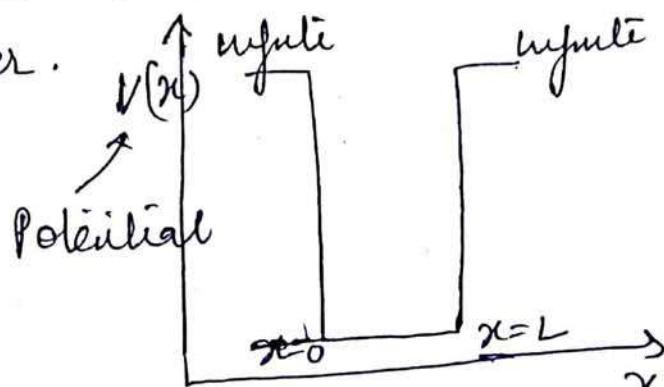


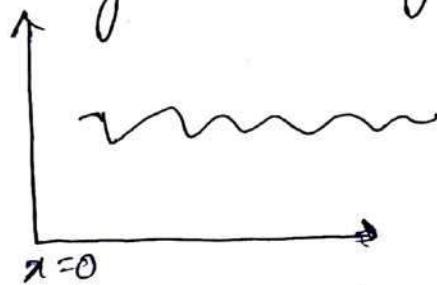
## Application of Schrodinger's Equations

- i) Particle in One dimensional Box: Infinite Potential Barrier.



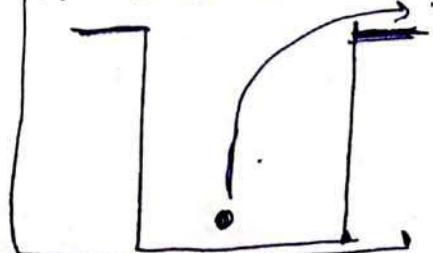
- The given diagram is the profile of potential v/s distance  $x$ .

- The particle may exist anywhere from  $x=0$  to  $x=\infty$



- But the Potential profile is such that for  $x > L \} \text{ potential is } \infty$  and for  $x = 0 \rightarrow L \} \text{ potential } = 0$

- So if the particle is located in b/w  $x=0$  to  $x=L$ , so particle has to have infinite amount of potential energy or we can say that, it requires infinite amount of ~~more~~ potential energy to reach beyond the distance  $L$  or outside the box of having length  $L$ .



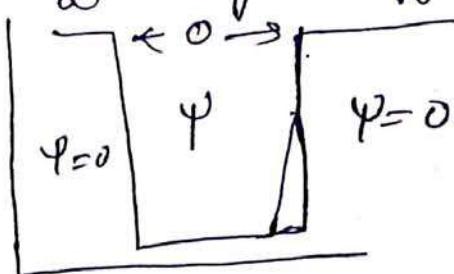
- Since potential energy required is infinitely large so it is impossible for the particle to be located outside the box, particle remains confined in Box.

- So magnitude of wave function outside the box will be zero, and inside the box we need to determine the nature of the wave function.

- Inside the Box  $V=0$

so Schrodinger eq<sup>n</sup> reduces to

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi \quad \text{--- (2)} \Rightarrow \frac{d^2\psi}{dx^2} = -\frac{E\psi}{\frac{2m}{\hbar^2}}$$



The general solution of eq (2) defined in this form is given by

$$\psi = A \sin(kx) + B \cos(kx) \quad \text{--- (3)}$$

$\downarrow$   
A and B are constant coefficient

- And the value of  $k$ , now from eq<sup>n</sup> (1) and (2)

$$\frac{d^2\psi}{dx^2} = -k^2 [A \sin(kx) + B \cos(kx)]$$

$$+ \frac{E\psi}{2m} = -k^2 \psi.$$

$$\Rightarrow k^2 = \frac{E2m}{\hbar^2} \Rightarrow k = \sqrt{\frac{2Em}{\hbar^2}}$$

(K)

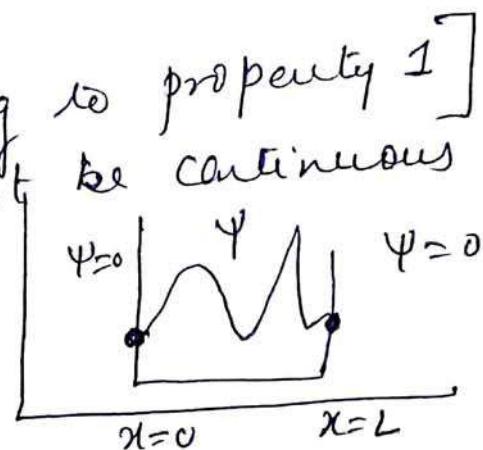
Apply Boundary Condition to identify the values of A, B and K.

→ at  $x=0$ ,  $\psi=0$  [According to property 1]  
 $\psi$  must be continuous

so

$$\psi(x=0) = A \sin 0 + B \cos 0$$

$$B=0$$



so from eq ③

$$\boxed{\psi = A \sin(Kx)} \quad \text{--- (4)}$$

sol<sup>n</sup>

→ at  $x=L$ ,  $\psi=0$  [According to property 1)

so

$$\psi(x=L) = A \sin(KL)$$

$$0 = A \sin(KL)$$

for  $K = \frac{n\pi}{L}$ , eq<sup>n</sup> will be satisfied.

Now from eq<sup>n</sup> ④

$$\Rightarrow \frac{n\pi}{L} = \sqrt{\frac{2E}{m}}$$

solve for E

$$\boxed{E_n = \frac{n^2\pi^2}{L^2} \frac{h^2}{2m}} \quad \text{--- (5)}$$

→ From eq ④

$$\boxed{\psi = A \sin\left(\frac{n\pi}{L}x\right).} \quad \text{sol<sup>n</sup>}$$

→ Apply fluid property

$$\int_0^L |\psi|^2 dx = 1$$

$$\cos^2 \alpha = 1 - 2 \sin^2 \alpha$$

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

$$\sin^2 \alpha = \frac{1 - \cos 2\alpha}{2}$$

$$\Rightarrow \int_0^L A^2 \left[ \frac{1 - \cos 2 \frac{n\pi}{L} x}{2} \right] dx = 1$$

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

$$\Rightarrow \frac{A^2 L}{2} - \frac{A^2}{2} \left( \frac{2n\pi}{L} \right) \sin \left( \frac{2n\pi L}{L} \right) + 0 = 1$$

Even integr. Always zero.

$$\therefore \frac{A^2 L}{2} = 1 \Rightarrow A = \sqrt{\frac{2}{L}}$$

$$\boxed{\psi = \sqrt{\frac{2}{L}} \sin \left( \frac{n\pi}{L} x \right)}$$

∴ the final sol<sup>n</sup> of our wave function.

- Now consider how the wave particle behaves inside the box.

$$\text{for } n=1, \psi = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}x\right)$$

$$\text{at } x=0, \psi = 0$$

$$\text{at } x=L, \psi = 0$$

$$\text{at } x=\frac{L}{2}, \psi = \sqrt{\frac{2}{L}}$$

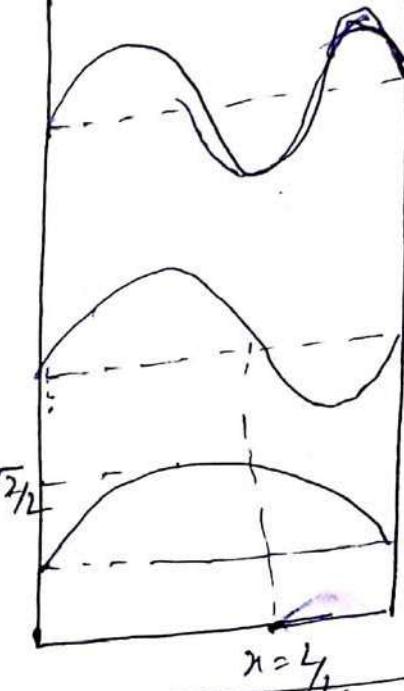
$$\text{for } n=2, \psi = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi}{L}x\right)$$

$$\text{at } x=0, \psi = 0$$

$$\text{at } x=\frac{L}{2}, \psi = 0$$

$$\text{at } x=L, \psi = 0$$

$$\text{at } x=\frac{L}{4}, \psi \rightarrow \text{maximum Amplitude}$$



$n=1$

$$\# \text{ at } n=1 \quad E_1 = \frac{\pi^2 \hbar^2}{2mL} \quad E_3 = \frac{3^2 \pi^2 \hbar^2}{2mL}$$

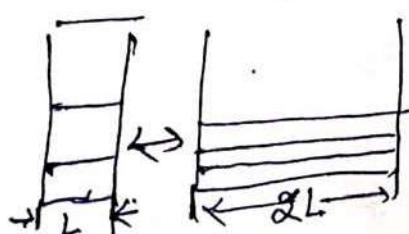
$$E_2 = \frac{2^2 \pi^2 \hbar^2}{2mL}$$

- So from the above we have observed that frequency or wavelength of all wave function changes as the value of  $n$  changes.. and at different values of  $n$  Energy of all wave function is different so the Energy is quantized bcoz it does not take values b/w  $E_1$  and  $E_2$

- The Energy gap b/w  $E_1$ ,  $E_2$  and  $E_2$ ,  $E_3$  is also different and this gap increases with value of  $n$ . and also depends on the length of the box.

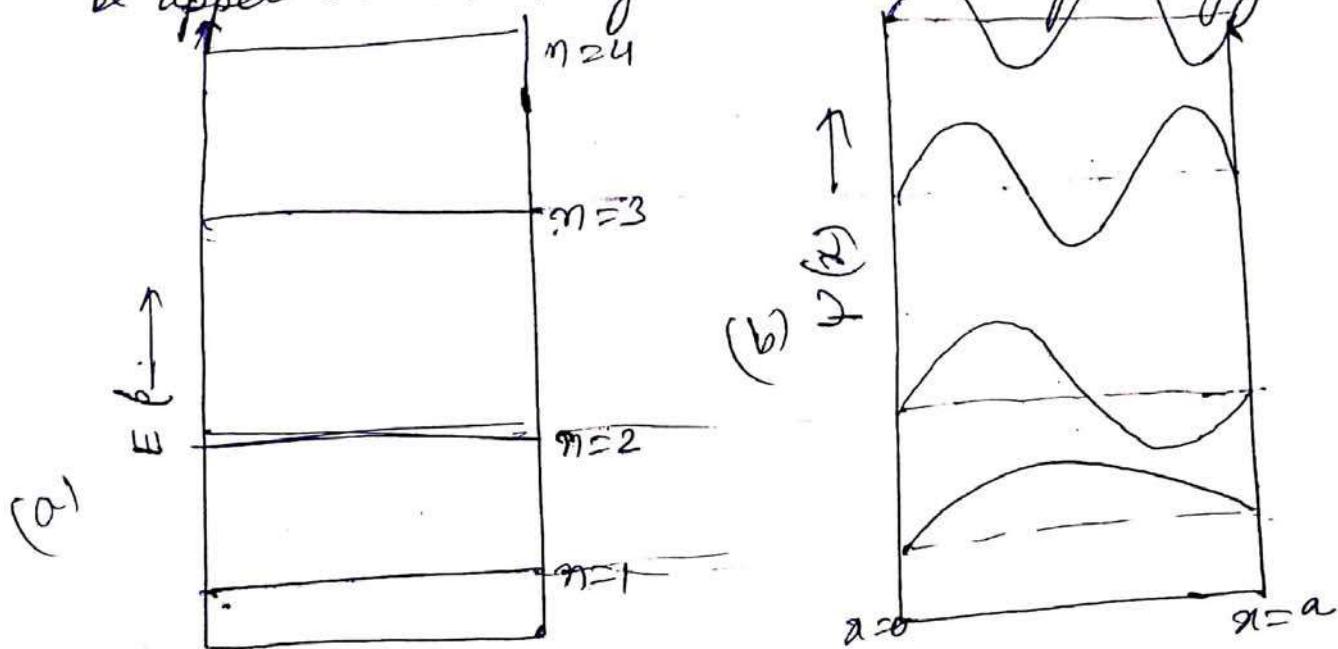
$$\therefore \Delta E_n = E_n - E_{n-1} = \frac{\pi^2 \hbar^2}{2mL^2} [n^2 - (n-1)^2]$$

$$= \frac{\pi^2 \hbar^2}{2mL^2} [2n-1]$$



$\Delta E \uparrow$  as  $L \downarrow$

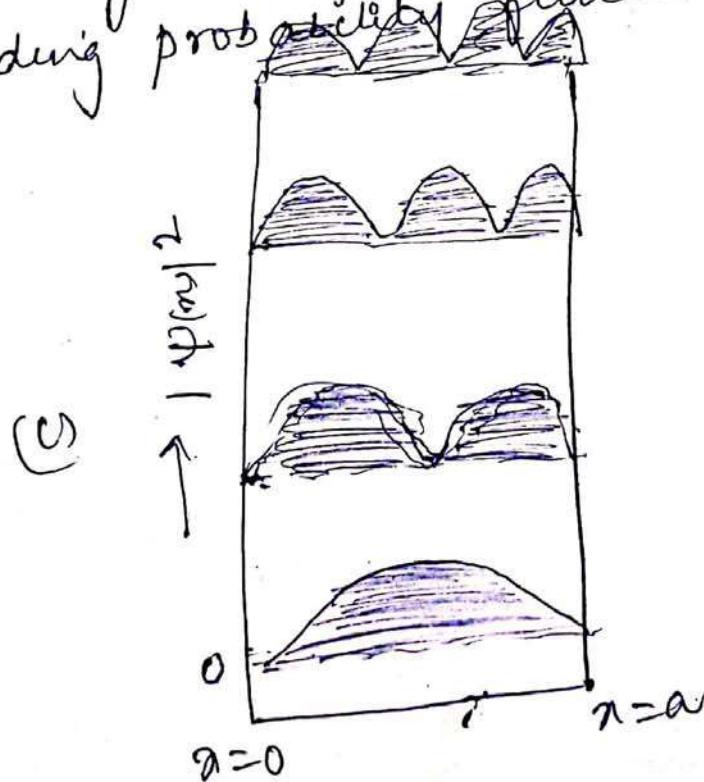
Also as the mass increases the Energy decrease so and also the gap decreases. For heavier mass bodies, the Energy of the particle is appeared to be continuous as the gap b/w the Energy level is very small, and it seems to be appear that taking all values of Energy.



(a) Four lowest discrete energy levels.

(b) Corresponding wave functions

(c) Corresponding probability functions



Tut

Q1 Calculate the first three energy levels of an electron in an infinite potential well.

Consider an electron in an infinite potential well of width  $5 \text{ Å}$ .

$$\text{Soln} \quad E_n = \frac{\hbar^2 n^2 \pi^2}{2 m A^2} = \frac{n^2 (1.054 \times 10^{-34})^2 \pi^2}{2 (9.11 \times 10^{-31})(5 \times 10^{-10})^2}$$

Length of the well  
 $= n^2 (2.41 \times 10^{-19}) \text{ J}$

$$\text{or } E_n = \frac{n^2 (2.41 \times 10^{-19})}{1.6 \times 10^{-19}} = n^2 (1.51) \text{ eV}$$

Then  $E_1 = 1.51 \text{ eV}$ ,  $E_2 = 6.04 \text{ eV}$ ,  $E_3 = 13.59 \text{ eV}$

Q2 Calculate the first three allowed energy level (in eV) for an electron. The width of an infinite potential well is  $12 \text{ Å}$ .

Q3 Calculate the penetration depth of a particle impinging on a potential barrier. Consider an incident electron that is travelling at a velocity of  $1 \times 10^5 \text{ m/s}$  in region II



$$E = \frac{1}{2} m v^2 = \frac{1}{2} (9.11 \times 10^{-31}) (1 \times 10^5)^2 \text{ J} = 2.85 \times 10^{-19} \text{ eV}$$

Assume barrier height is twice the energy,

$$V_0 = 2E$$

The wave function soln in region 3.

$$\Psi(n) = B_3 e^{-\alpha x} \quad \text{where } \alpha = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

In this, we want to determine the distance at which the wave function magnitude decayed to  $e^{-1}$  of its value.

$$\therefore \frac{1}{\alpha} = \frac{1}{\sqrt{2m(V_0 - E) / h^2}}$$

$$\text{when } \alpha = \sqrt{\frac{2m(V_0 - E)}{h^2}}$$

$$\frac{1}{\alpha} = \sqrt{\frac{2m(V_0 - E)}{h^2}}$$

$$I = \alpha \propto \sqrt{\frac{2m(V_0 - E)}{h^2}} \quad V_0 = 2E$$

$$\frac{1}{\alpha} = \sqrt{\frac{2mE}{h^2}}$$

$$\alpha \propto \sqrt{\frac{h^2}{2mE}}$$

$$= \frac{1.0054 \times 10^{-34}}{\sqrt{2(9.11 \times 10^{-31})(1.58 \times 10^{-24})}}$$

$$= 11.6 \times 10^{-10} \text{ m}$$

$$\text{or. } d = 11.6 \text{ Å}$$

$$\begin{matrix} 10^{-3} \\ 10^{-2} \\ 10^{-1} \\ 10^0 \end{matrix}$$

$$\begin{matrix} 10^{-2} \\ 10^{-1} \end{matrix}$$

$$\begin{matrix} 10^{-2} \\ 10^{-1} \end{matrix}$$

Tut

Transmission Coefficient: it is defined as the ratio of the transmitted flux to the incident flux in region 2  
 for special case when  $E \ll V_0$ , we find that

$$T = 16 \left( \frac{E}{V_0} \right) \left( 1 - \frac{E}{V_0} \right) \exp(-2k_2 a) \quad \text{--- (1)}$$

↳ Transmission coefficient when  $k_2 = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$

Q. Calculate the probability of an electron tunneling through a potential barrier.  
 consider an electron with an energy of 2 eV impinging on a potential barrier with  $V_0 = 20$  eV and a width of  $3\text{A}^\circ$

Soln

convert unit Joul & Nm

$$k_2 = \sqrt{\frac{(2 \times 9.11 \times 10^{-31})(20-2)(1.6 \times 10^{-19})}{(1.054 \times 10^{-34})^2}}$$

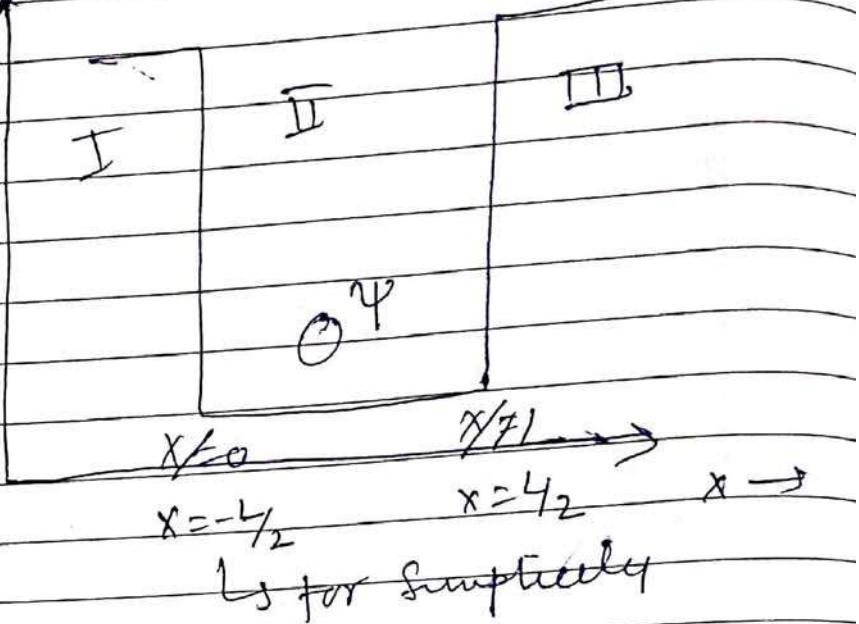
$$k_2 = 2.17 \times 10^{10} \text{ m}^{-1}$$

when  $T = 16 \left( \frac{2}{20} \right) \left( 1 - \frac{2}{20} \right) e^{(-2 \times 2.17 \times 10^{10})(3 \times 10^{-10})}$

$$\boxed{T = 3.17 \times 10^{-6}} \quad \underline{\text{Ans}}$$

## 2. Particle in a 1 D Box : Finite Potential Barrier

- Outside the Box in the previous example,  $V = \infty$  we assumed that wave function does not exist there but now we can write Schrödinger equation outside the box. Using the same idea here we can write while.



- As we know

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

- Inside the Box, the Schrödinger eq<sup>n</sup> is for  $-L/2 < x < L/2$

$$\frac{-\hbar^2}{2m} \frac{d^2 \psi_2}{dx^2} = E \psi_2 \quad (1)$$

or  $\frac{d^2 \psi_2}{dx^2} = -\frac{E}{2m} \frac{1}{\hbar^2} \Rightarrow \frac{d^2 \psi_2}{dx^2} + \frac{E}{2m} \frac{1}{\hbar^2} = 0$

- We can also write the Schrödinger eq<sup>n</sup> outside the box also.

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi_1}{dx^2} + V_0 \psi_1 = E \psi_1 \quad (for Region I, III)$$

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi_3}{dx^2} + V_0 \psi_3 = E \psi_3 \quad (3)$$

Let us assume that potential height in region 3 is  $V_0$ . When  $E < V_0$ , it means the particle is dying somewhere in region 2.

But as  $E < V_0$ , it is quite odd, but it is one of the feature of Quantum Mechanics. so we can write Schrödinger eq<sup>n</sup> in region 1 and region 3.

This seems to be difficult assumption, if  $E < V_0$ , it means particle exist somewhere in region 2, and its got total Energy  $E$ , and that Energy  $E$  is less than the potential height ( $V_0$ ). It sounds a bit odd, but is one of the feature of Quantum mechanics. and if  $E < V_0$ , then K.E becomes.

From eq<sup>n</sup> ① ② and ③ we, that is the

$$\frac{d^2\psi_1}{dx^2} (V_0 - E) \psi_1 =$$

implication of it is that what classical mechanics tells according to that if K.E is negative then particle can not have existence. But here we are able to write the eq<sup>n</sup> outside the box

$$\frac{d^2\psi_1}{dx^2} = \frac{2m(V_0 - E)}{\hbar^2} \psi_1 \Rightarrow \frac{d^2\psi_1}{dx^2} = -K^2 \psi_1$$

$$K = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

$$\frac{d^2\psi_2}{dx^2} = -\frac{2mE}{\hbar^2} \psi_2 \Rightarrow \frac{d^2\psi_2}{dx^2} = -K^2 \psi_2 \quad \text{if } E < V_0$$

$$\frac{d^2\psi_3}{dx^2} = \frac{2m(V_0 - E)}{\hbar^2} \psi_3 \Rightarrow \frac{d^2\psi_3}{dx^2} = -K^2 \psi_3.$$

Sols to above eq<sup>n</sup> is

$$\psi_1 = A_1 e^{Kx} + B_1 e^{-Kx} \quad \text{--- (1)}$$

$$\psi_2 = A_2 e^{-ikx} + B_2 e^{ikx} \quad \text{--- (2)}$$

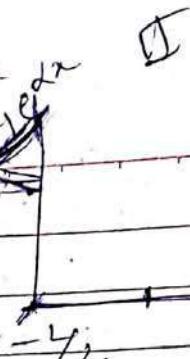
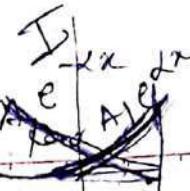
$$\psi_3 = A_3 e^{Kx} + B_3 e^{-Kx} \quad \text{--- (3)}$$

\* as  $n$  is -ve (Region I)

$$\Psi_1 = A_1 e^{+lx} + B_1 e^{-lx}$$

$$= A_1 e^{+lx} + (B_1 e^{-lx})$$

$$\text{so } \Psi_1 = A_1 e^{-lx}$$



$$-y_2 \quad y_2$$

(A)

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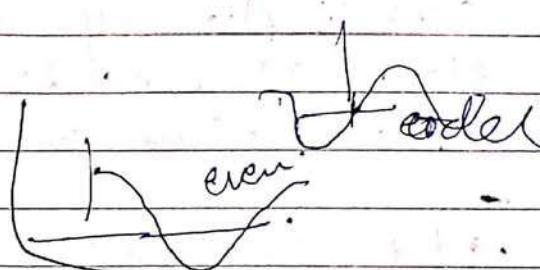
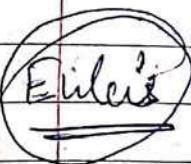
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→

$$/ \text{water} \quad v = w P Z L R t y v E g o$$

youtube link for Quantum tunneling

<https://www.youtube.com/watch?v=RF7d03trm>



→ The wave function in region 3 is given by  $\psi_3 = A_3 e^{kx} + B_3 e^{-kx}$

for the case  $E < V_0$ , the coefficient  $B_3$  is not zero. If  $B_3$  is not zero, then probability density function of the particle being found in region 3 is not equal to zero.

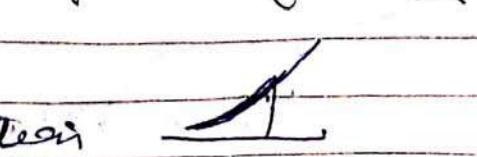
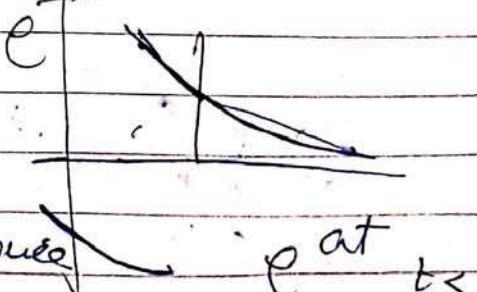
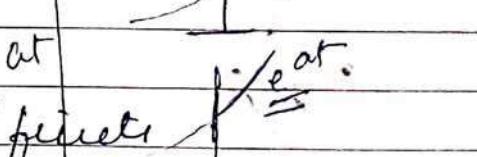
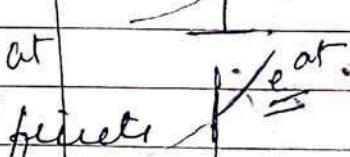
This result implies that there is a finite probability that the incident

particle will penetrate the potential barrier and exist in region 3.

The probability of a particle penetrating the potential barrier is another difference b/w classical and quantum mechanics.

The quantum mechanical penetration is classically not allowed.

for  $E < V_0$ .



## Molecular orbital formation

(1) To understand what happens when these atoms come together to form solids.

- Consider the Hydrogen atom.
- Hydrogen has one electron, with electronic configuration  $1s^1$ . When two H-atoms come together there are two  $1s$  atomic orbitals (AOs) and these form two molecular orbitals (MOs).

(2) For simplicity, let us denote the AO of H atom by  $\psi_{1s}$ .

(3) In Quantum Mechanics  $\Psi$  refers to the wave function of the electron and the product of  $\Psi$  with its complex conjugate  $\Psi^*$  gives the probability distribution of electrons.

(4) The wave function can be solved using Schrodinger equation in spherical coordinates and the wave function  $SOI^n$  for the  $1s$  orbital is given by

$$\Psi(r) = \frac{1}{\sqrt{\pi}} \left(\frac{1}{a_0}\right)^{3/2} e^{-\frac{r}{a_0}}$$

where  $a_0$  refers to Bohr radius and has a value of  $0.53 \text{ \AA}$ ,

The  $SOI^n$  is an exponential function with its value decreasing as  $r$  increases i.e moving away from the nucleus.

- Consider two H atoms A and B with AO's  $\Psi_{1s}^A$  and  $\Psi_{1s}^B$ .

There are two ways in which AO's can come together to form two MO's.

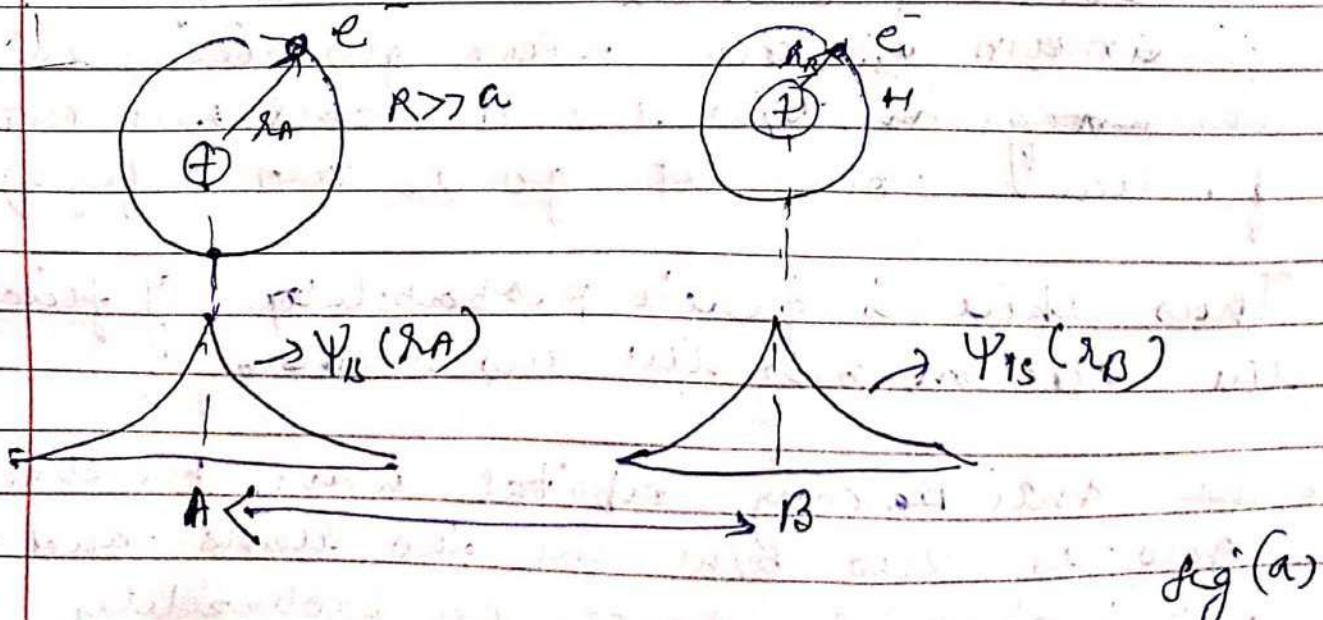
- The two AO's can be added, and this is called the bonding orbital, ( $\sigma_s$ ) or they can be subtracted giving antibonding orbital ( $\sigma^{*}$ ).
- The orbital can be represented by

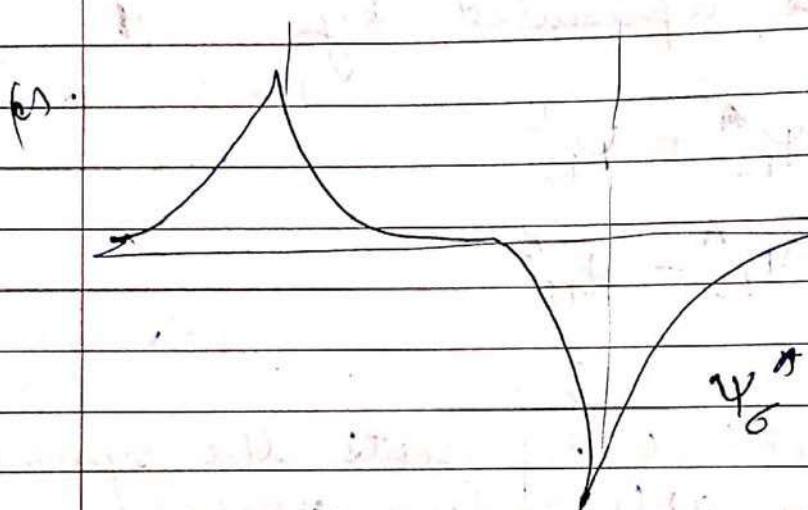
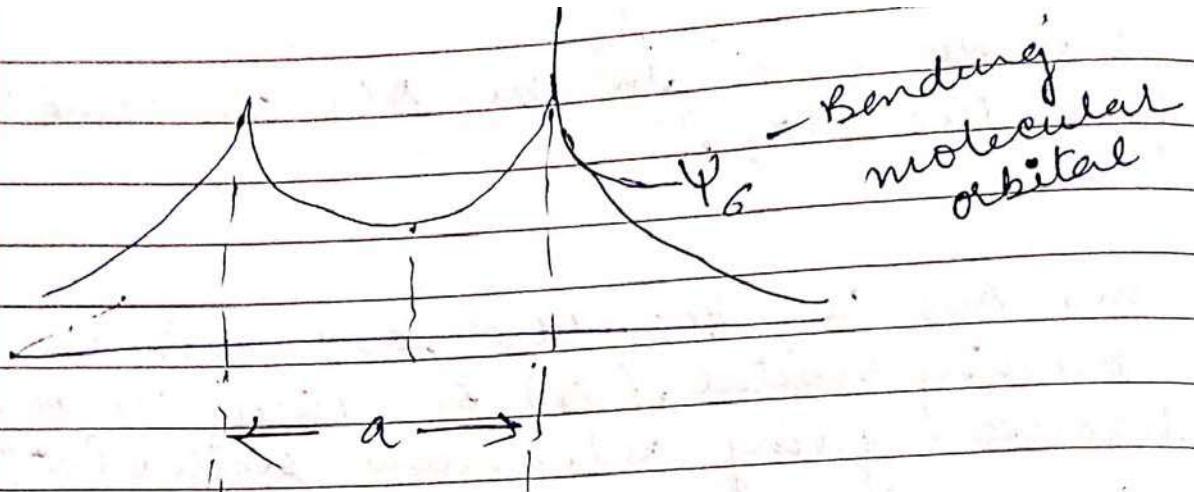
$$\sigma = \Psi_{1s}^A + \Psi_{1s}^B$$

and

$$\sigma^* = \Psi_{1s}^A - \Psi_{1s}^B$$

- The Bonding Orbital represents the symmetric MO, while the antibonding orbital represents the anti-symmetric MO.





- The Bonding Orbital shows a local minimum in the wave function in the region b/w the two H-atoms but the function does not go to zero (fig a)

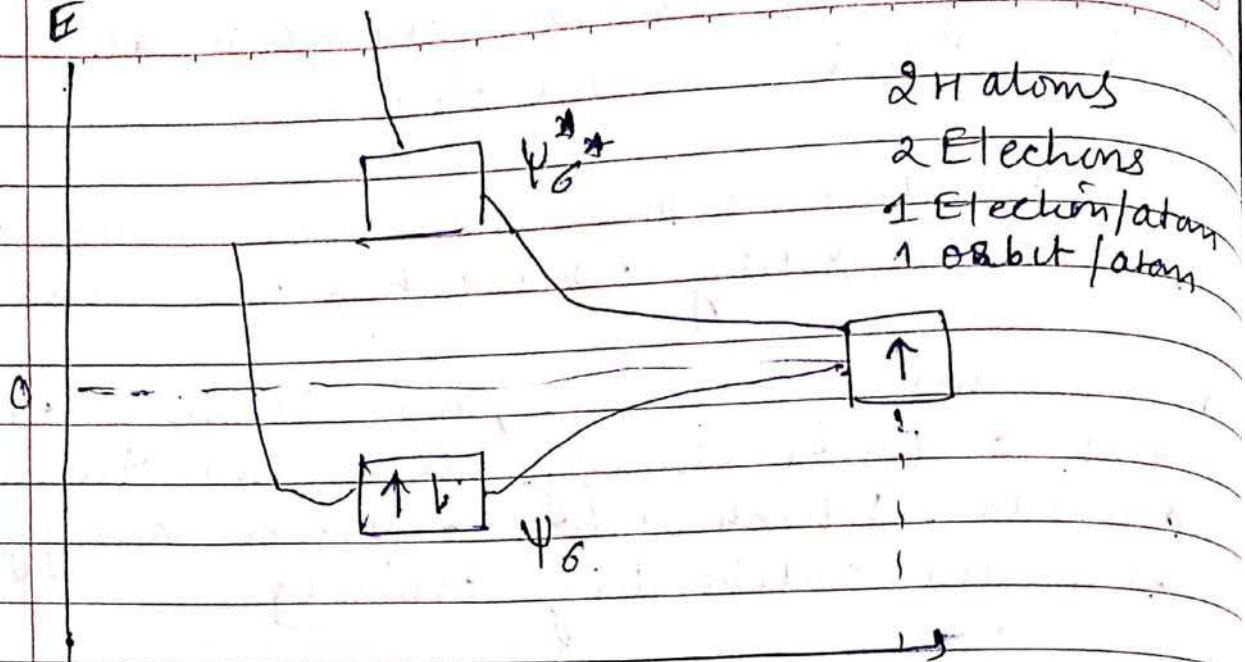
Thus there is finite probability of finding the electron b/w the two atoms.

- The Anti-Bonding orbital wave function goes to zero b/w the two atoms and the probability hence the probability

of finding the electron in the two atoms is zero. This is called node.

- The Bonding orbital has zero node and the antibonding orbital has one node.
- In terms of energy, the bonding orbital has a lower energy than the individual orbitals, which have a lower energy than the antibonding orbital.  
This is because in bonding orbital ( $\sigma$ ) the electron is 'Shared' by both nuclei. Which leads to a lower energy.
- If two H-atoms come together, then both electrons will go to the bonding  $\sigma$  orbital (the electron will have opposite spin; in accordance with Pauli exclusion principle) since this will lower the overall energy of the system.
- The electron filling can be represented by an energy versus bond length plot. Shown in fig below

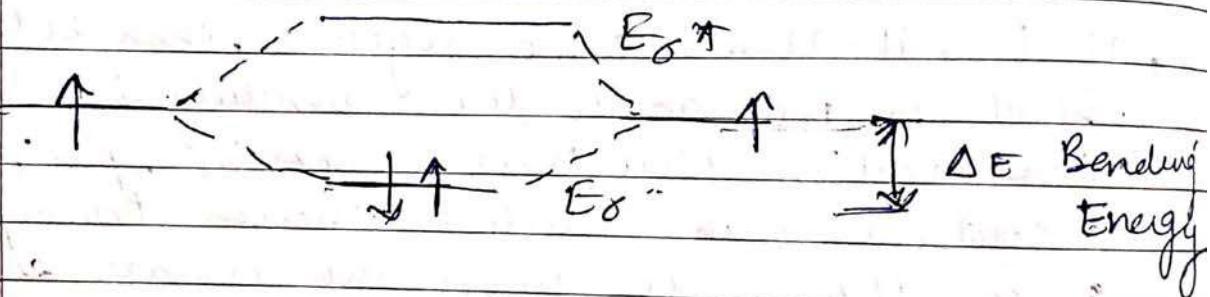
E



fig(d)

Large distance  
Energy bond length plot for two H atoms

fig(e)



The schematic representations of the formation of the  $H_2$  molecule.

Both electrons go to the bonding orbital while the antibonding orbital is empty.

- At large interatomic distance, the H atoms occupy their individual atomic energy levels.
- When they start to come together the two atoms start to feel each

other, the AOs then mix and form MOs.

- There is an equilibrium distance of separation where the energy of the system is minimum. Both electrons occupy this minimum in the bonding orbital. shown in fig(d).
- Formation of Bands in n Atoms
- Consider the splitting of energy levels. here it is a plot of energy versus distance b/w the atoms (from A-H not)

## (6) Electrons in periodic lattice:-

Now consider several atoms and they are arranged in a very periodic linear arrangement. So these different atoms are placed in a nice periodic arrangement; one-dimensional or along this dimension, atoms are placed.

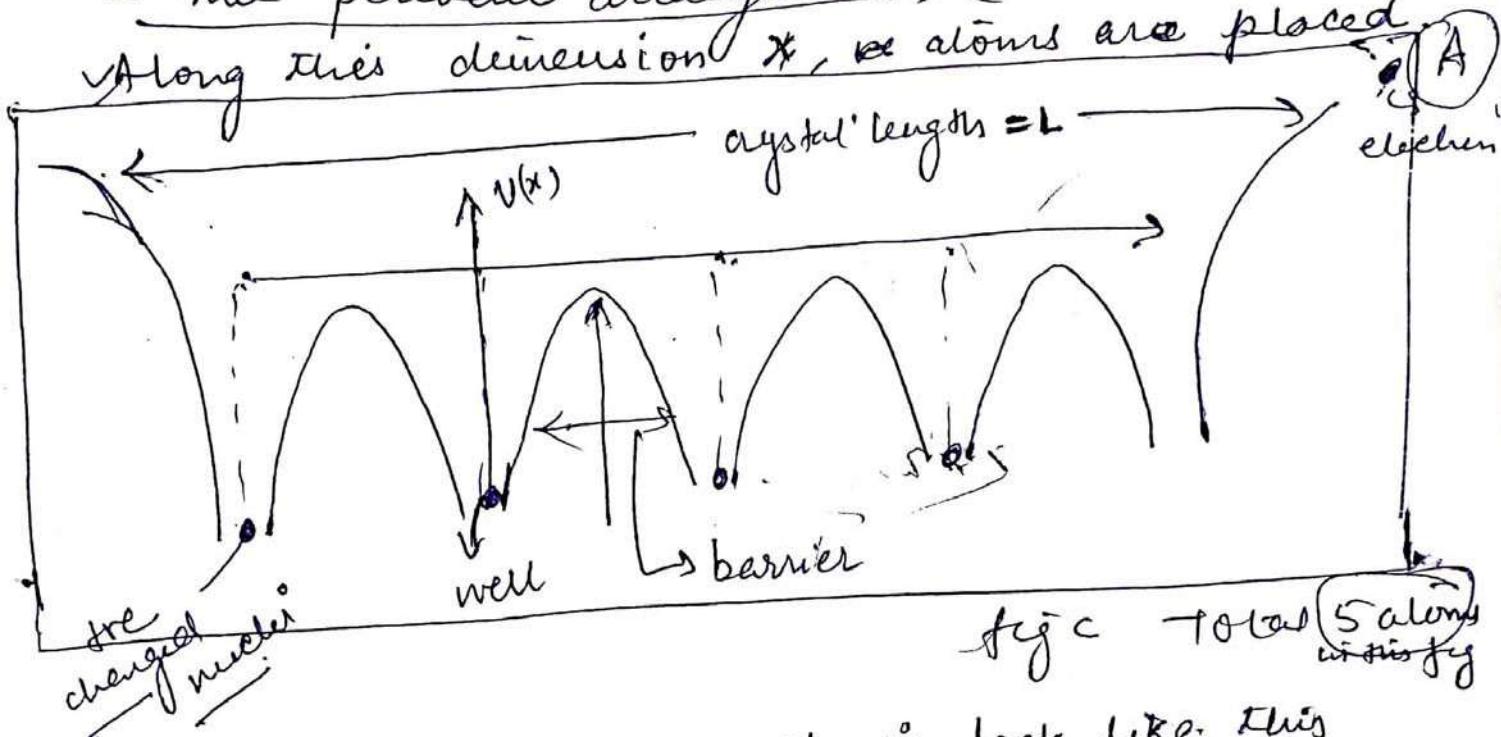
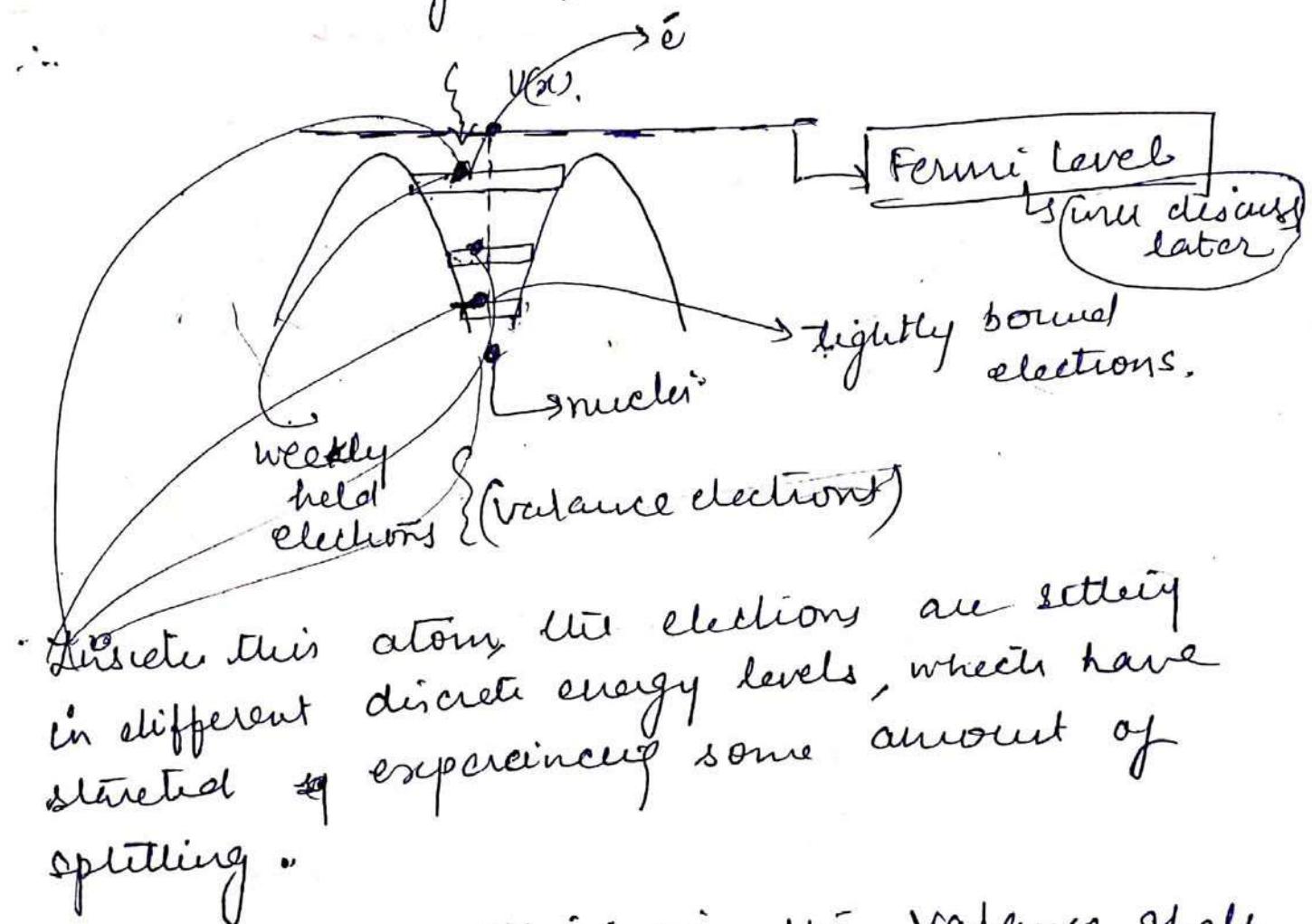


fig c Total 5 atoms

- The potential energy profile is look like this as shown in above fig when they are placed close to each other.
- Crystal  $\rightarrow$  is the periodic arrangement of atoms.
- and length of the crystal is  $L$ .
- Consider a electron which is sitting a position (A), does not sit at the edges of the crystal as it is completed where the potential is zero at the edges and electron here is completely free and does not have any knowledge about the structure.
- We have periodic arrangement of potential wells. and also have well of periodic barrier potential b/w these wells.

- In the fig we have represented the potential term by  $V(x)$ . It is the potential energy term in a Schrödinger equation.

- Inside this crystal, take a particular atom.



- Inside this atom the electrons are sitting in different discrete energy levels, which have started experiencing some amount of splitting.

- The electron sitting in the valence shell gets excited & got some thermal energy and could jump into higher energy level higher and occupy the energy level above the Fermi level. Now we can say this electron is <sup>now</sup> setting in different potential wells and is free to move about the solid.

So we can say there are two kind  
of boxes, or potential well  
~~two kind of potential~~  
when ~~one~~ The first is the potential well  
prescribed by each atom and the second  
when they escape from the clutch of the  
atom, and enter into higher energy states.

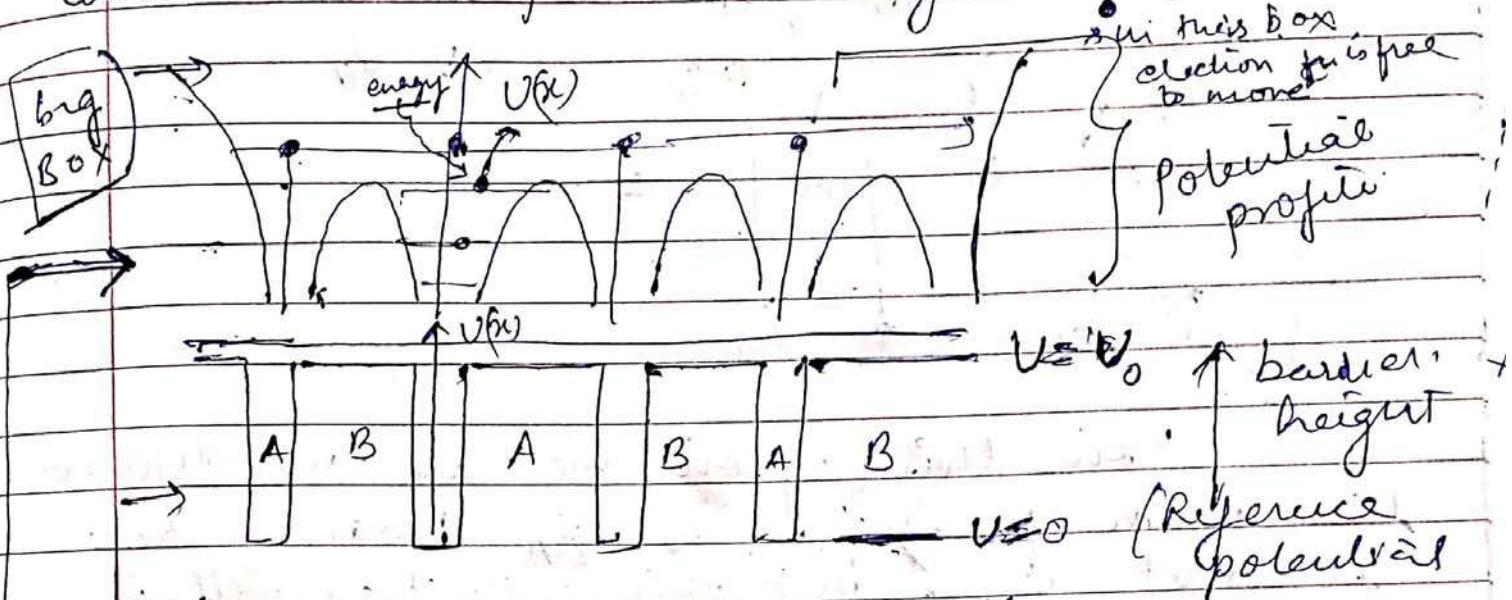
- so now we are going to use all these  
ideas to develop more mathematical estimate  
i.e in regard with the formation of energy  
bands, and energy gaps in a solid. and  
all this is done by called Kroneq  
Penney Model

19, 29, 35, ~~37~~, 45, 48 | (L-~~4~~-20/08/19)  
L-6-31/08/19

4, 15, 20, 28, ~~30~~, 31, ~~33~~, 35, 38, ~~42~~, 51, ~~54~~, ~~58~~, 62, ~~65~~

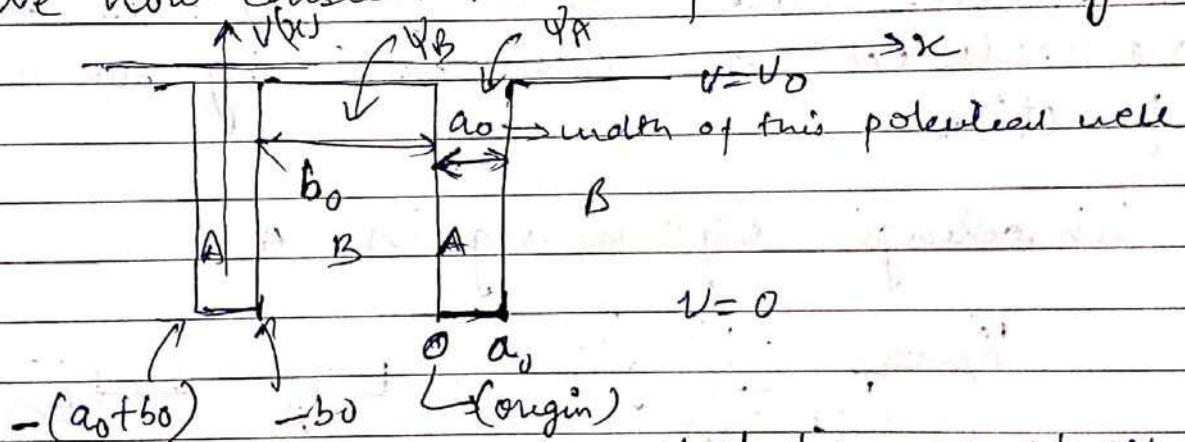
# Kronig Penney Model

Consider one dimensional linear periodic arrangement of atoms



mode of above potential profile:

- we now consider the two potential valleys as



In order to qualify the nature of electron, we need to solve Schrödinger equation  
Let us consider periodic potential in 1 D crystal

$$a_0 + b_0 = a = \text{lattice constant}$$

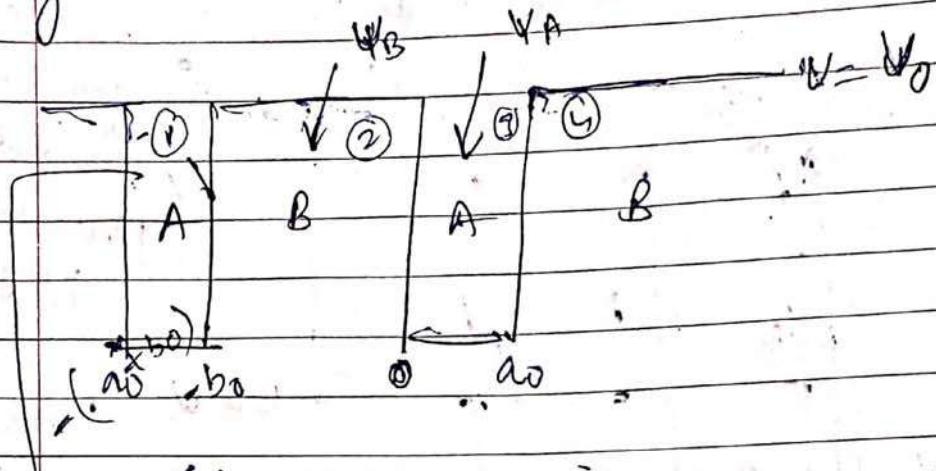
represents the periodicity of this potential well

Let wave function in region A is  $\psi_A$

B is  $\psi_B$

- True potential profile  $\rightarrow$  but for convenience it is shown as in rectangular form representation
- periodic arrangement of these atom in one dimensional is also called 1-D crystal

Write the Schrodinger equation in different regions.



In this region we are not defining the wavefunction as  $\Psi_A$  because here it is not  $\Psi_A$ . but this potential well is very similar to the potential well where the wavefunction is  $\Psi_A$ . So, these wells are related to each other by some function.

The Schrodinger eq<sup>n</sup> in region A

$$\frac{\hbar^2}{2m} \frac{d^2 \Psi_A}{dx^2} = E \Psi_A \quad (1)$$

in region B.

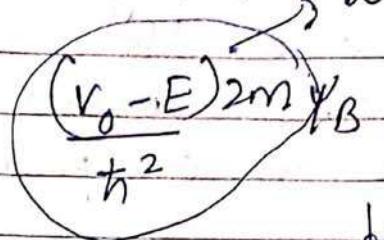
$$\frac{-\hbar^2}{2m} \frac{d^2 \Psi_B}{dx^2} + \Theta V_0 \Psi_B = E \Psi_B \quad (2)$$

From eq<sup>n</sup> (1)

$$\frac{d^2 \Psi_A}{dx^2} = -\frac{2mE}{\hbar^2} \Psi_A \quad (3)$$

✓ from eq<sup>n</sup> ②

$$\frac{d^2 \psi_B}{dx^2} = \frac{(V_0 - E) 2m}{\hbar^2} \psi_B \quad \text{--- (4)}$$



for  $E < V_0$

(Tunneling case)

Consider the Boundary condition

Sol<sup>n</sup> of eq (3) is given by

$$\psi_A(x) = A \sin \beta x + B \cos \beta x \quad \text{--- (5)}$$

and sol<sup>n</sup> of eq (4) is given by

$$\psi_B(x) = A_1 e^{i k x} + A_2 e^{-i k x} \quad \text{--- (6)}$$

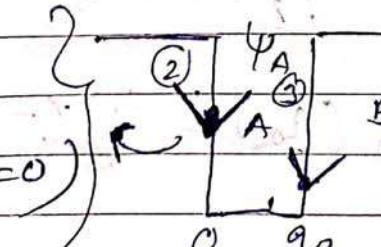
or may be of form ④ of eq<sup>n</sup> (5)

so from ④ and ⑥ we need to find the four coefficient i.e. A, B, A<sub>1</sub> and A<sub>2</sub>

# So apply the Boundary condition

$$(1) \psi_A(x=0) = \psi_B(x=0)$$

$$(4) \frac{d \psi_A(x=0)}{dx} = \frac{d \psi_B(x=0)}{dx}$$



(iii) Nature does not differentiate b/w regions

① and ③ i.e. ① could be ③ and vice versa

② could be ①

$$i \ell K \left( \frac{a_0 + b}{a_0} \right)^{\frac{1}{2}}$$

$$\text{so } \psi_A(x=a_0) = \psi_B(-b) e^{\frac{i \ell K (a_0 + b)}{a_0}}$$

C. Bloch's theorem

~~Date~~

This boundary condition is not familiar. and this arise something called Bloch's theorem  $\rightarrow$  it is applied when we have periodic potential profile  $\rightarrow$

Bloch's theorem  $\rightarrow$  says that nature does not differential <sup>b/w</sup> the coordinates, the choice of its coordinates is arbitrary.

So therefore wave function in region ① must be related to wave function in region ③

so,

$$\Psi_A(x=a_0)$$

$\geq \Psi_A^0(x=-b_0)$  These edges are turns  $e^{ikR}$   $\Rightarrow$  lattice constant

and  $\Psi_A^0(x=-b_0) \rightarrow$  is exactly same as

$$\Psi_B(x=-b_0)$$

$$\therefore \boxed{\Psi_A(a_0) \approx \Psi_B(-b_0) e^{ik(a_0+b_0)}}.$$

and

$$\frac{d\Psi_A(a_0)}{dx}(x=a_0) = \frac{d\Psi_B(-b_0)}{dx} e^{ik(a_0+b_0)}$$

Now By using all these boundary conditions and solving eq ① and ②

$$\frac{(\alpha^2 + \beta^2) \sin(\alpha a_0) \sin(\beta b_0) + \cos(\alpha a_0) \cos(\beta b_0)}{2\alpha\beta} = \cos(k(a_0 + b_0)) = F_0(E)$$

$\alpha, \beta$  are both function of energy

$a_0 \rightarrow$  width of potential well

$b_0 \rightarrow$  width of potential barrier

so this entire term in the bracket is

the function of energy and denoted

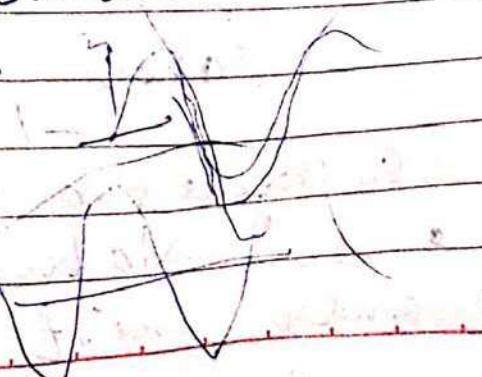
$F_0(E)$

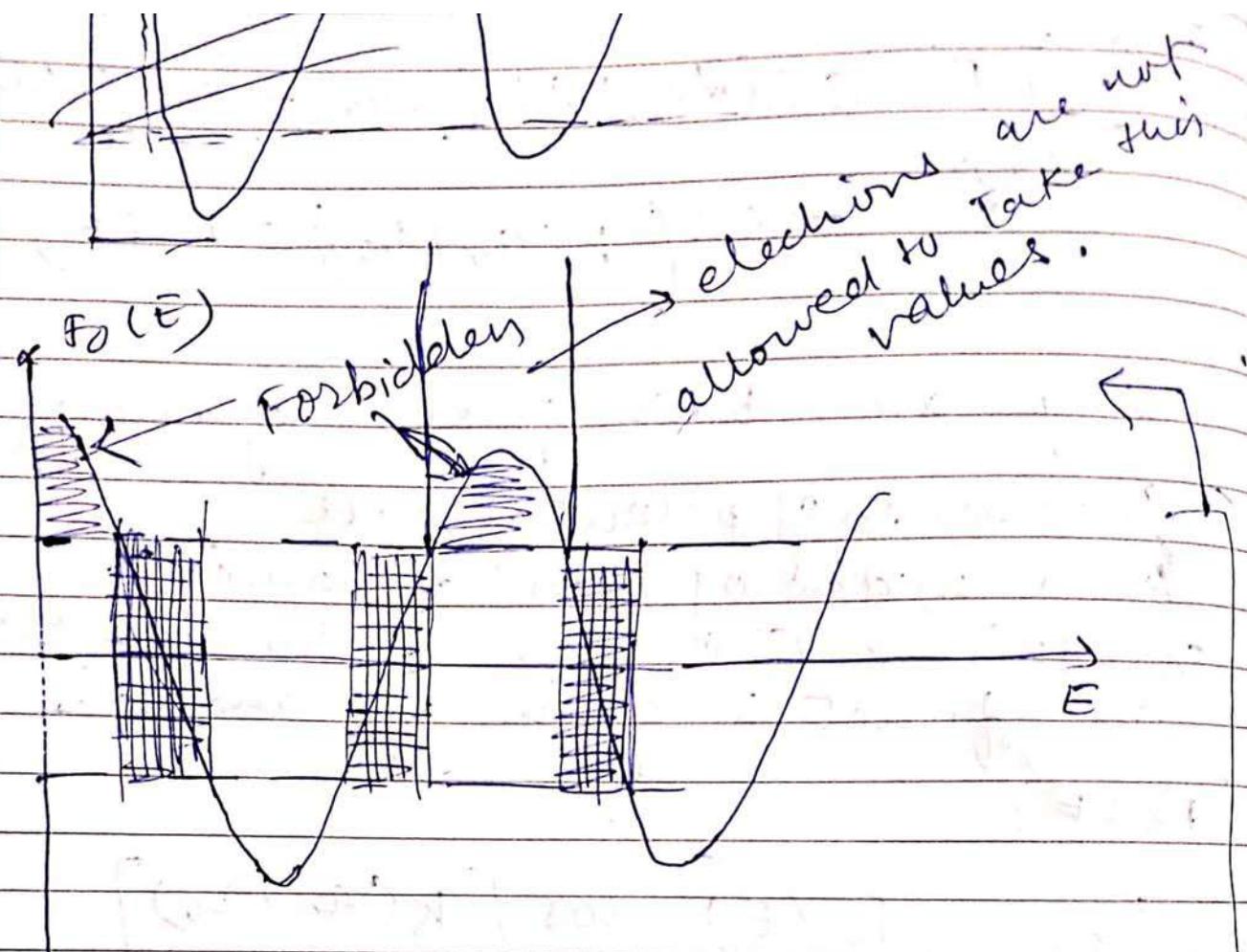
$$F_0(E) = \cos[k(a_0 + b_0)]$$

$k \rightarrow$  is a wave vector.

Note L.H.S of the above equations produces an oscillating function that could be greater than +1 or less -ve.

But R.H.S is a cosine function and hence bounded b/w -1 and +1.





• But Nature imposes a limit on  $f_0(E)$ .  
And that limit is  $f_0(E)$  must be equal to  $\cos[k(a_0 + b_0)]$ .

and this function must satisfy

$$-1 \leq f_0(E) \leq 1$$

also

$$-1 \leq f_0(E) \leq 1$$

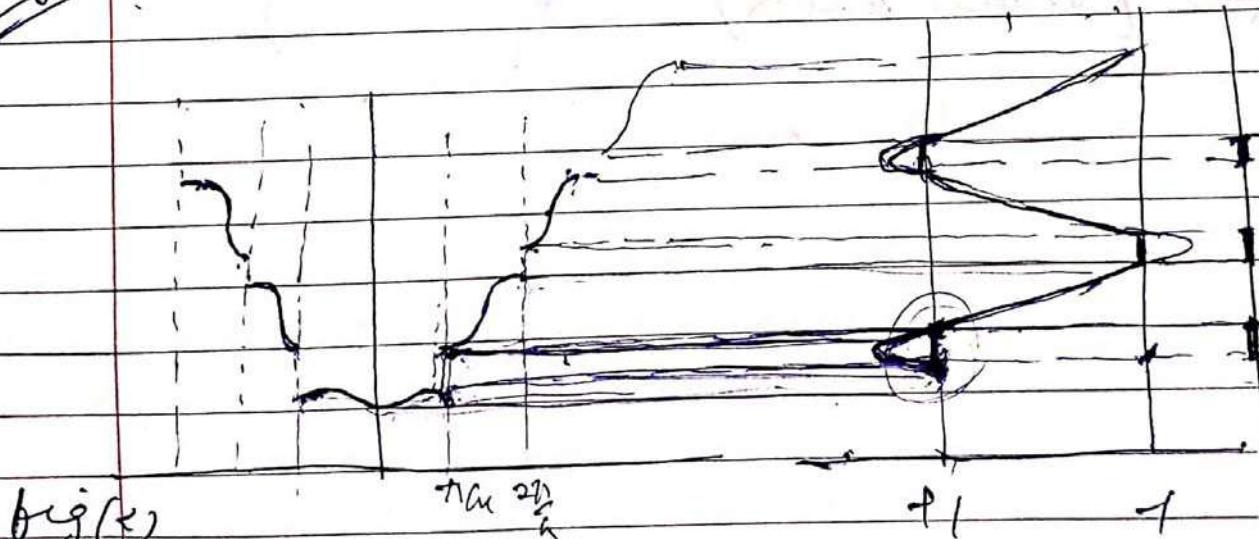
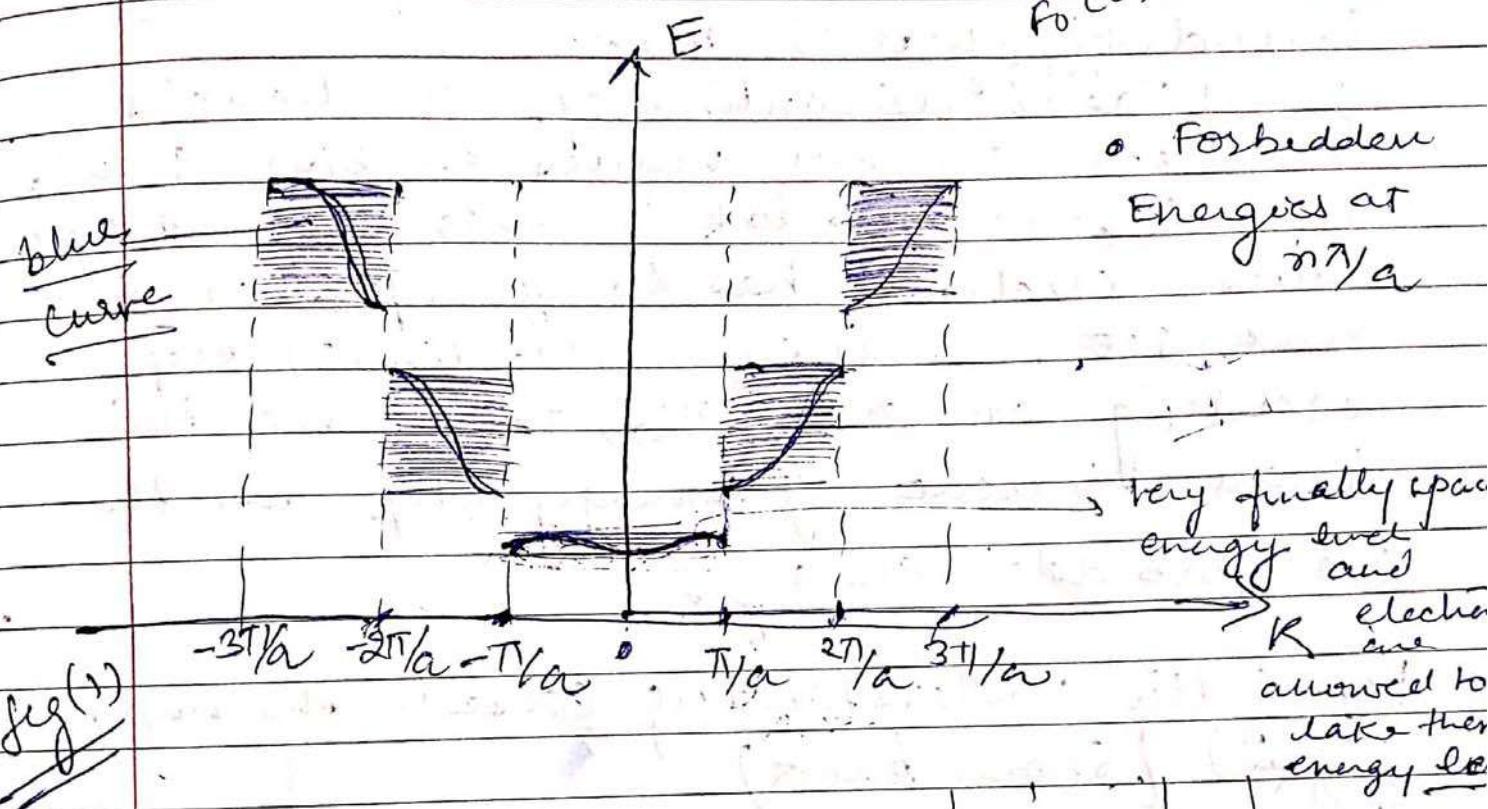
So therefore this mathematical is bounded  
• So Nature allows the electrons to only exist in this bound.

and All of these places the  $F_0(E)$  exceeds 1 or goes below -1 are all forbidden so electron can not sit.

Now Plot w/o EV(s) K

$$F_0(E) = \frac{w}{\cos(\frac{\pi}{L}ka)}$$

$$F_0(E) = \frac{w}{\cos(\frac{\pi}{L}ka)}$$



- Forbidden Energies at  $n\pi/a$
- Each continuous band is actually discrete points spaced at  $n\pi/L$
- $L$  = crystal size

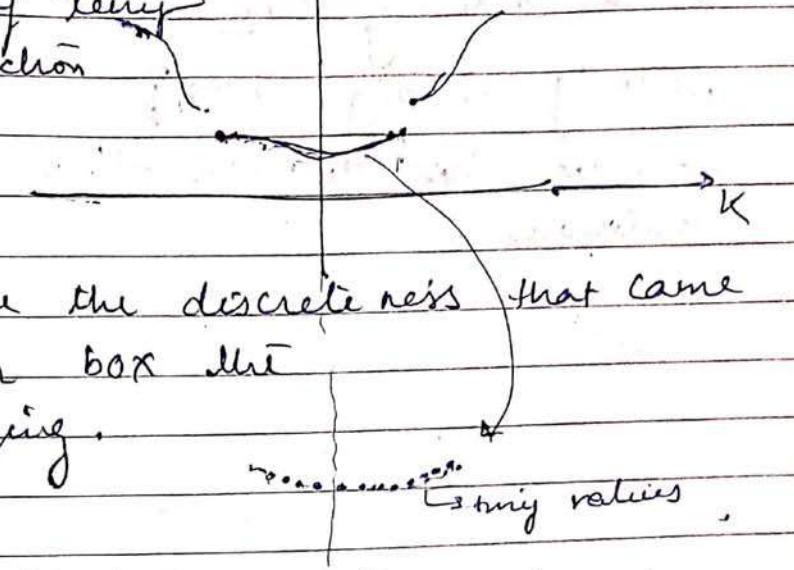
- The curves in fig (1) shows that electrons are allowed to occupy these energy levels or curves.

- As  $k$  takes all values of  $n\pi/a$  at these boundaries there is sudden jump in energy or discontinuity. So electrons can take all the values in b/w  $0 \rightarrow \pi/a$

then  $\pi/a \rightarrow 2\pi/a$ . but at those beyond these values electrons has to jump into the next set. so these discontinuity keep occurring at  $\pi/a, 2\pi/a, 3\pi/a$  and this is the presence of energy gap and these are forbidden energy.

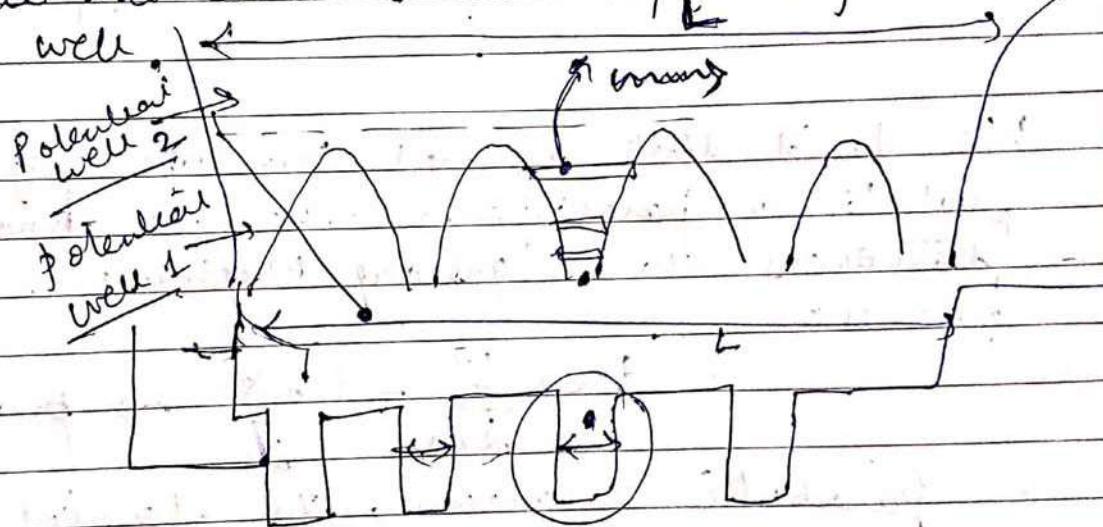
For better understanding consider the next fig (2) [shown back]

- Consider one line curve, it looks very continuous, but in fact it composed of very tiny values (energy) the electron could take up.



- These tiny values are the discrete ness that came bcs of the very large box the electron are occupying.

- Consider the 1D Initiat fig of Kronig-penney model. here the electrons are experiencing two potential well.

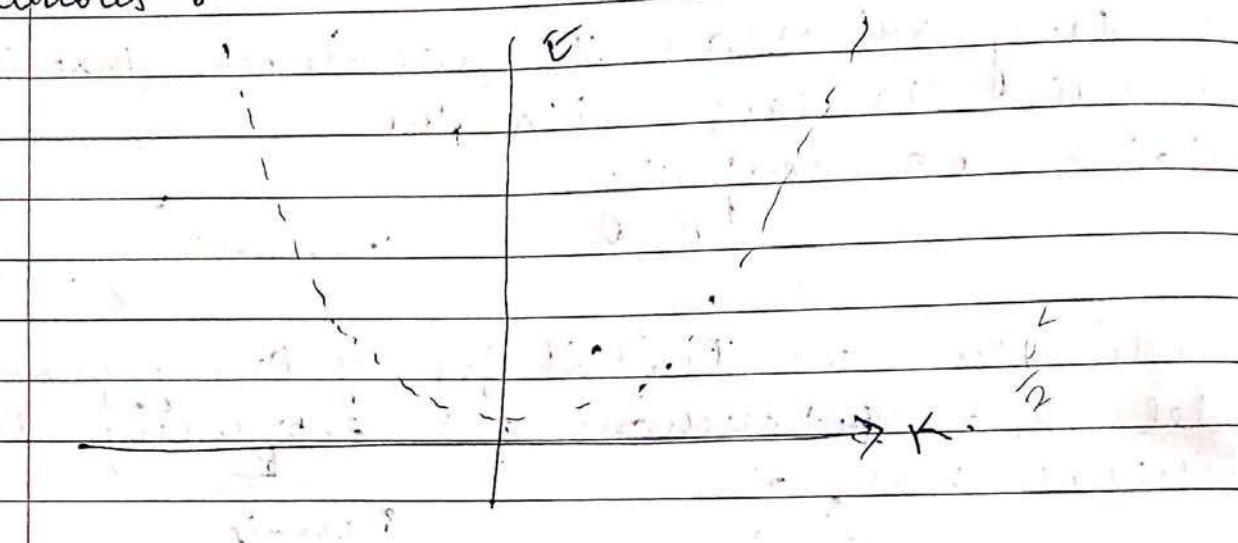


- so when the electron escape from the cluster of one potential well and jump to another potential well when the electron is free to roam about the crystal.

- As the length of the box increases, the difference b/w the Energy level drops down significantly.

.....  
indicating the same

- Difference in  $\Delta K$ , is order of  $\pi/a$   
 but if look at the finally space k points, and  
 it in order of  $\pi/L$  where the electrons are  
 settling in big ~~box~~. and the energy levels  
 are more close to each other and looks like  
 continuous.

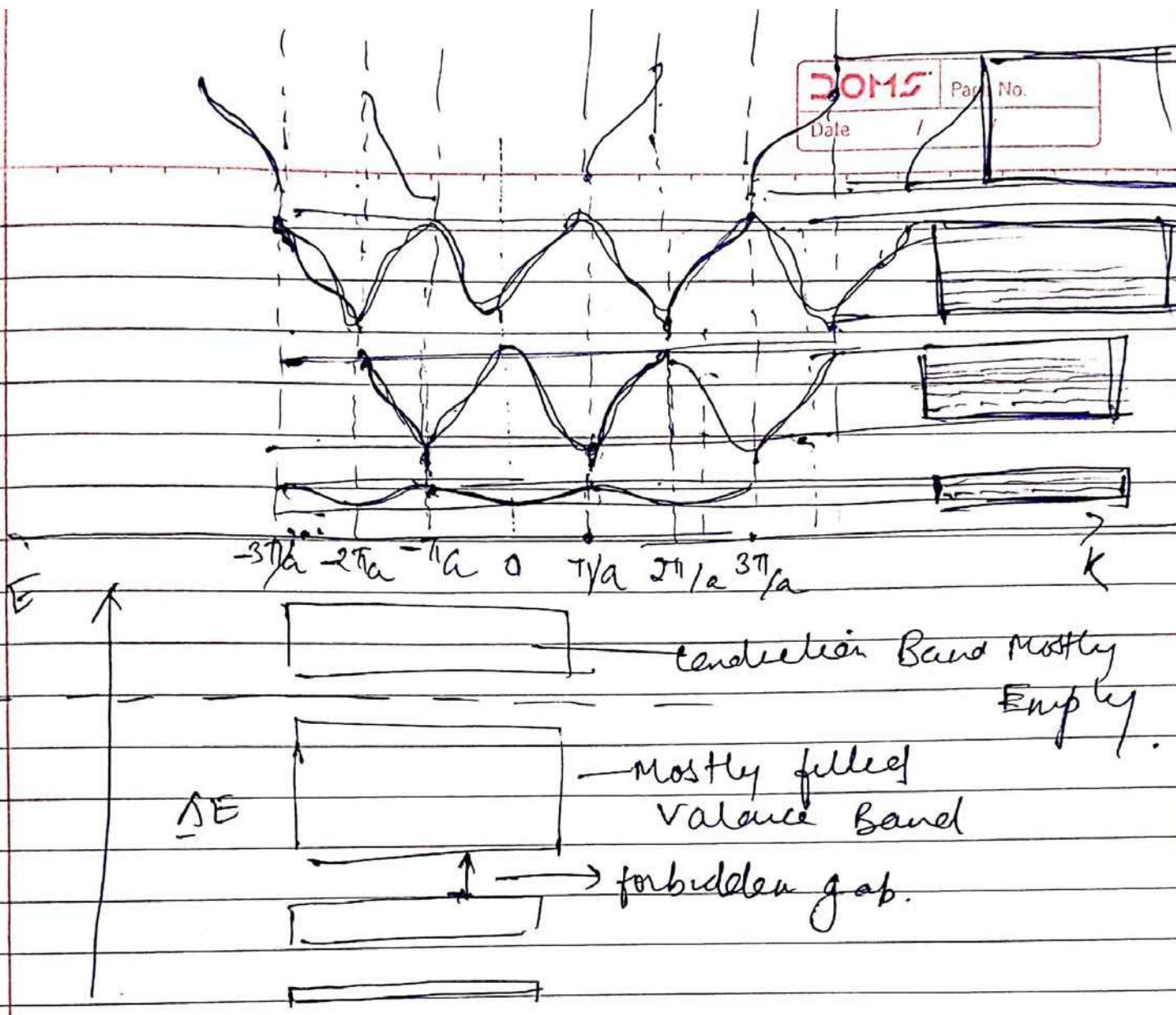


We find that general Envelope of all plot is a parabola  $\rightarrow$  when we head towards the Classical Mechanics, we find that

$$E = \frac{p^2}{2m} = \frac{(\hbar k)^2}{2m} \rightarrow \text{parabola.}$$

a parabolic relation, In classical Mechanics the discreteness disappears.

The freq(1) of E-k diagram can be drawn in different manner, we arbitrarily define the origin, but nature does not differentiate.



$a_0 + a$

$a_0 + b$