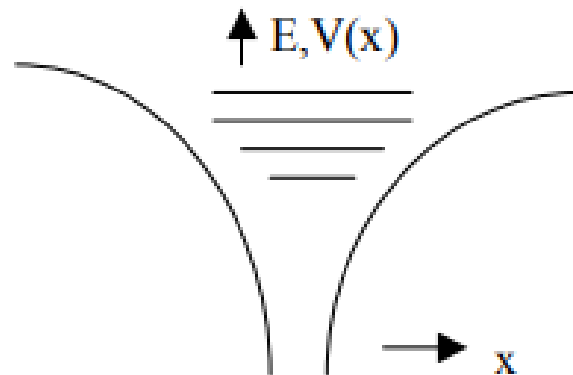


We therefore find there are  $\alpha$ 's for which there is no valid K. As  $E = \frac{\hbar^2}{2m} \alpha^2$

This means there are disallowed regions of energy, i.e., energy gaps.

## Energies and wave functions for electrons in crystal (periodic potential $V(x)$ )

### a) Isolated Potential well





b) Free Electrons

$$\psi(x) = Ce^{jkx}$$

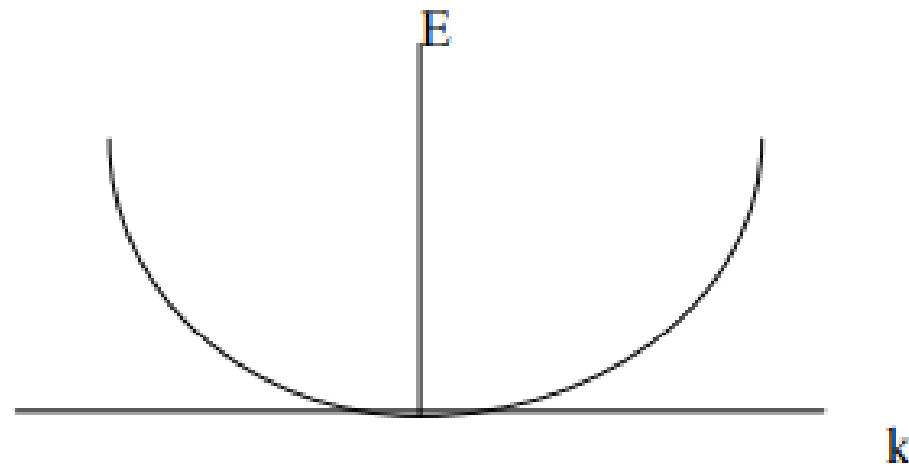
$$\Psi(x,t) = Ce^{j(kx - \omega t)}$$

- plane wave solutions

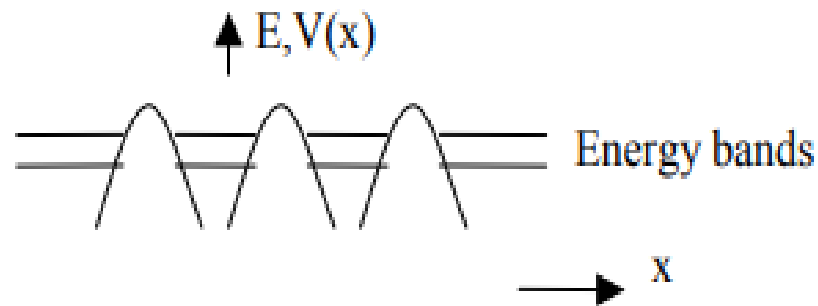
- any energy allowed:

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

- Parabolic E versus k



### c) Periodic Potential



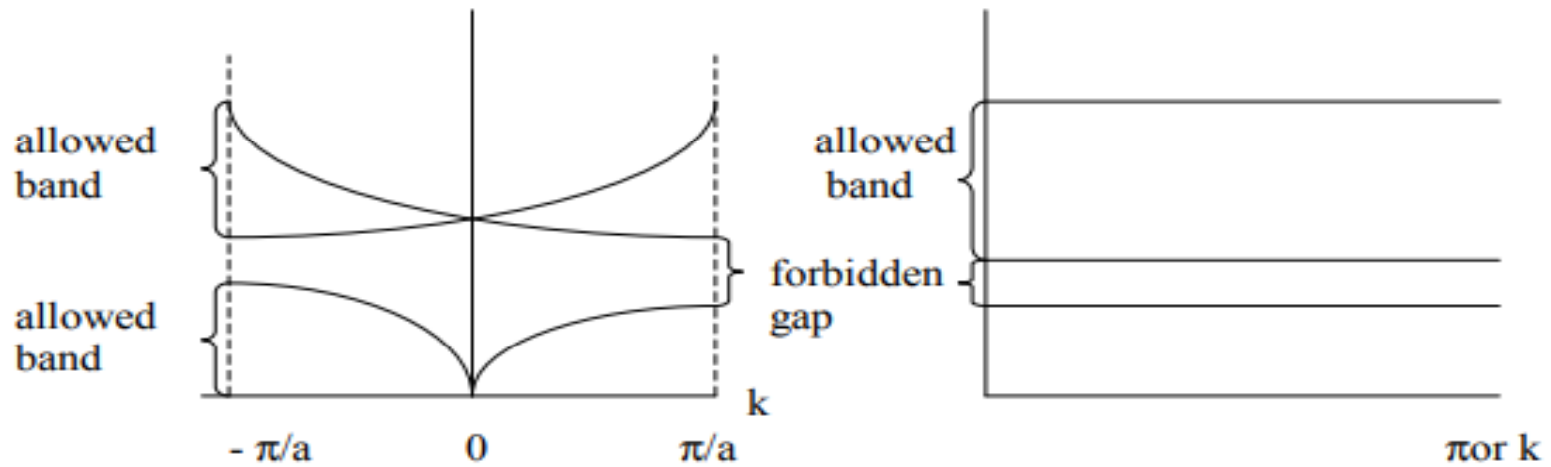
- ability of electrons to tunnel between barrier walls spreads out the discrete energy levels seen for isolated wells into bands

- We find a number of bands of energies are allowed.
- We have restricted  $k$  values:  $(-\pi / a \leq k \leq \pi / a)$
- The wave functions are Bloch waves:  $\psi_k(x) = U_k(x)Ce^{jkx}$

$\psi_k(x, t) = U_k(x)e^{j(kx - \omega t)}$  - which is modulated travelling wave

- Waves functions act like free electrons (almost)

Simplified energy diagram:



General results from Kronig-Penney model:

- if potential barrier between wells is strong, energy bands are narrowed and spaced far apart

(Corresponds to crystals in which electrons are tightly bond to ion cores, and wavefunctions do not overlap much with adjacent cores. Also true for lowest energy bands)

- if potential barrier between wells is weak, energy bands are wide and spaced close together (this is typically situation for metals with weakly bond electrons – e.g. alkali metals. Here the “nearly free” electron model works well.)