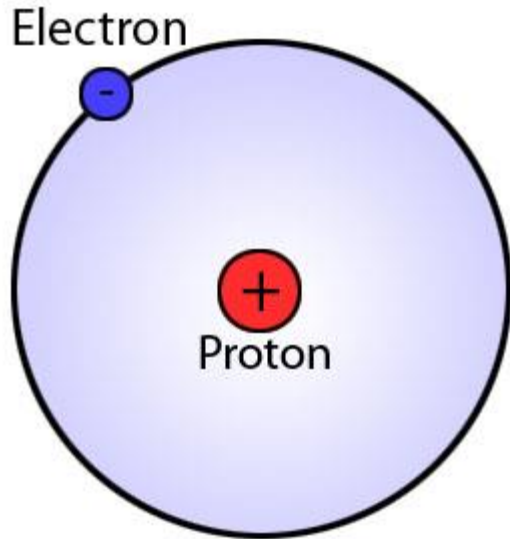


Physics of Semiconductor: Lecture # Lec 1

Dr. Sudipta Som

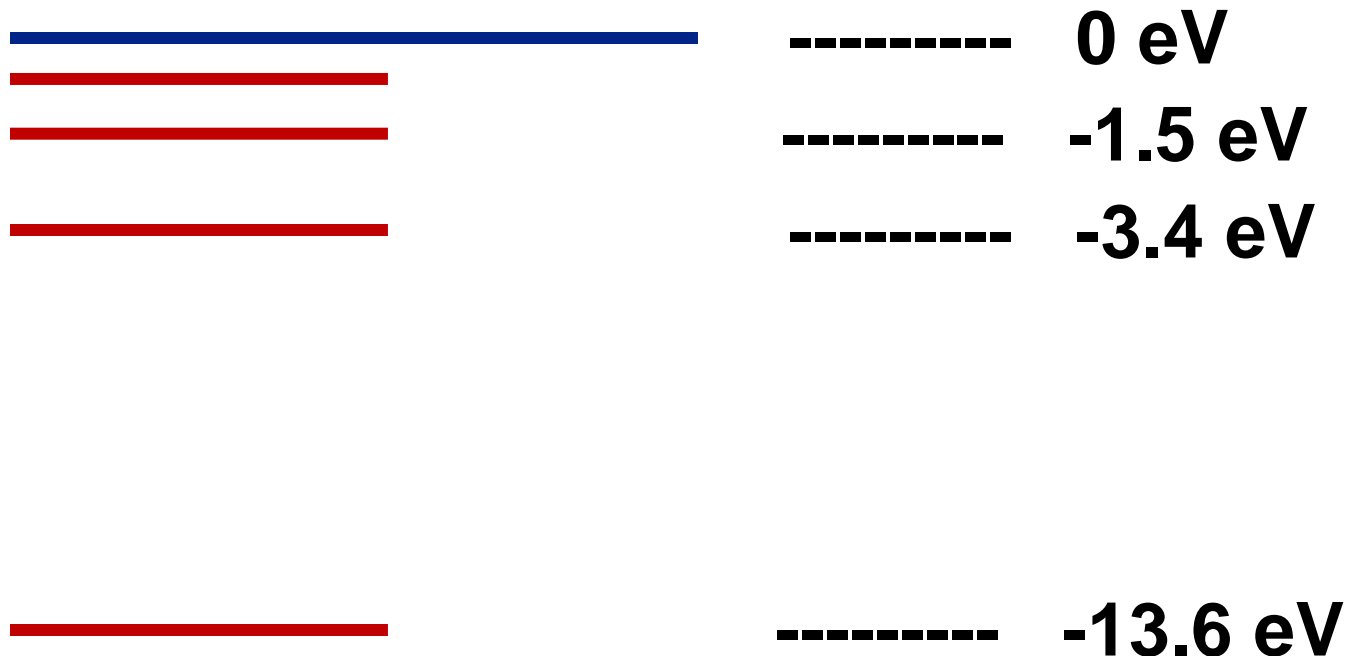
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Shiv Nadar University Chennai



$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V\psi(x) = E\psi(x)$$

$$E_n = -13.6/n^2 \quad \text{-----} \quad \psi_n$$



For more than one electron---

ψ_{nlm}

n can be integer no. 1, 2, 3,

l starts from 0 to n-1

m starts from -l to +l

l = 0 --- s l = 1 --- p

l = 2 --- d l = 3 --- f

Say for example $n = 3$

$l = 0, 1, 2$ s, p, d

3s, 3p, 3d----- orbitals

Now, $l = 2$ ----- $m = -2, -1, 0, 1, 2$ (total 05 orbital)

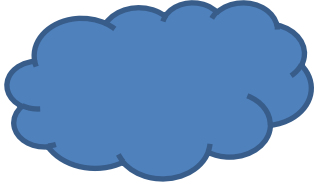
Each orbital can contain two electrons with opposite spin

For Na---- 11

$1s^2 2s^2 2p^6 3s^1$

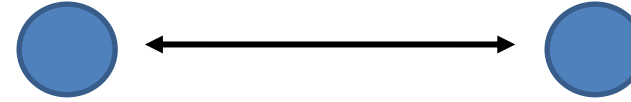
No of electron		No of state
 3p ⁰ -----	
1	3s ¹ -----	2
6	2p ⁶ -----	6
2	2s ² -----	2
2	1s ² -----	2

Gas



E.g. N no of particles

No interaction



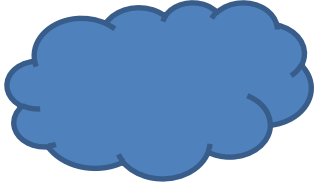
For Na vapor

No of electron

No of state

	
	3p ⁰	
	3s ¹	
N		2N
	2p ⁶	
6N		6N
	2s ²	
2N		2N
	1s ²	
2N		2N

Now Na atom
For Na vapor



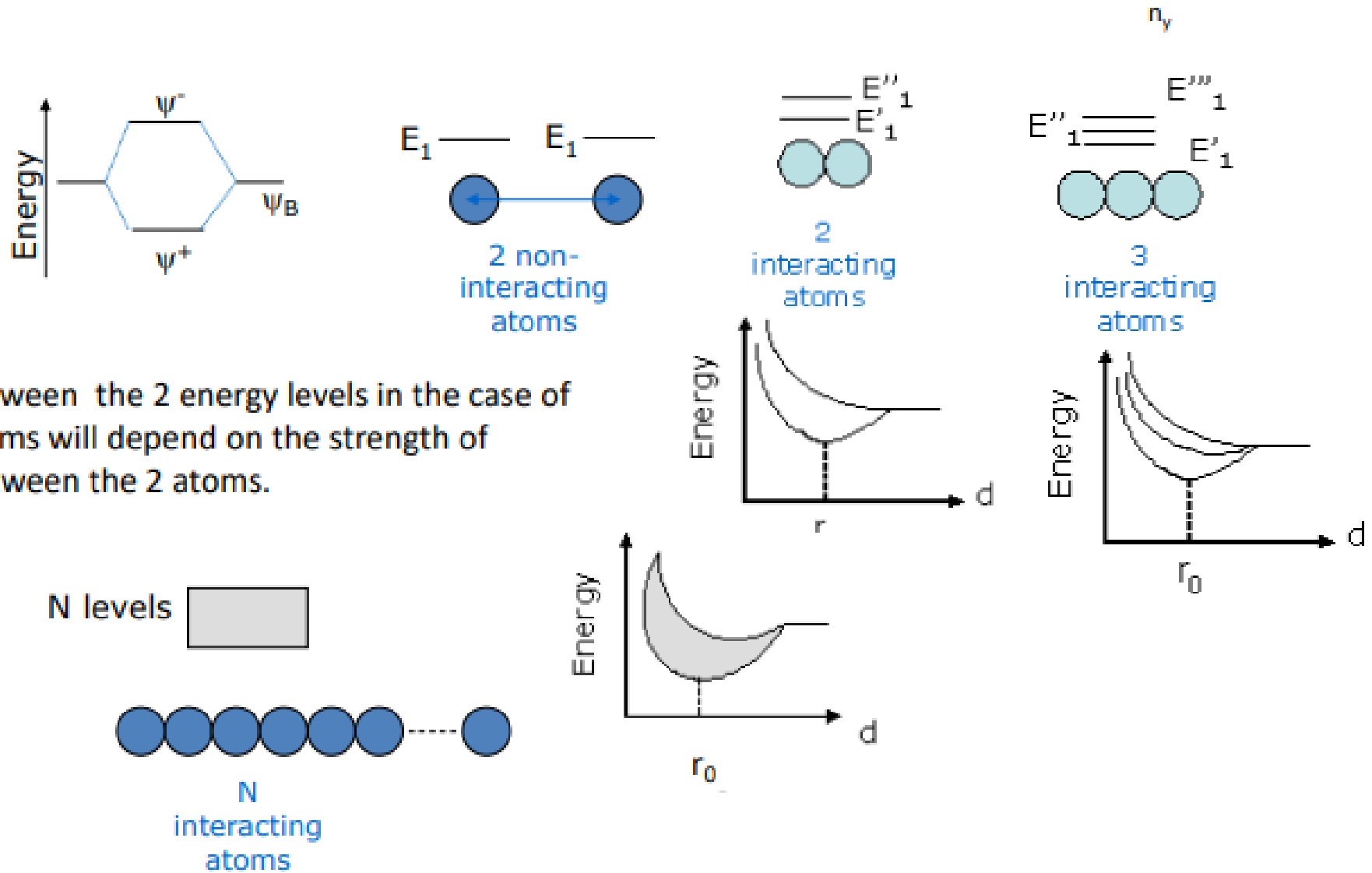
E.g. N no of particles



Interaction b/w electron
started

Band theory of solids

- Atomicity model (tight binding approximation)
- Electron in a periodic potential –Bloch theorem

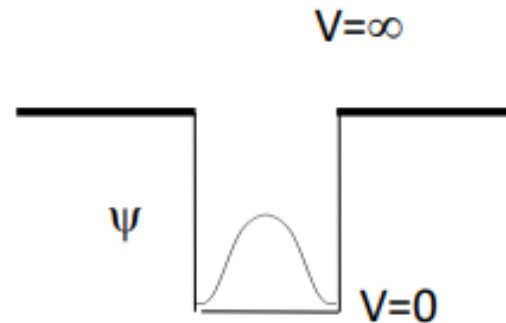


The Atomicity model (tight binding approximation)

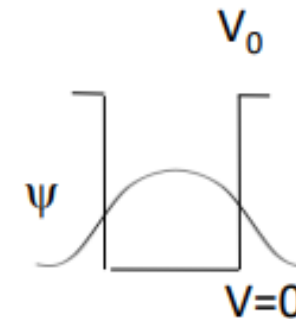
Imagine two identical isolated atoms (hydrogen?)
[separated by a large distance d ($d \gg \text{radius of atom, } r$)]

Allowed energy levels are similar to that of electron in a potential well

What is the difference?

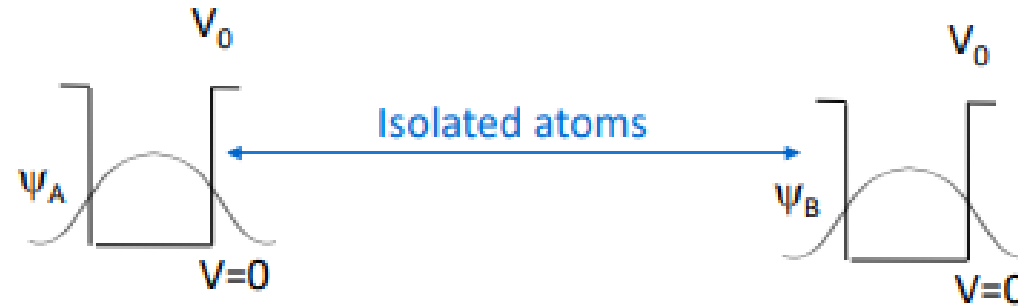


1D potential well
Width of wall,
 $W = \infty$ on either side,
 $V = \infty$



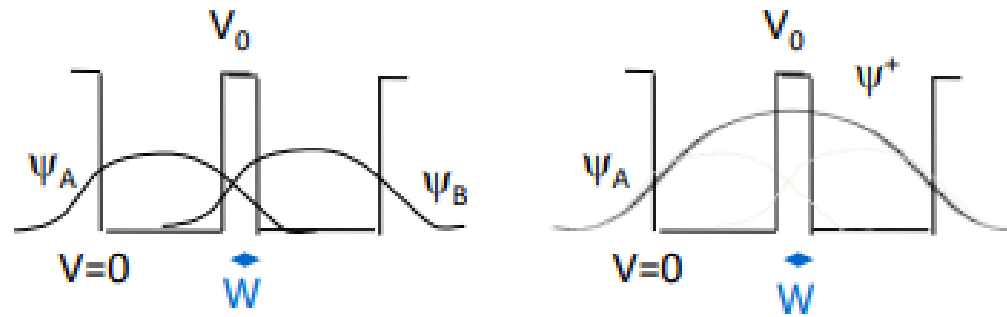
In reality
 $V \neq \infty$, $W \neq \infty$

Let the 2 atoms A, B that we are considering have electrons
in the same energy level (i.e say the ground state)



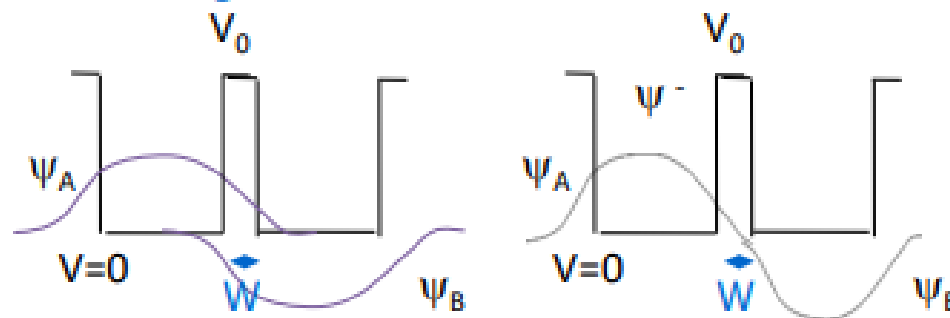
Possibilities when they come so close to each other that the potential of one affects the other

Symmetric bonding



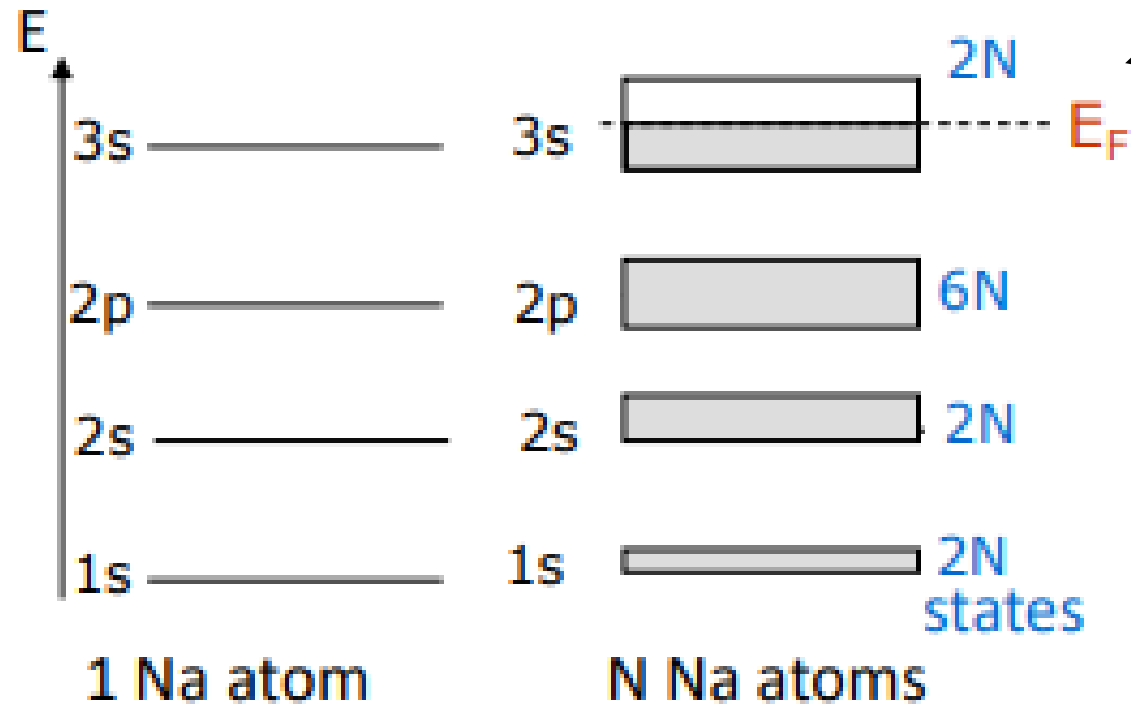
ψ^+ looks like the ground state $n=1$, eigen function of a potential well of width $2L + W(\text{small})$

Antisymmetric bonding



ψ^- looks like the first excited state $n=2$, eigen function of a potential well of width $2L + W(\text{small})$

Let us take the example of Na,
 $Z = 11$ ($1s^2, 2s^2, 2p^6, 3s^1$)



N no of quantum states are empty

@ RT, with thermal energy those electron which are posited in the quantum states can move to the empty states.

Thereby, takes part in conduction

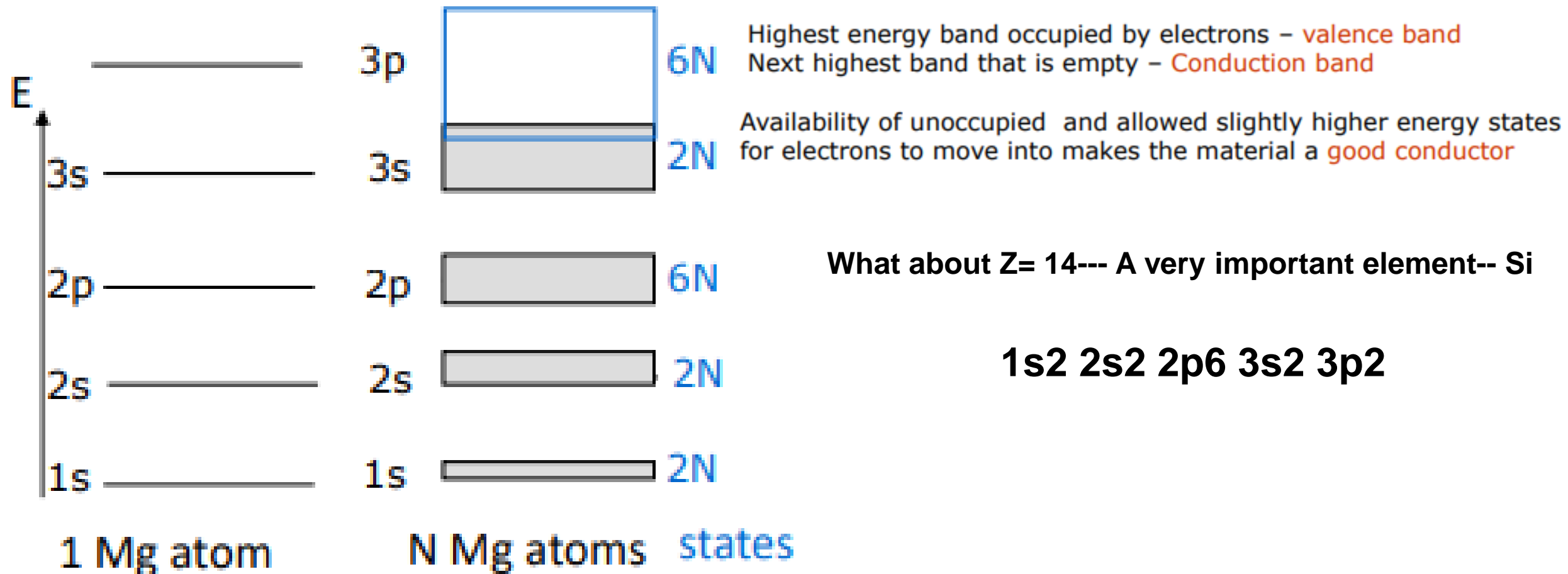
As the conduction electrons are available, this band is called as conduction band

LUMO and HOMO

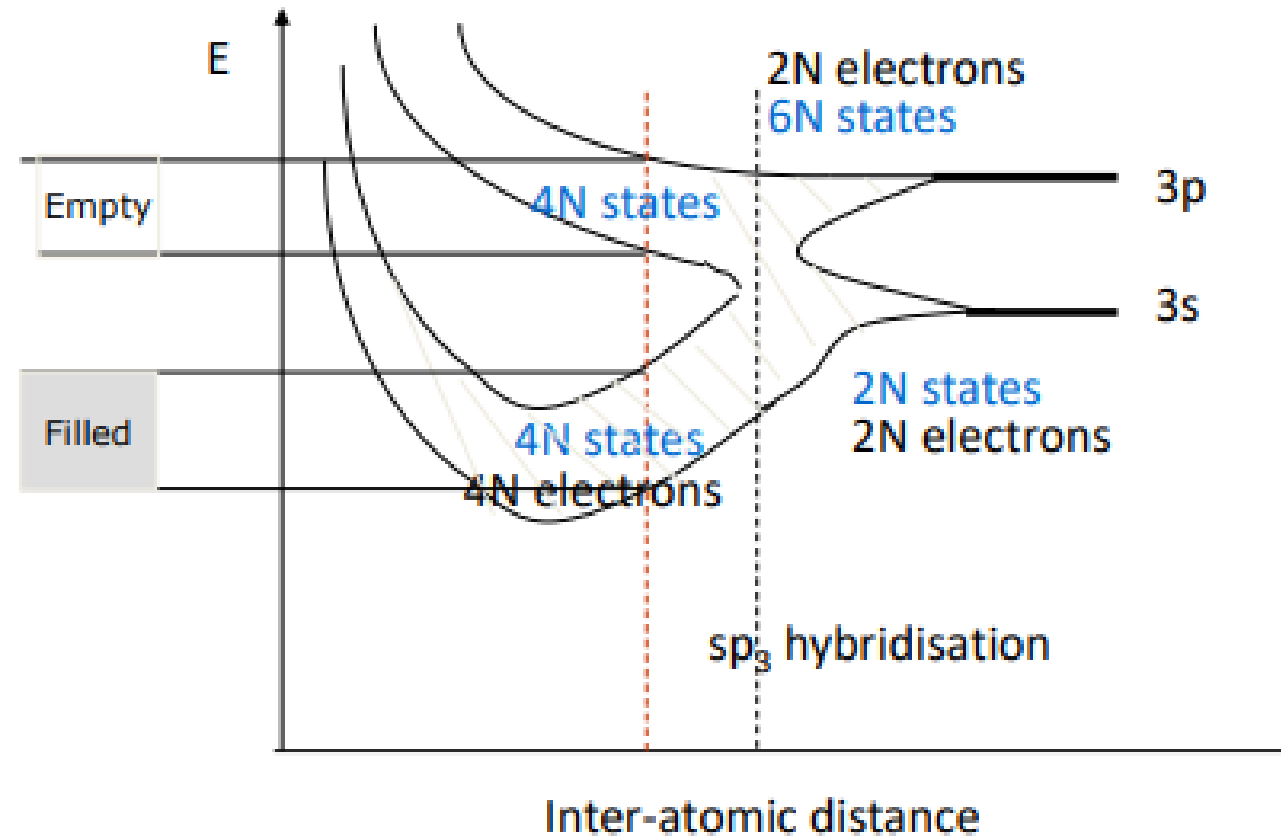
Metal

Example 2: of Mg,
 $Z = 12$ ($1s^2, 2s^2, 2p^6, 3s^2$)

Semi-metal
(overlapping conduction band)



Hybrid energy band structure of silicon $1s^2, 2s^2, 2p^6, 3s^2, 3p^2$



When N atoms come together to form a solid

Electron in a periodic potential

For, electron in a periodic potential,

$$\frac{d^2\psi}{dx^2} + \left(\left(\frac{2m}{\hbar^2} \right) (E - V(x)) \right) = 0 \quad V(x) = V(x+a).$$

$\Psi(x)$ will also be periodic with same period p as the periodic potential energy $V(x)$

Solution that satisfies T.I.S.E for both well and wall region is

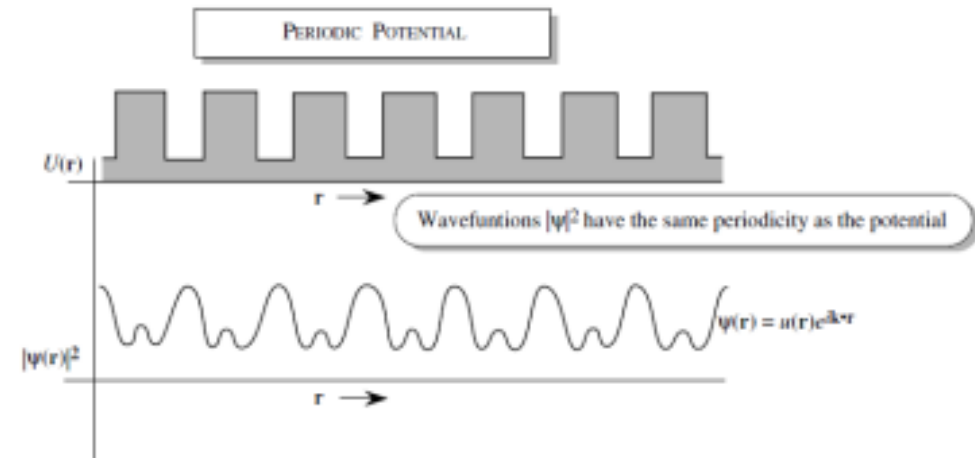
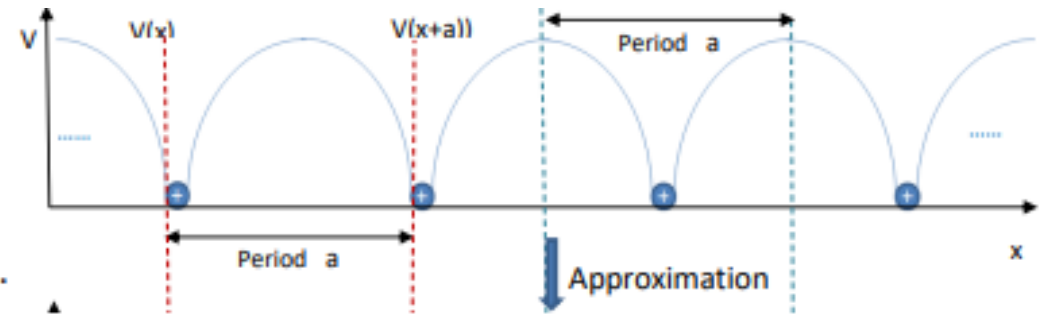
$$\psi(x) = e^{\pm ik \cdot x} u_k(x) \quad \text{where} \quad u_k(x) \text{ is periodic in } x \text{ with same periodicity}$$

$$\text{i.e. } u_k(x) = u_k(x+a). \quad \text{as the potential energy}$$

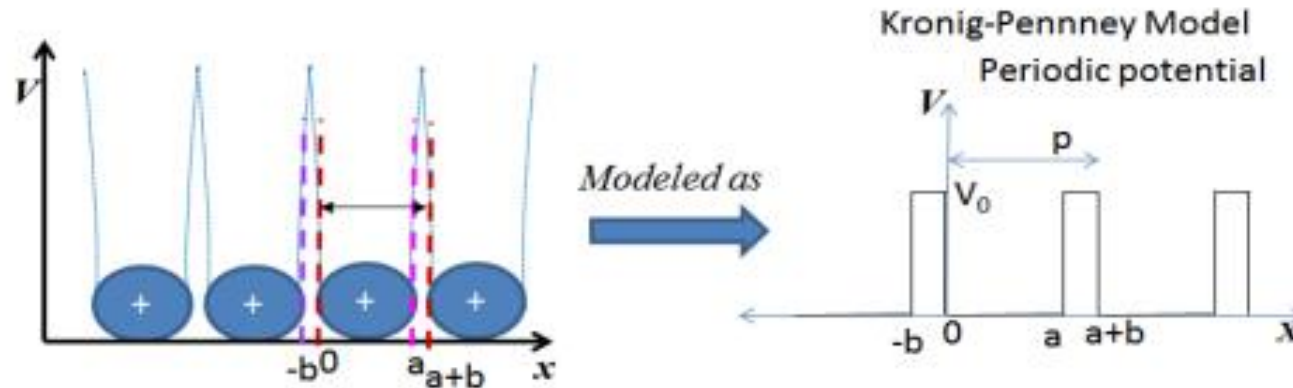
Bloch theorem also called Fouquet's theorem for 1D systems

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

But $\psi(x+a) = \psi(x)$, $\therefore e^{\pm ik \cdot a} \psi(x) = \psi(x)$
or $e^{\pm ik \cdot a} = 1$;



$$k = \pm \frac{n2\pi}{a}; \text{ with } n = 0, 1, 2, \dots$$



$$\frac{d^2\psi}{dx^2} + \left(\left(\frac{2m}{\hbar^2} \right) (E - V(x)) \right) = 0 \quad V(x) = V(x + p).$$

$\Psi(x)$ will also be periodic with same period p as the periodic potential energy $V(x)$

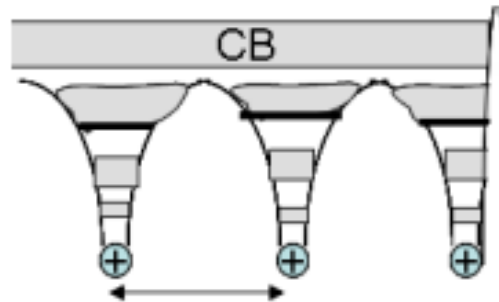
Solution that satisfies T.I.S.E for both well and wall region is

$\psi(x) = e^{\pm ik \cdot x} u_k(x)$ where $u_k(x)$ is periodic in x with same periodicity as the potential energy

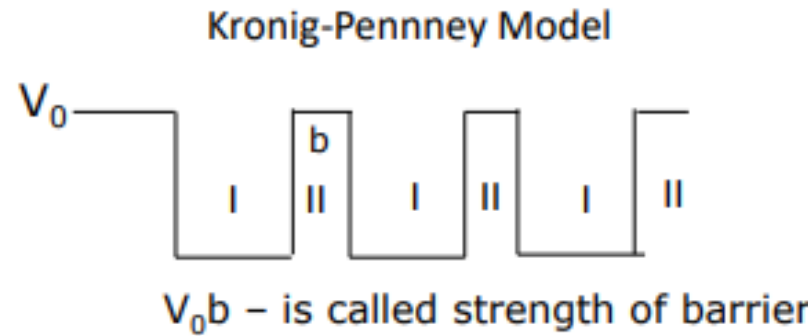
$$u_k(x) = u_k(x + p).$$

Bloch theorem also called Fouquet's theorem for 1D systems

Kronig-Penney Model – electron moving in a periodic potential



$$V(x) = V(x+p)$$



$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} (E - V(x)) \psi = 0$$

As per Kronig-Penney Model,

In Region I

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

$$\frac{d^2 \psi}{dx^2} + \alpha^2 \psi = 0$$

In Region II

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

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

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

Using Bloch function $\psi(x) = e^{\pm ikx} u_k(x)$, as the solution valid for both regions

$$\frac{d\psi}{dx} = ike^{ikx} u_k(x) + e^{ikx} u_k'(x)$$

$$\frac{d^2\psi}{dx^2} = -k^2 e^{ikx} u_k(x) + 2ike^{ikx} u_k'(x) + e^{ikx} u_k''(x)$$

These equations are substituted into the Schrodinger equation for Region I and Region II. *Applying boundary conditions that both the wave function and its first derivative must be continuous at points such as $x = 0$ for both regions and that the solution of region I at $x=a$ should be same as that of Region 2 at $x=-b$ due to periodicity*

$$u_1(a) = u_2(-b)$$

$$u_1(0) = u_2(0)$$

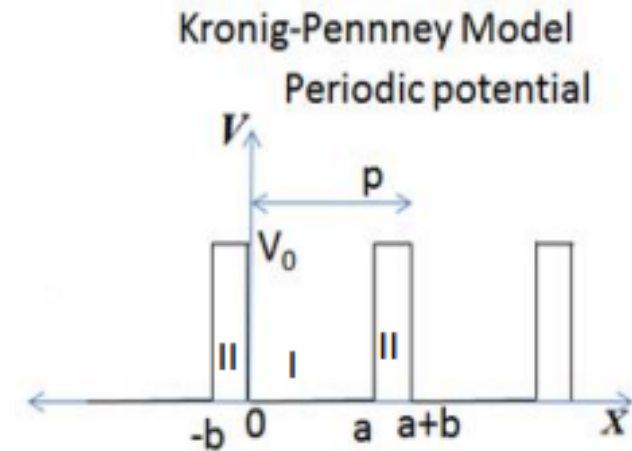
$$\frac{du_1(a)}{dx} = \frac{du_2(-b)}{dx}$$

$$\frac{du_1(0)}{dx} = \frac{du_2(0)}{dx}$$

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

With the approximation that $V_0 b$ (barrier strength) is finite, $\alpha^2 \ll \beta^2$, $\sinh(\beta b) = \beta b$, $\cosh(\beta b) = 1$ leads to the condition that valid solutions for energy are those that satisfy the following equation

$$\frac{P \sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka \quad \text{where} \quad P = \frac{ma}{\hbar^2} V_0 b; \quad \alpha = \frac{\sqrt{2mE}}{\hbar}$$



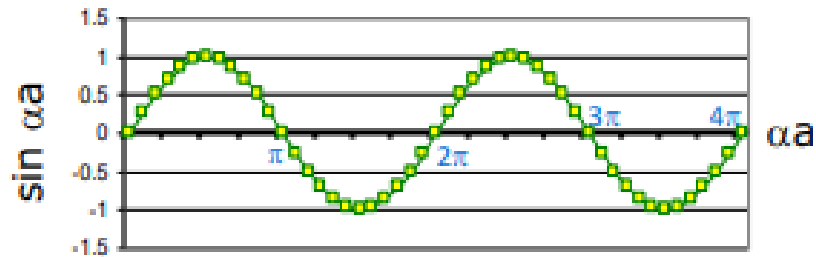
$$\frac{P \sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka \quad \text{where} \quad P = \frac{ma}{\hbar^2} V_0 b ; \quad \alpha = \frac{\sqrt{2mE}}{\hbar}$$

The RHS is a cosine function and therefore can take values between +1 and -1 only.

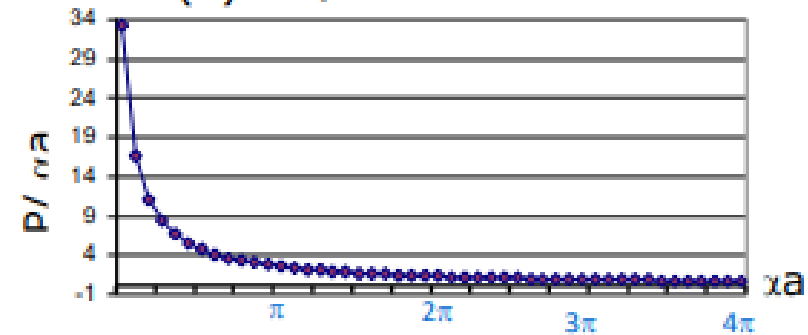
The restriction that the allowed value of LHS are those which fall between +1 and -1 gives rise to allowed and forbidden energy bands.

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

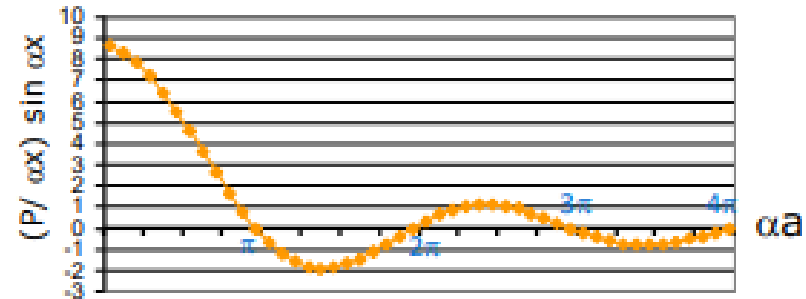
(i) $\sin \alpha a$

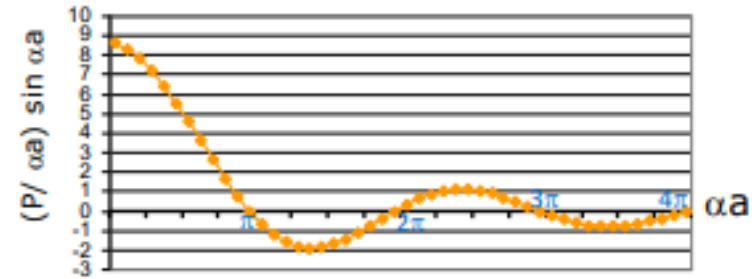
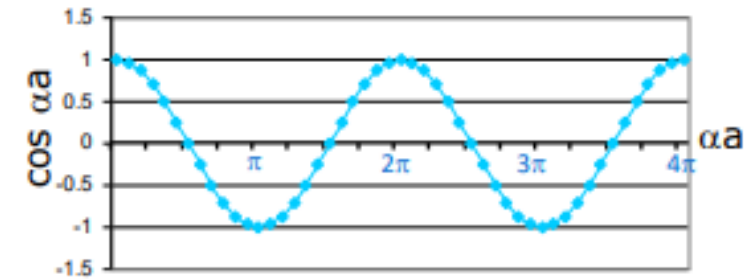
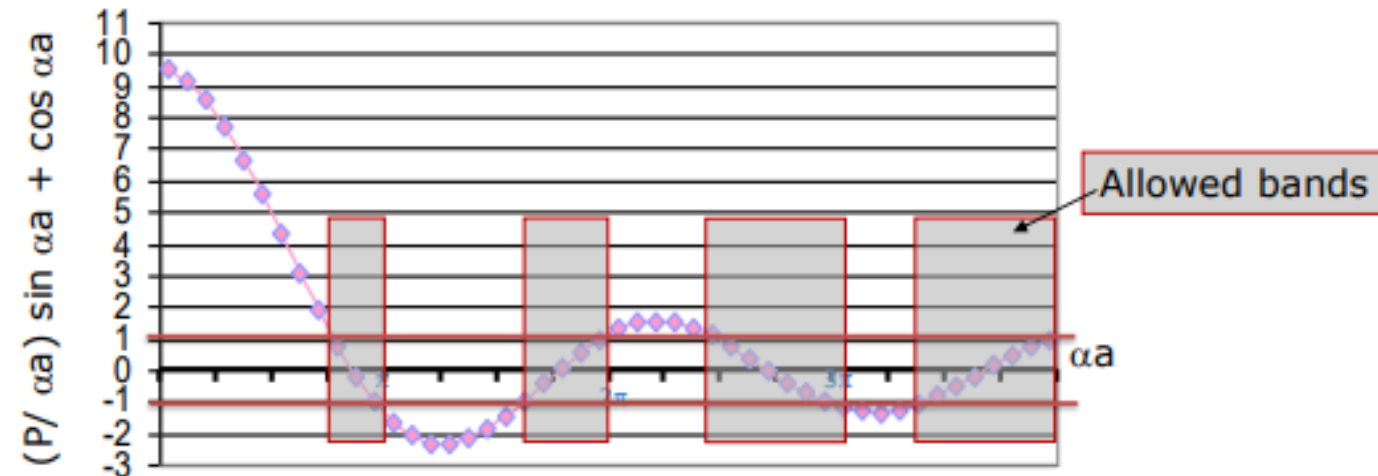


(ii) $P/\alpha a$

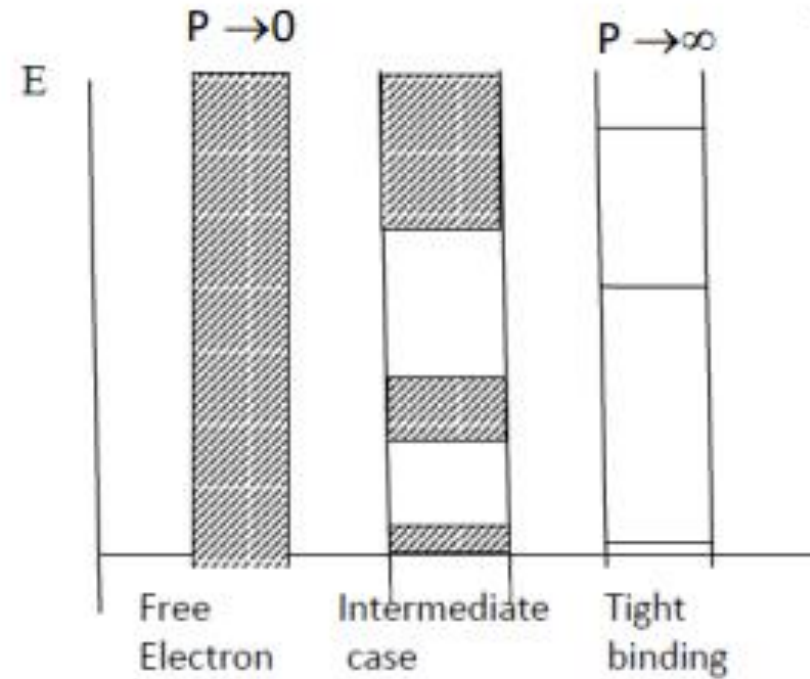


(iii) $(P/\alpha a) \sin \alpha a$



(iii) $(P/\alpha a) \sin \alpha a$ (iv) $\cos \alpha a$ (v) $(P/\alpha a) \sin \alpha a + \cos \alpha a = \cos ka$ 

Influence on P on the band formation



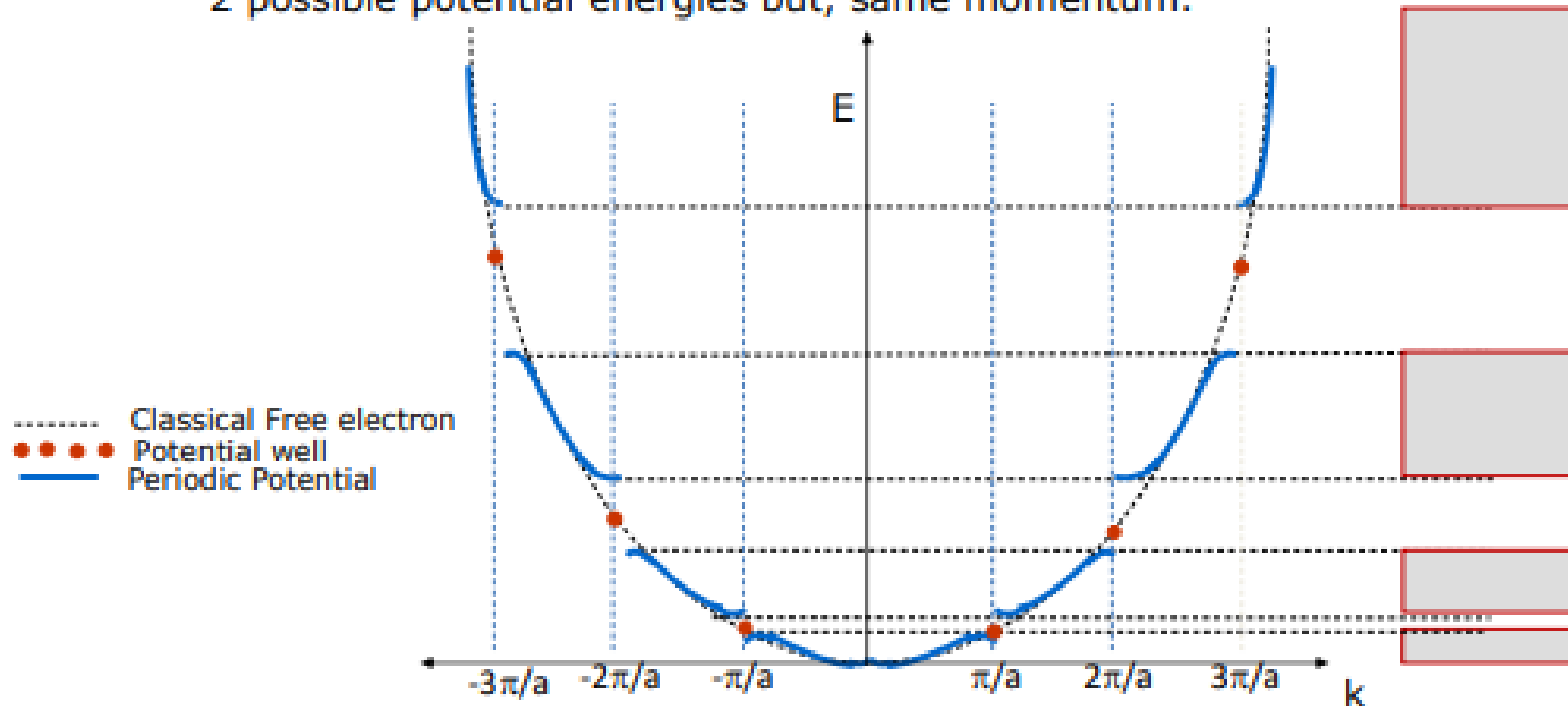
$$P = \frac{ma}{\hbar^2} V_o b ; \alpha = \frac{\sqrt{2mE}}{\hbar}$$

Breaks in the band occurs whenever $ka = \pm n\pi$ or $k = \pm n\pi/a$

a =lattice
constant

At zone boundary, solutions are 2 standing waves (due to Bragg reflection- constructive interference between reflected electron waves from the successive lattice points) leading to 2 possible potential energies but, same momentum.

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



- ▶ When N identical atoms come close together, each energy level of the isolated atom becomes a band of N levels and this causes the formation of energy band structure
- ▶ The energy gaps between the allowed energy levels indicate regions where Bragg reflection of the matter waves dominates i.e electrons having those energies undergo Bragg reflection and is not transmitted through the lattice (Breaks occur at $k = \pm n\pi/a$, where a is the periodicity of the potential)
- ▶ Highest energy band occupied by electrons – valence band
- ▶ Next highest band that is empty – Conduction band
- ▶ Availability of unoccupied and allowed slightly higher energy states for electrons to move into and presence of free electrons makes the material a good conductor and is classified as a metal
- ▶ Some materials exhibit hybrid band structure and the bandgap between valence band and conduction band [depends on their interatomic spacing] determines whether they are classified into semiconductors or insulators

Bonding in Solids

Atoms are held together to form a solid by bonding forces.

Bonding forces – attractive force (F_a) function of inter-atomic distance, r
 $\propto 1 / r^N$

-repulsive force (F_r) function of inter-atomic distance, $r \propto 1 / r^M$
- $M > N$

At some inter-atomic distance " r_0 ", $F_a = F_r$, resultant force = 0; the energy of this system of 2 atoms will be minimum (Binding energy)

B.E varies from 0.02eV (H_2) to 10eV (LiF)

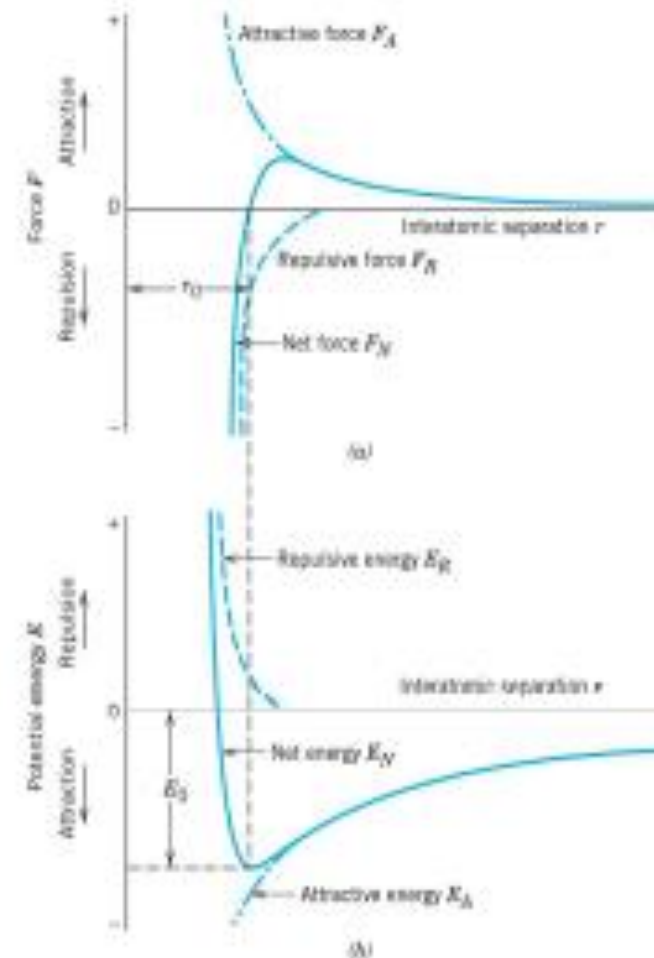
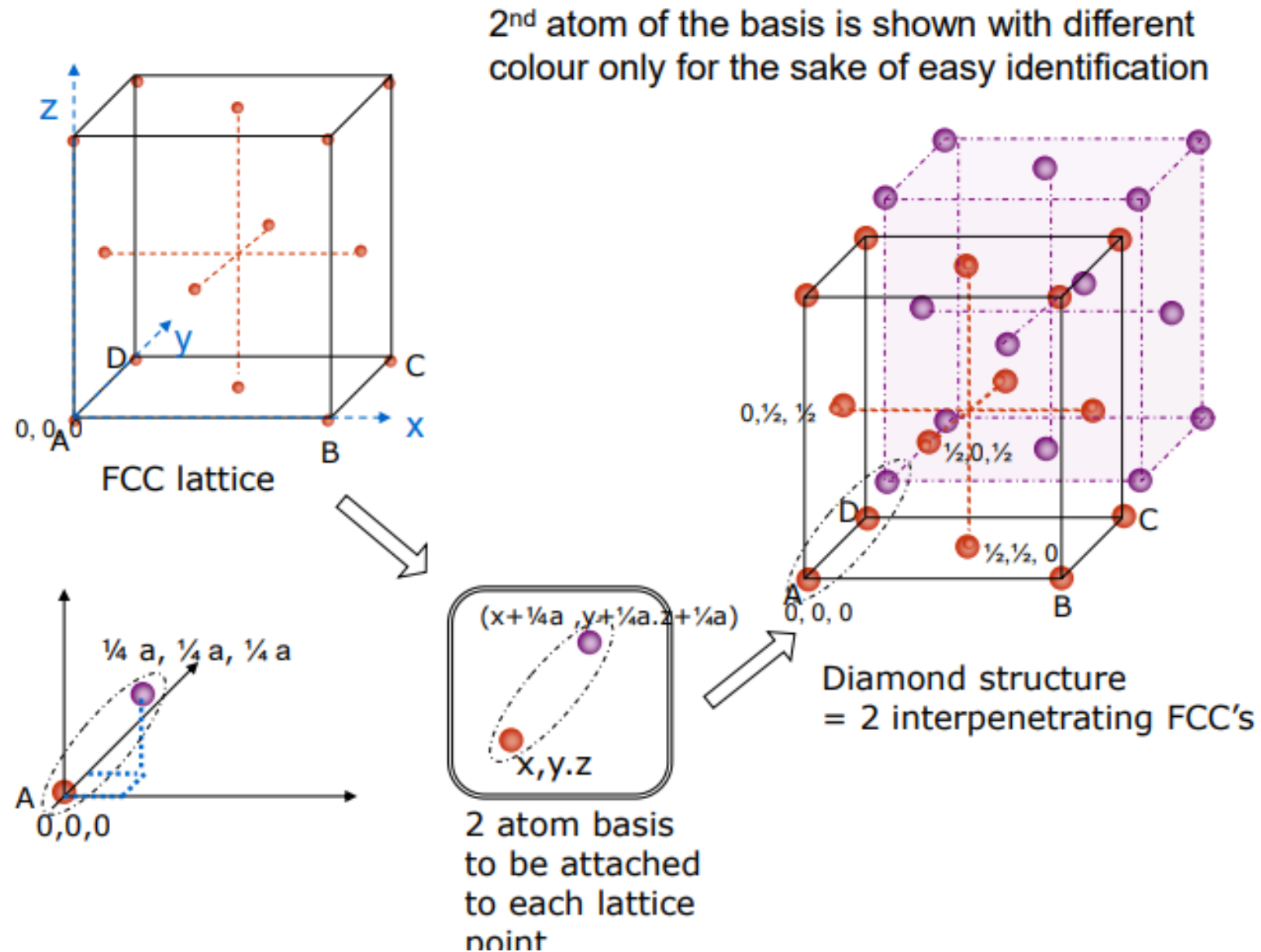


FIGURE 2.8 (a) The dependence of repulsive, attractive, and net forces on interatomic separation for two isolated atoms. (b) The dependence of repulsive, attractive, and net potential energies on interatomic separation for two isolated atoms.

Diamond crystal structure is actually an FCC lattice with a 2 atom basis, where one atom is at the lattice point, say at the origin $(0,0,0)$, and the second atom of the basis is at a distance $(\frac{1}{4}a, \frac{1}{4}a, \frac{1}{4}a)$ from it.

To get the diamond structure:

- ▶ Start with FCC lattice
- ▶ Attach 2 atom basis one atom at lattice pt and the other $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ from it, to each lattice point of the FCC.
- ▶ Connect the second atom of the basis to see the interpenetrating 2nd FCC lattice.



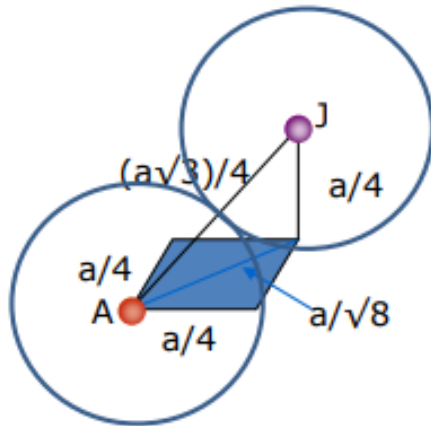
Atomic packing factor for diamond structure

Co-ordination number = 4

No. of atoms per cell =

$$\begin{array}{l} \left(\frac{1}{8}\right) \times 8 \quad + \quad \left(\frac{1}{2}\right) \times 6 \quad + \quad 4 = \quad \mathbf{8} \\ \text{(corner atoms)} \quad \quad \quad \text{(fc atoms)} \end{array}$$

Nearest neighbour distance



$$2r = (a\sqrt{3})/4; \quad r = (a\sqrt{3})/8$$

Volume occupied by atoms, $v =$

$$\frac{4}{3} \pi r^3 \times 8 = \frac{4}{3} \pi a^3 \frac{3\sqrt{3}}{64} = \pi a^3 \sqrt{3} / 16$$

Volume of unit cell, $V = a^3$

$$\text{Packing fraction} = v/V = \pi\sqrt{3} / 16 = \mathbf{0.34}$$

Lowest packing fraction!

