

**DEPARTMENT OF PHYSICS AND NANOTECHNOLOGY**  
**SRM INSTITUTE OF SCIENCE AND TECHNOLOGY**

**21PYB102J – Physics: Semiconductor Physics and Computational methods**  
**Module-I, Lecture-1**

Introduction to Classical Free electron theory-Introduction to Quantum Free electron theory-Concepts-Energy band in solids-Kronig-Penney model--E-k diagram-Direct and Indirect band gap-Concept of phonons-Concept of Brillouin Zone



**SRM**  
Institute of Science and Technology

# Classical Free Electron Theory of Metals



## Free Electron Theory

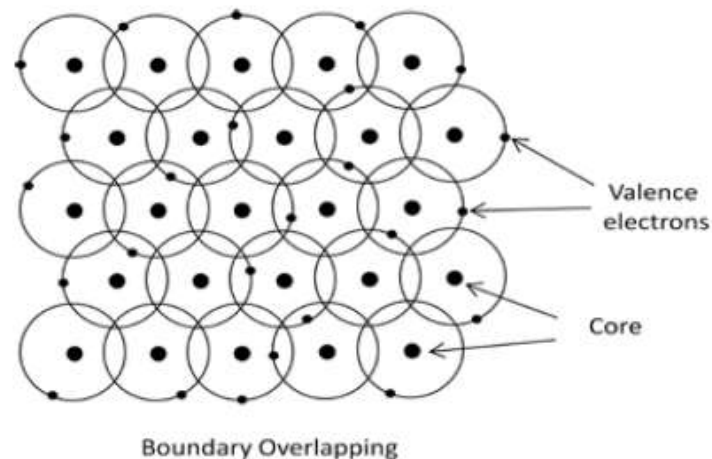
### ► The Classical free electron theory

A classical free electron theory is a macroscopic theory proposed by Paul Drude in 1900. After the discovery of electron by JJ Thomson, this theory was elaborated by Lorentz in 1909. Hence this theory is also known as Drude & Lorentz. According to this theory metals contains free electrons which are responsible for the electrical conductivity in metals and obeys the laws of classical mechanics (Maxwell-Boltzmann distribution)



## Free Electron Theory

According to Drude-Lorentz theory, when a large number of atoms arranged in three dimensional lattice points to form a metal, the boundaries of the neighbouring atoms slightly overlap with each other as shown in figure. Due to this overlapping, the valance electrons of all the atoms are free to move within the metal lattice. These electrons are called free electrons.





**SRM**  
Institute of Science and Technology

# Classical Free Electron Theory of Metals



**SRM**  
Institute of Science and Technology

## Free Electron Theory

These electrons are called free electrons. These free electrons are move randomly in all directions through the conductor with average speed of the order of  $10^6$  m/s. This is similar to the motion of gas molecules confined in a vessel. Since the free electrons are responsible for electrical and thermal conduction in metals, they are also called as conduction electrons.

All metals contain free electrons which act just as a gas molecules moving in every direction throughout the lattice. The average velocity due to the thermal energy is zero since the electrons are going in every direction. There is a way of affecting this free motion of electrons, which is by use of an electric field. This process is known as electrical conduction and theory is called Drude-Lorentz theory. The assumptions of the Drude-Lorentz classical theory of freeelectrons are the following



## Assumptions of Classical free-electron theory:

1. All metals contain large number of free electrons which move freely through the positive ionic core of the metals. Since these free electrons causes conduction in metal under the application of electrical field, they are called as conduction electrons.
2. The free electrons are treated as equivalent to gas molecules; the laws of classical kinetic theory of gases can be applied to them. Therefore these electrons have mean free path ( $\lambda$ ), mean collision time ( $T$ ), average speed ( $v$ ).
3. In the absence of the electric field, the kinetic energy associated with an electron at a temperature  $T$  is given by  $\frac{1}{2} mv^2 = \frac{3}{2} kT$  Where  $v$  is the thermal velocity of the electron.
4. Since the motion of the electrons is random, the net current is zero in the absence of electric field. But when an electric field is applied, current is produced due to the drift velocity of the electrons.
5. The electric field (or Potential) due to positive ionic cores is considered to be uniform throughout the metal and hence neglected. But the force of attraction between the electrons & lattice ions and the force of repulsion between the electrons themselves are considered to be negligible.



**SRM**  
Institute of Science and Technology

# Classical Free Electron Theory of Metals



**SRM**  
Institute of Science and Technology

**Drift velocity ( $V_d$ )** : It is the average velocity acquired by the electrons in a direction opposite to the direction of the applied electric field.

**Mean Free Path ( $\lambda$ )**: The average distance travelled by the conduction electrons between two successive collisions with lattice ions is known as mean free path.

**Mean Collision Time** : It is the average time that elapses between two successive collisions of an electron with lattice points.

**Relaxation time**: It is time during which the average velocity decreases to  $(1/e)$  times its value of time when the field is turned off (OR) it can be defined as the time taken for the drift velocity of the electron to decay to  $1/e$  of its initial value.



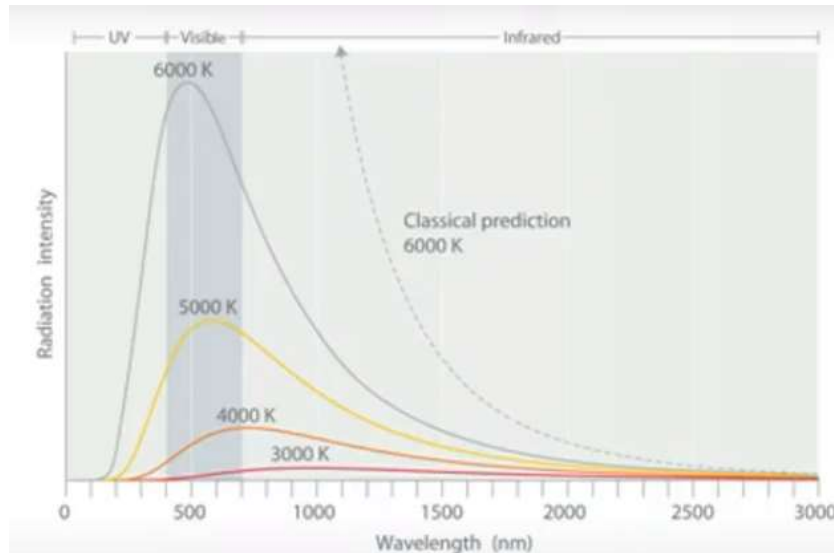
## Success of classical free electron theory:

- (1). It verifies Ohm's law.
- (2). It explains the electrical and thermal conductivities of metals.
- (3). It derives Wiedemann – Franz law. (i.e., the relation between electrical conductivity and thermal conductivity)
- (4). It explains optical properties of metals.



## Drawbacks of classical free electron theory:

The phenomena such as Photoelectric effect, Compton effect and the black body radiation couldn't be explained by classical free electron theory.

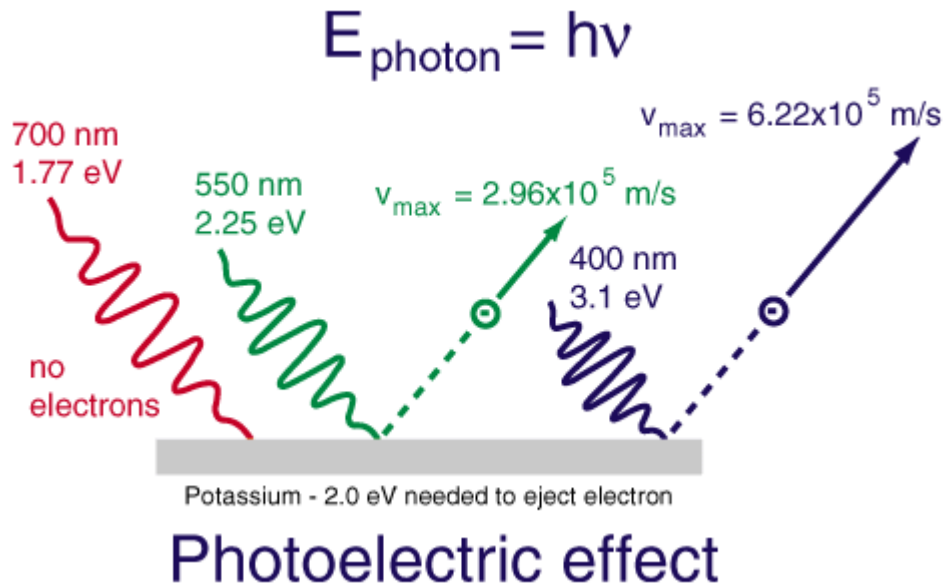


Max Planck (1858-1947)  
Nobel Prize (1918)

Classical explanation: electron can oscillate at any frequency, up to infinity. As a result the amount of energy emitted has no upper limit.

Planck's explanation: the energy from oscillating electrons can only happen at certain fixed values, called packets (or quanta) of energy, with  $E_{\text{one packet}} = nh\nu$





Classical physics do not apply to the photoelectric effect. Scientists believed that whether electrons are ejected from a metal and how much kinetic energy these electrons have all depend on the intensity of the light. The truth is that it is not the intensity of the light that causes this, but the frequency of the light. The intensity of the light will change the number of photoelectron emitted from a metal. Classical physics also say that at low intensities, the ejection of an electron takes time. Again, this is not the truth.

➤Electrical conductivity couldn't explained with temperature using this model. Electrical conductivity is inversely proportional to temperature  $T$ , while theory predicts that it is inversely proportional to square root of temperature  $T$ .

➤specific heat capacity.

➤The theoretical value of paramagnetic susceptibility is greater than the experimental value. Ferromagnetism cannot be explained by this theory.

➤Cannot explain the electrical conductivity of semiconductors and Insulators



**SRM**  
Institute of Science and Technology

# Classical Free Electron Theory of Metals



## ► The Quantum free electron theory

To overcome the drawbacks of classical free electron theory, Sommerfeld proposed quantum free electron theory. He treated electron as a quantum particle. He retains the vital features of classical free electron theory and included the Pauli Exclusion Principle & Fermi-Dirac statistics. The following are the assumptions of quantum free electron theory.

## Postulates

- 1. The free electrons in a metal can have only discrete energy values. Thus the energies are quantized.
- 2. The electrons obey Pauli's Exclusion Principle, which states that there cannot be more than two electrons in any energy level.
- 3. The distribution of electrons in various energy levels obey the Fermi-Dirac quantum statistics.
- 4. Free electrons have the same potential energy everywhere within the metal, because the potential due to ionic cores is uniform throughout the metal.
- 5. Electrons are treated as wave-like particles.



## **MERITS OF QUANTUM FREE ELECTRON THEORY**

1. It successfully explains the electrical and thermal conductivity of metals.
2. We can explain the Thermionic phenomenon.
3. Temperature dependence of conductivity of metals can be explained by this theory.
4. It can explain the specific heat of metals.
5. It explains magnetic susceptibility of metals.

## Failures of Quantum Free electron theory

- Fails to explain “why some crystals have metallic properties and other do not”.
- Fails to differentiate metals, semiconductors and insulators.
- Fails to explain the positive value of Hall coefficient.



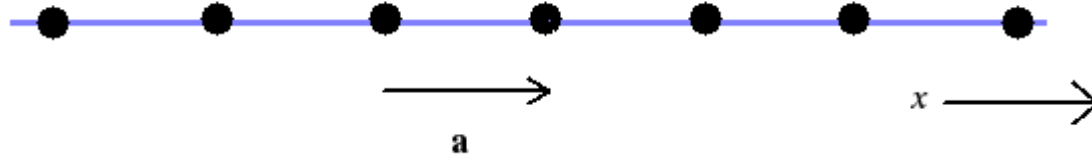
Zone theory was developed by Bloch in 1928. According to this theory, free electrons move in periodic potential provided by lattice. This theory is also known as band theory of solids.

## **Band Theory of Solids – Brillouin Zone and Kronig-Penney Model**



# 1D Lattice

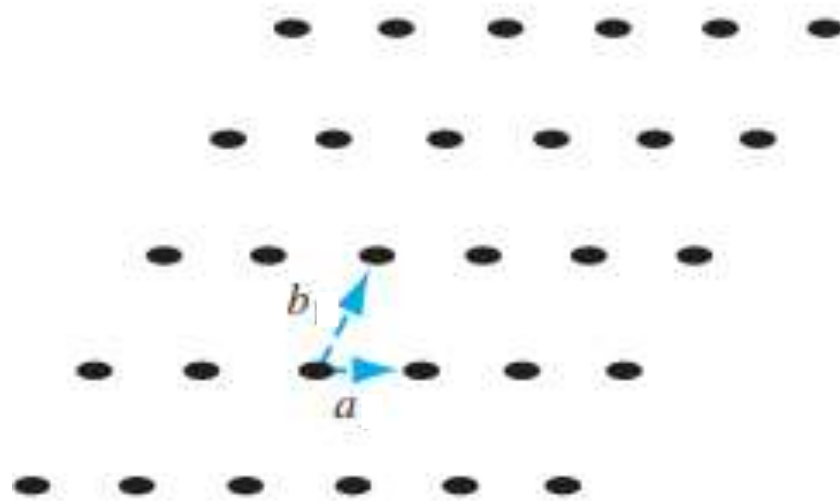
---



- Atoms (or ions) are arranged with equal spacing  $a$  called **lattice parameter**.

## 2D Lattice

---

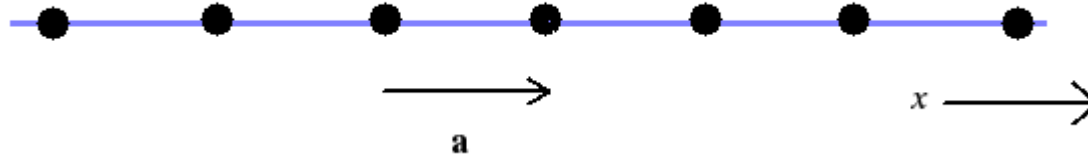


- Atoms (or ions) are periodically arranged in 2D space.
- Two lattice parameters  $a$  and  $b$  uniquely define the 2D lattice.

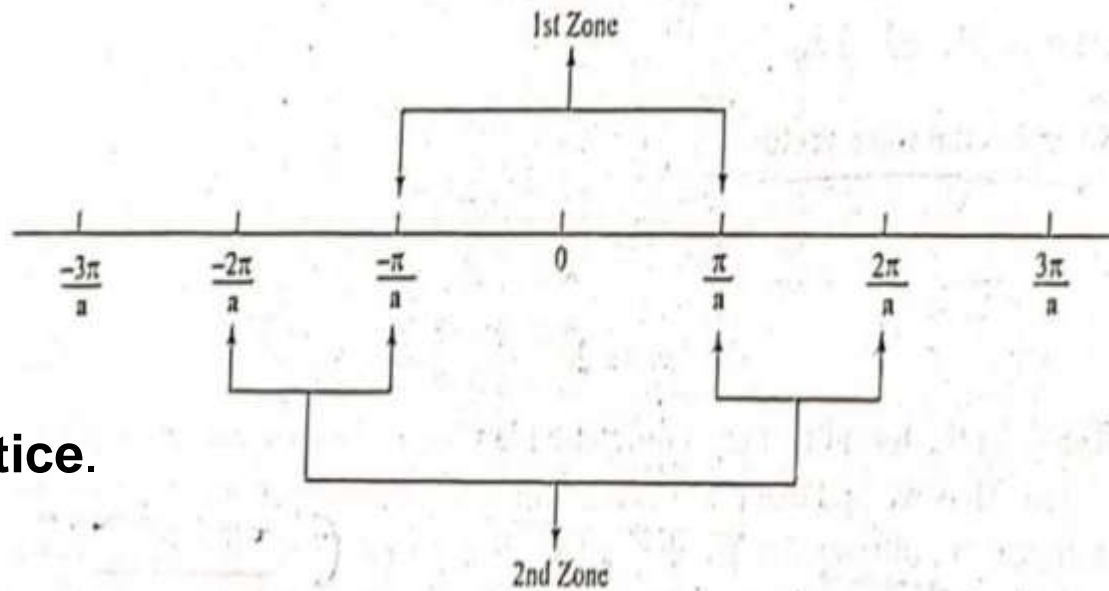
# Reciprocal Lattice and Brillouin Zone in 1D

---

Direct lattice.

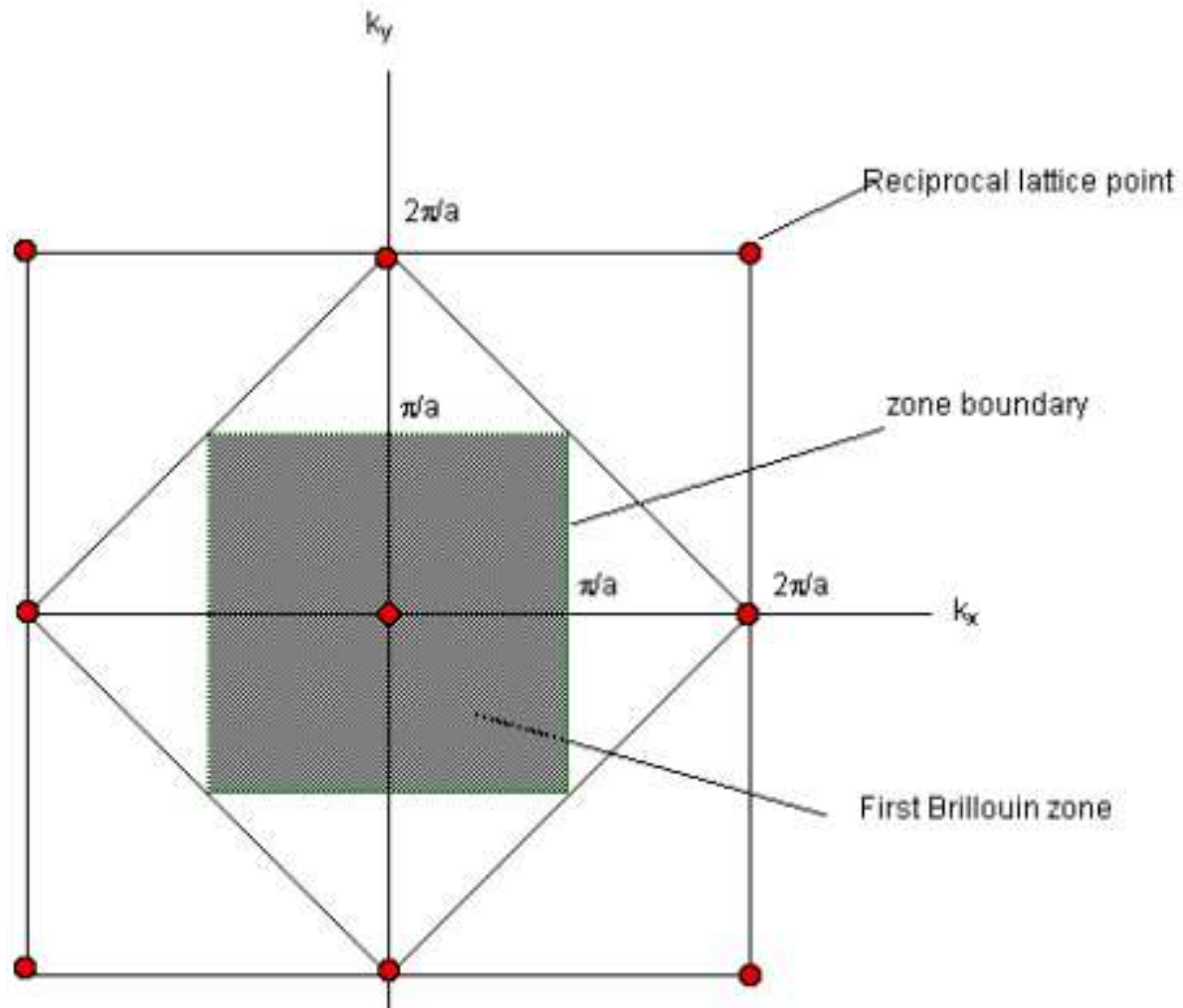


Reciprocal lattice.



# Brillouin Zone in 2D

---



- Also called **Wigner-Seitz primitive cell** in the reciprocal lattice.

# Band Theory of Solids

---

- Developed by Felix Bloch in 1928. (PhD thesis)
- **Free-electron approximation** is abandoned.
- Coulombic interaction between valence electrons and positively charged metal ions is included.
- **Independent-electron approximation** is retained.
- Gives rise to band structure in solids.



Felix Bloch (1905 -1983)

Nobel Prize in Physics, 1952

# Bloch's Theorem

---

- A fundamental theorem in the quantum theory of crystalline solids.
- **Statement:** The wave function of an electron moving in a periodic 1D lattice is of the form

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

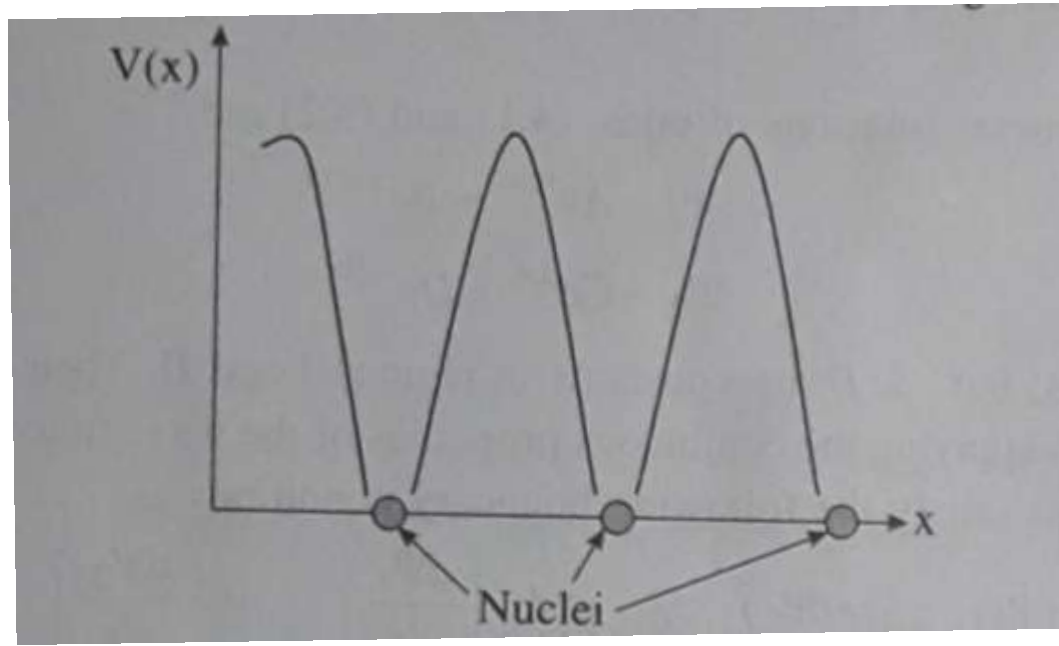
- $u(x)$  has the same periodicity as the lattice.

$$u(x + a) = u(x)$$

- **Alternate statement** of Bloch's theorem:

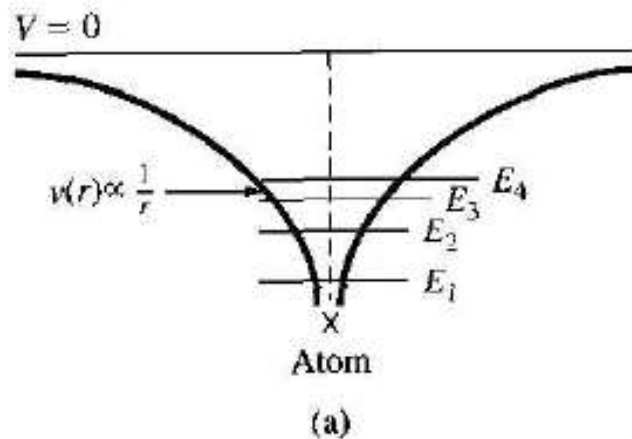
$$\psi(x + a) = e^{ika}\psi(x)$$

## The motion of an electron under actual periodic potential in Crystal lattice

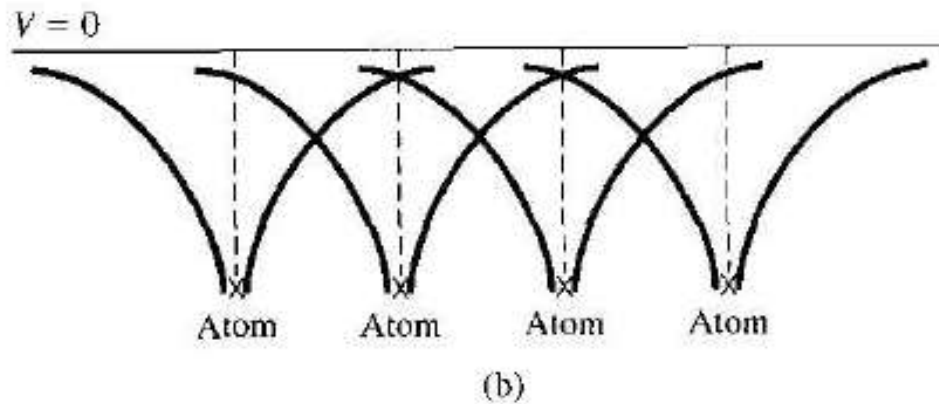


Electron move to close enough to a nucleus, a very strong attractive Coulomb potential is seen in fig. Of course, on a line that does not pass exactly through nuclei, the potential will not plunge that low.

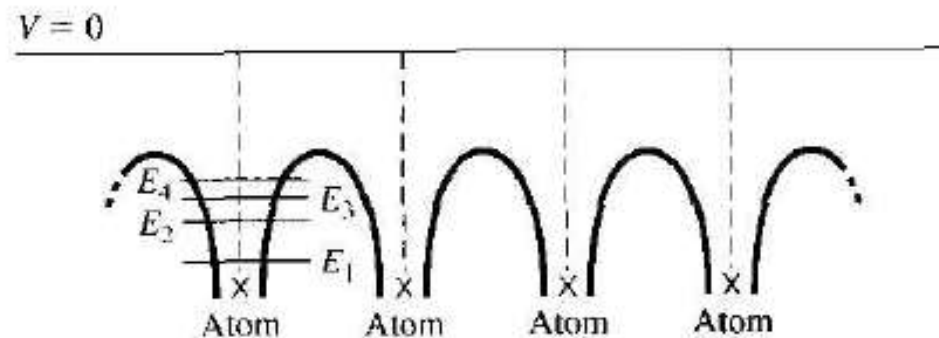




(a) Potential function if a single isolated atom.

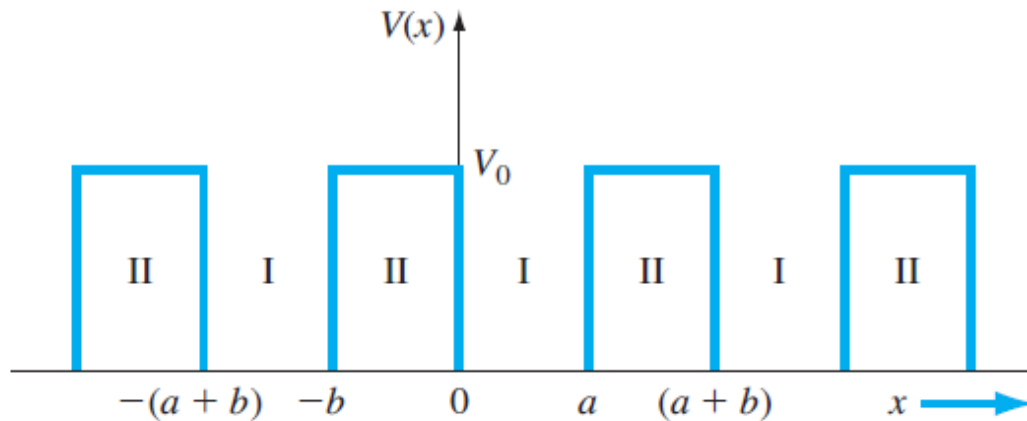


(b) Overlapping potential functions of adjacent atoms.



(c) Net potential function of a one-dimensional single crystal.

## ELECTRON IN A PERIODIC FIELD OF A CRYSTAL (THE KRONIG - PENNEY MODEL)



**The one-dimensional periodic potential function of the Kronig-Penney model.**

For the treatment of our problem, a periodic repetition of the potential well of Fig.3, a periodic arrangement of potential wells and potential barriers, is most probably very close to reality and is also best suited for the calculation. Such a periodic potential is shown in Fig. for the one-dimensional case. Although this model is highly artificial, yet it illustrates many of the characteristic features of the behaviour of electrons in a periodic lattice. The wave functions associated with this model can be calculated by solving Schrodinger equations for the two regions I and II. The time- independent Schrodinger equation takes the following forms for the two regions

The Periodic Square well Potential has the period  $(a+b)$  and Satisfy the following boundary conditions:

$$V(x) = 0 \quad \text{for } 0 < x < a$$

$$V(x) = V_0 \quad \text{for } -b < x < 0$$

The Corresponding Schrodinger eqn.  
for the above two boundary condition

$$\frac{d^2 \psi_x}{dx^2} + \frac{2mE}{\hbar^2} \psi(x) = 0 \quad \text{for } 0 < x < a \quad \text{--- (1)}$$

and

$$\frac{d^2 \psi_x}{dx^2} - \frac{2m}{\hbar^2} (V_0 - E) \psi(x) = 0 \quad \text{for } -b < x < 0 \quad \text{--- (2)}$$

Take two real quantities  $\alpha$  and  $\beta$  as

$$\alpha^2 = \frac{2mE}{\hbar^2}$$

equivalently

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

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

$$k^2 = \frac{2mE}{\hbar^2}$$

So eqn (1) & (2) written as

$$\frac{d^2 \psi}{dx^2} + \alpha^2 \psi(x) = 0 \quad \text{--- (3)}$$

$$\frac{d^2 \psi}{dx^2} - \beta^2 \psi(x) = 0. \quad \text{--- (4)}$$

The wave function  $\Psi = e^{ikx} \cdot u_k(x)$

$\swarrow$   $\searrow$   
 Traveling wave Block Function

$$\frac{d\Psi}{dx} = ik e^{ikx} u(x) + e^{ikx} \frac{du}{dx}$$

$$\frac{d^2\Psi}{dx^2} = -k^2 e^{ikx} u(x) + 2ik e^{ikx} \frac{du}{dx} + e^{ikx} \frac{d^2u}{dx^2}$$

Sub. the above value in eqn (3) & (4)  
and simplify the eqn (3) & (4)

$$\frac{d^2u_1}{dx^2} + 2ik \frac{du_1}{dx} + (\alpha^2 - k^2)u_1 = 0 \quad \text{--- (5)}$$

$$\frac{d^2u_2}{dx^2} + 2ik \frac{du_2}{dx} - (\beta^2 + k^2)u_2 = 0 \quad \text{--- (6)}$$

The solution of eqn (5) & (6)

$$u_1 = A e^{i(\alpha - k)x} + B e^{-i(\alpha + k)x} \quad \text{--- (7)}$$

$$u_2 = C e^{i(\beta - ik)x} + D e^{-i(\beta + ik)x} \quad \text{--- (8)}$$

A, B, C, D are constant

The value of constant will be Findout  
using Boundary conditions and the  
Function should be continuous

$$u_1(0) = u_2(0) \text{ \& } \left( \frac{du_1}{dx} \right)_{x=0} = \left( \frac{du_2}{dx} \right)_{x=0}$$

$$u_1(a) = u_2(-b) \text{ \& } \left( \frac{du_1}{dx} \right)_{x=a} = \left( \frac{du_2}{dx} \right)_{x=-b}$$

applying the boundary Condition the  
eqn (7) \& (8) becomes.

$$u_1 = Ae^{i(\alpha - K)x} + Be^{-i(\alpha + K)x} \quad \text{--- (7)}$$

$$u_2 = Ce^{i(\beta - iK)x} + De^{-i(\beta + iK)x} \quad \text{--- (8)}$$

A, B, C, D are constant



Then we get,  $A + B = C + D$  — (9)

$$Ai(\alpha - K) - Bi(\alpha + K) = C(\beta - iK) - D(\beta + iK) \quad (10)$$

$$Ae^{i(\alpha - K)a} + Be^{-i(\alpha + K)a} = Ce^{-i(\beta - iK)b} + De^{i(\beta + iK)b} \quad (11)$$

$$Ai(\alpha - K)e^{i(\alpha - K)a} - Bi(\alpha + K)e^{i(\alpha + K)a} = C(\beta - iK)e^{-i(\beta - iK)b} - D(\beta + iK)e^{i(\beta + iK)b} \quad (12)$$

For eqn (9), (10), (11) & (12) a non zero solution exist only if the determinant of the coefficient A, B, C, D vanishes

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ i(\alpha - K) & -i(\alpha + K) & (\beta - iK) & -(\beta + iK) \\ e^{i(\alpha - K)a} & e^{-i(\alpha + K)a} & e^{-i(\beta - iK)b} & e^{i(\beta + iK)b} \\ i(\alpha - K)e^{i(\alpha - K)a} & -i(\alpha + K)e^{i(\alpha + K)a} & -(\beta - iK)e^{-i(\beta - iK)b} & -(\beta + iK)e^{i(\beta + iK)b} \end{bmatrix} = 0$$



It turns out that solutions are possible only for energies given by the relation

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

The above equation is a **transcendental** equation. No analytical solutions are possible. Only graphical solutions can be obtained.

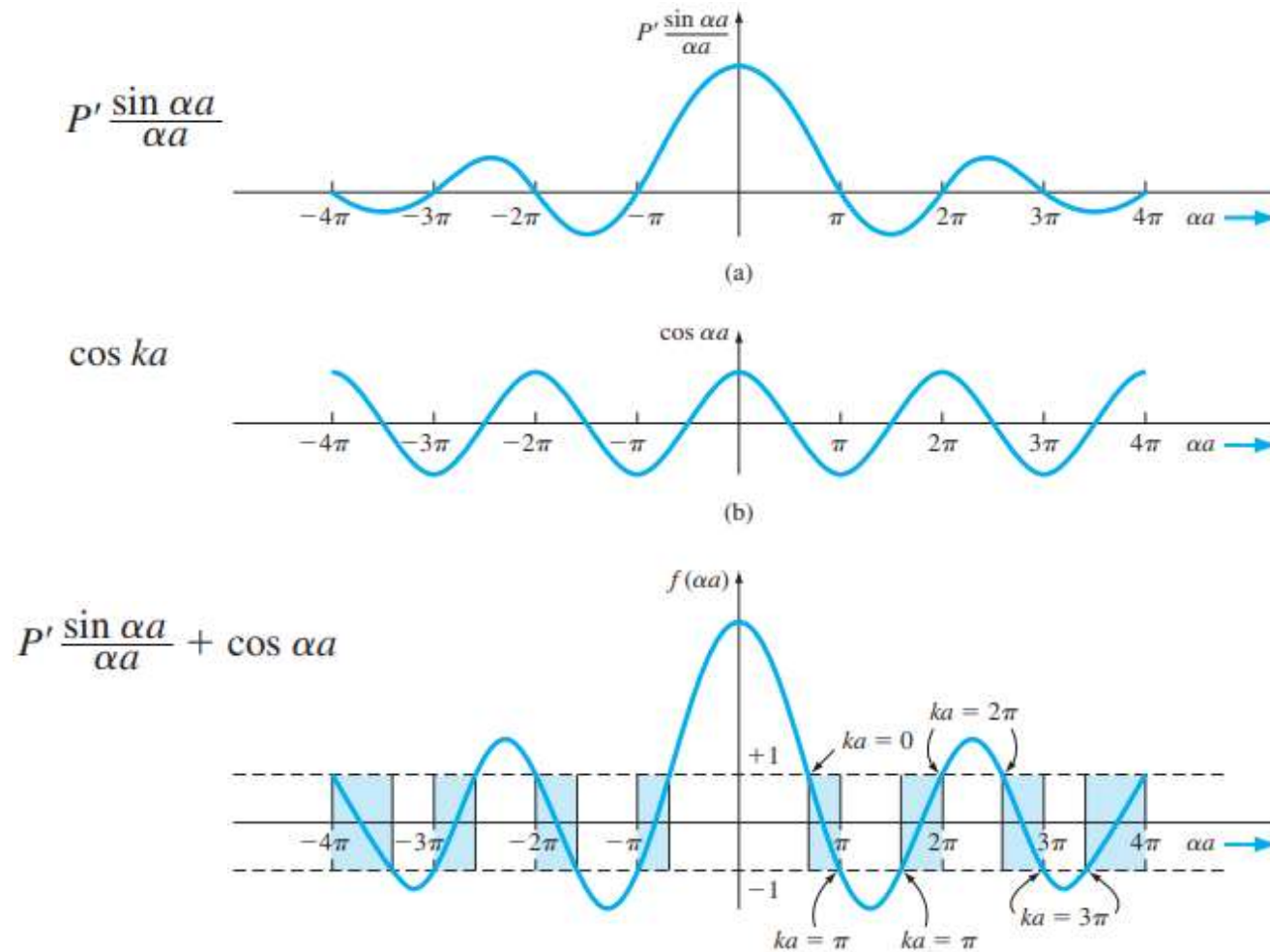
$$\text{Where } P = \frac{4\pi^2 ma}{h^2} V_0 a \text{ and } \alpha = \frac{2\pi}{h} \sqrt{2mE}$$

P is called scattering power of the barrier and  $V_0 a$  is called barrier strength.

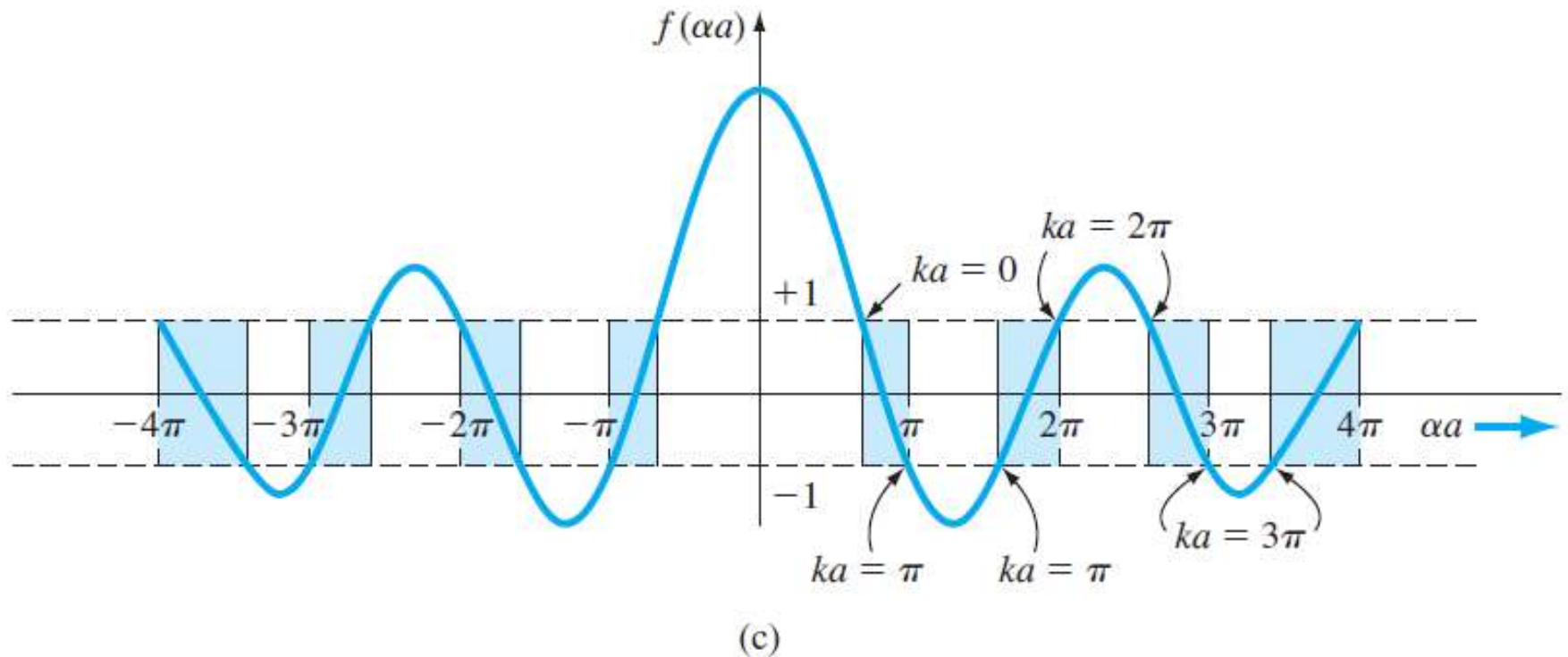
The left hand side of the equation (3) is plotted as a function of ' $\alpha a$ ' for the value of  $P = 3\pi/2$  which is shown in fig, the right hand side takes values between -1 to +1 as indicated by the horizontal lines in fig. Therefore the equation (3) is satisfied only for those values of ' $ka$ ' for which left hand side between  $\pm 1$ .

From fig , the following conclusions are drawn.

# Electron in a Periodic Potential

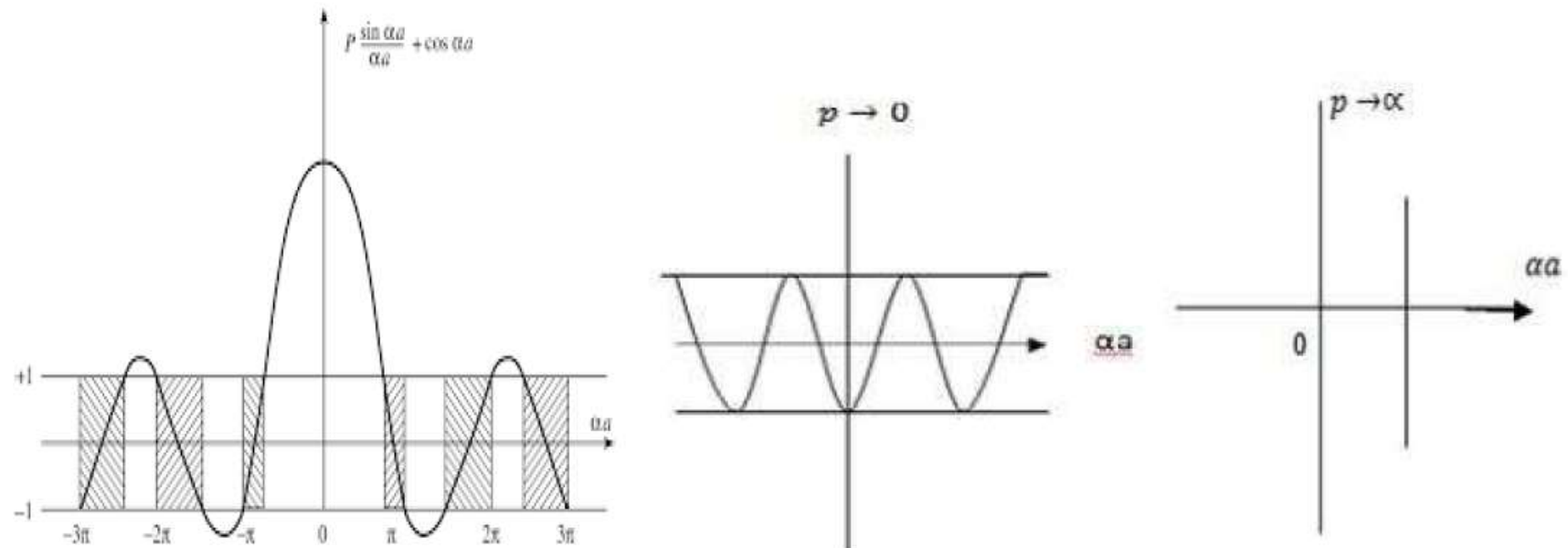


- Only values of  $\alpha a$  for which  $f$  lies between  $+1$  and  $-1$  are allowed.



**The  $\cos ka$  is only defined within the limits between  $+1$  and  $-1$ , indicating that, since  $\alpha$  is related to  $E$ , the solution for energies should also be between those limits. This essentially implies that the electrons, moving in a periodically varying potential field, may possess energies within certain energy bands only, i.e., within shaded regions. These allowed energy bands are separated by ranges of  $\alpha a$  corresponding to  $\cos ka$  being either greater than  $+1$  or less than  $-1$ , i.e., corresponding to forbidden energy ranges.**

- 1) The energy spectrum of the electron consists of a number of allowed and forbidden energy bands.
- 2) As ' $\alpha a$ ' increases the width of the allowed energy band increases and the width of forbidden band decreases.
- 3) With increasing potential barrier  $P$ , the width of an allowed band decreases.
- 4) As  $P \rightarrow \infty$ , the allowed energy becomes infinitely narrow and the energy spectrum is a line spectrum as shown in fig.
- 5) When  $P \rightarrow 0$  then all the electrons are completely free to move in the crystal without any constraints. Hence, no energy level exists that is all the energies are allowed to the electrons as shown in fig. This case supports the classical free electrons theory.

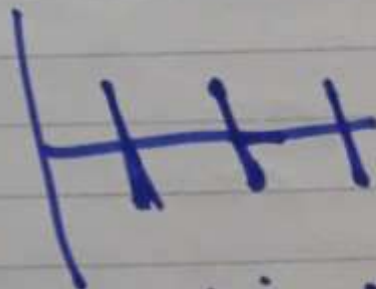


for  $p \rightarrow \infty$  Spectrum becomes a line.

$$\text{So, } \sin \frac{\alpha a}{a} = 0 \quad \alpha a = \pm n\pi \Rightarrow \alpha = \frac{n\pi}{a}$$

$$\alpha^2 = \frac{n^2 \pi^2}{a^2} = \frac{8\pi^2 m E}{h^2}$$

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



(like particle in a potential well)



4. on the other hand, if  $p=0$

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

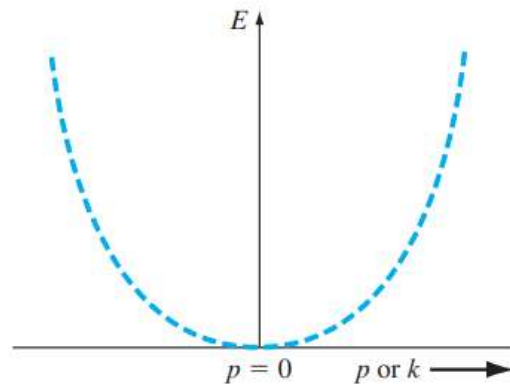
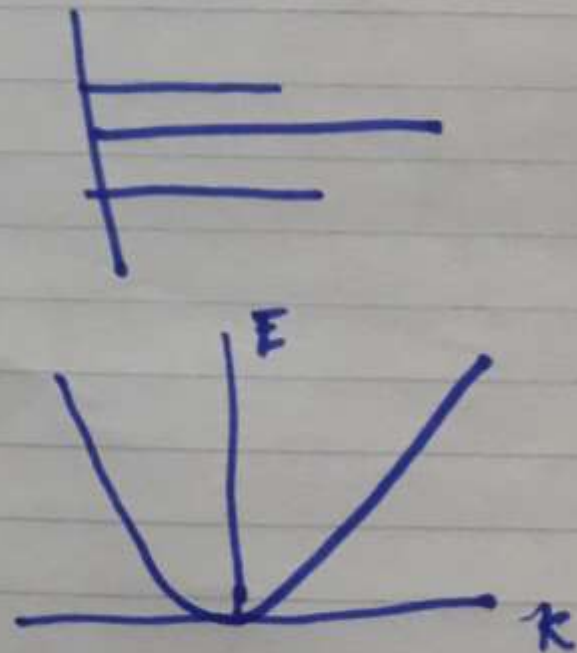
$$\alpha = k \Rightarrow k^2 = \alpha^2 = \frac{8\pi^2 m E}{h^2}$$

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

$$\text{So } E = \frac{h^2 \left( \frac{2\pi}{\lambda} \right)^2}{8\pi^2 m} = \frac{h^2}{2m\lambda^2}$$

Using de-Broglie's formula

$$E = h^2 / 2m \left( \frac{p}{h} \right)^2 = \frac{p^2}{2m} = \frac{1}{2} m v^2 \text{ (Free particle)}$$



# Kronig-Penney Model: Conclusion

---

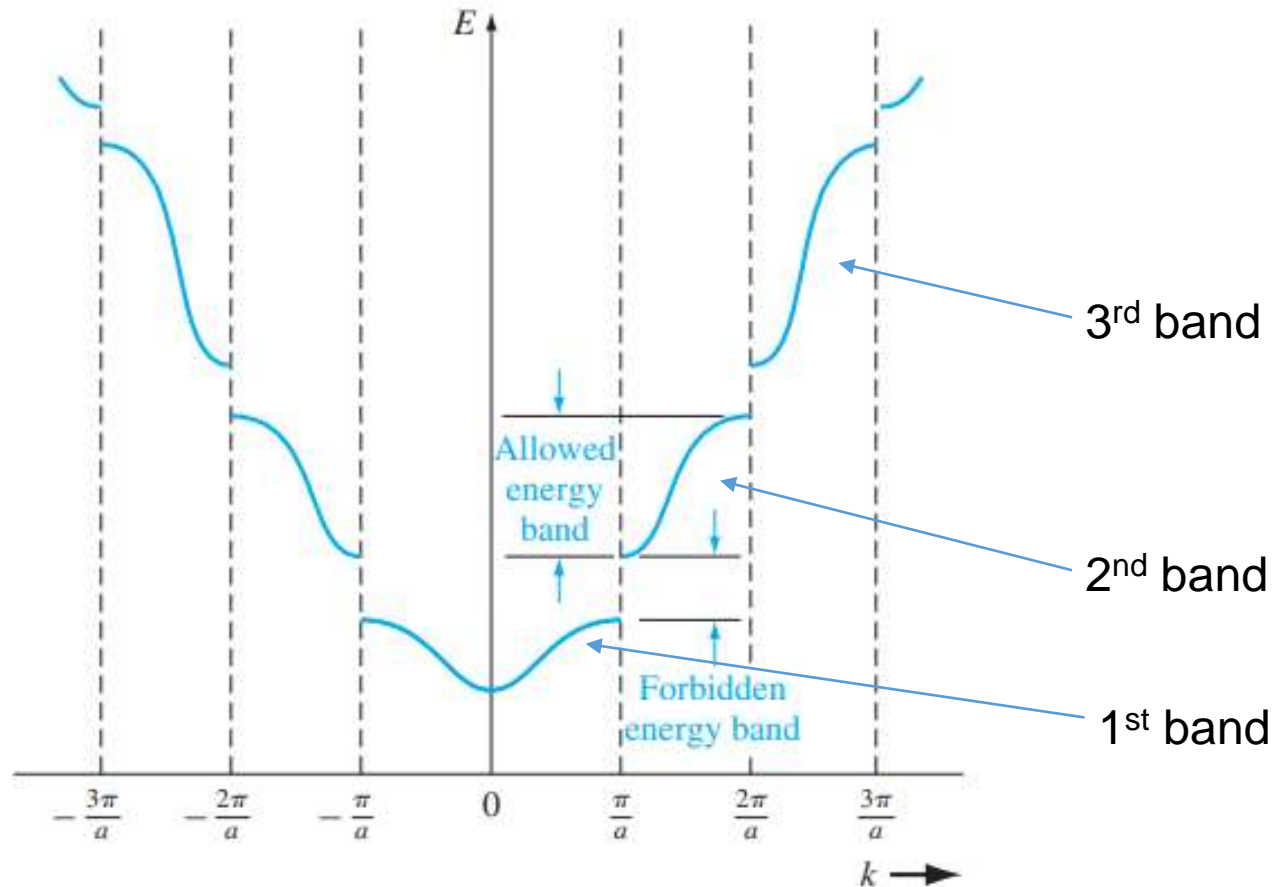
*We have been considering the Kronig–Penney model, which is a one-dimensional periodic potential function used to model a single-crystal lattice. The principal result of this analysis, so far, is that electrons in the crystal occupy certain allowed energy bands and are excluded from the forbidden energy bands.*

There are three types of E-K diagram

- Periodic zone
- Extended zone
- Reduced zone



# E-k Diagram for an Electron in a Periodic Potential



- Discontinuities in  $E$  indicate forbidden energies of the electron.

## **Extended Zone Scheme:**

In this scheme, different bands are drawn in different zones  
In  $k$ - space.

A discontinuities is obtained at  $K = \pm \frac{n\pi}{a}$  where  $n = \pm 1, \pm 2, \dots$

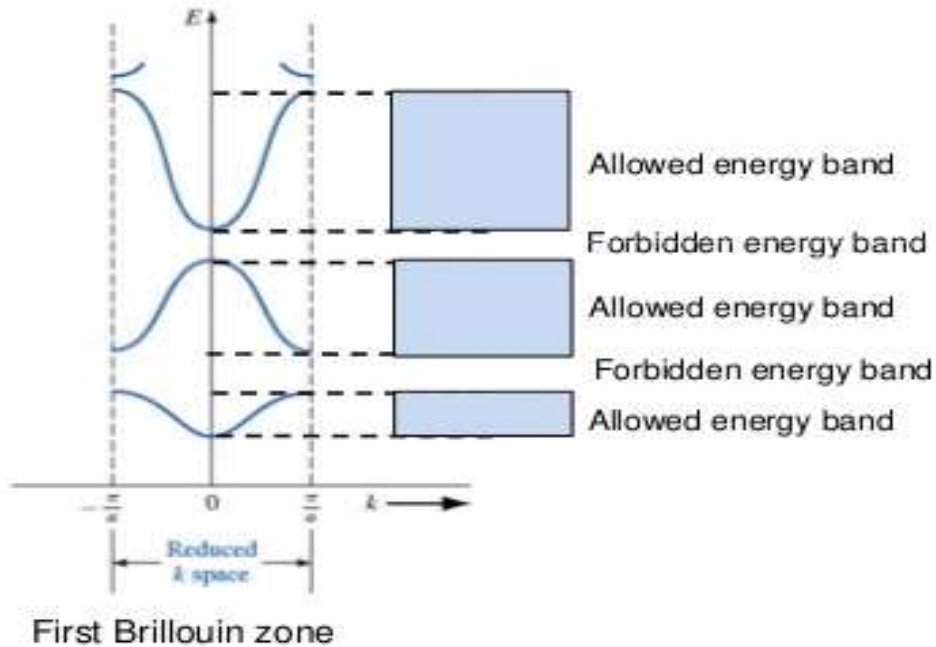
For  $k = \frac{\pi}{a}$  to  $\frac{\pi}{a}$  is first Brillouin zone

For  $k = -\frac{\pi}{a}$  to  $-\frac{2\pi}{a}$  and  $\frac{\pi}{a}$  to  $\frac{2\pi}{a}$  is second Brillouin zone

The discontinuities in the curve is due to Braggs law of reflection

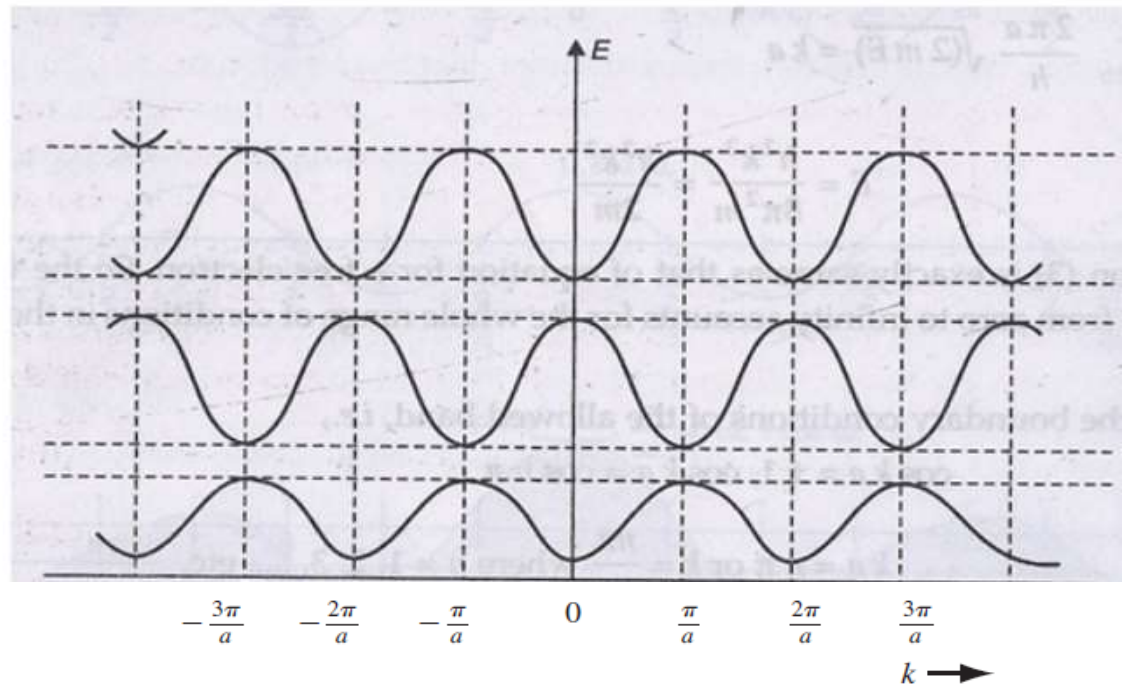
at the edges of allowed bands (i.e)  $K = \pm \frac{n\pi}{a}$

## Reduced zone



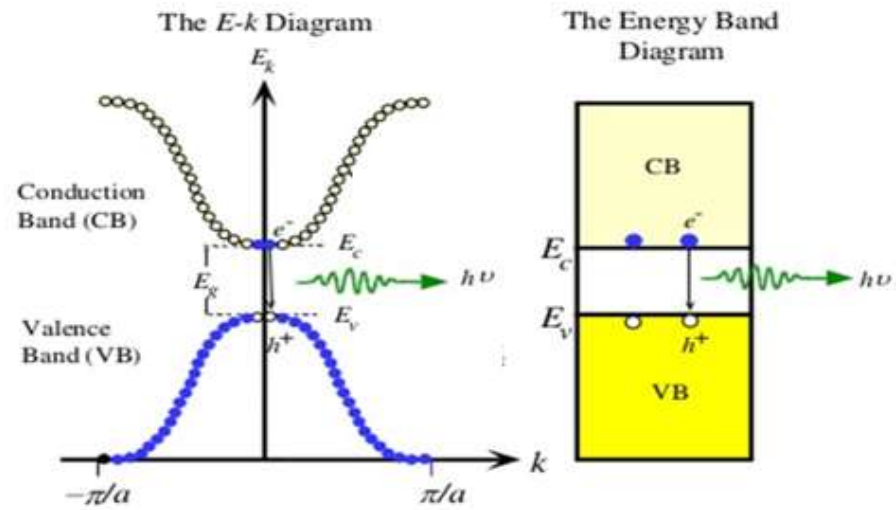
**When the bands (in extended zone) are all folded back into the first Brillouin zone is called reduced zone**

## E – k diagram – Periodic zone



### Periodic zone scheme:

The periodic repetition of allowed energy values corresponding to each allowed band, which is obtained by the periodic repetition of the region of  $-\frac{\pi}{a} < k < \frac{\pi}{a}$  through whole k-space.



## What are the significance of E-K diagram

- No theoretical study, experimentation and technological application can take place without E-K diagram.
- This diagram indicates the band gap  $E_g$  which is the difference in energy between top of the valance band and bottom of the conduction band
- This diagram demonstrate electron (hole) mobility
- This diagram explains electron (hole) effective mass
- This diagram indicate how the electron states are equally spaced in K-Space
- This diagram clearly shows direct vs indirect band gap

We know

$$P = \hbar k$$

$$\text{Kinetic energy (K)} = \frac{1}{2}mv^2, \text{ and}$$

$$\text{Momentum (p)} = mv$$

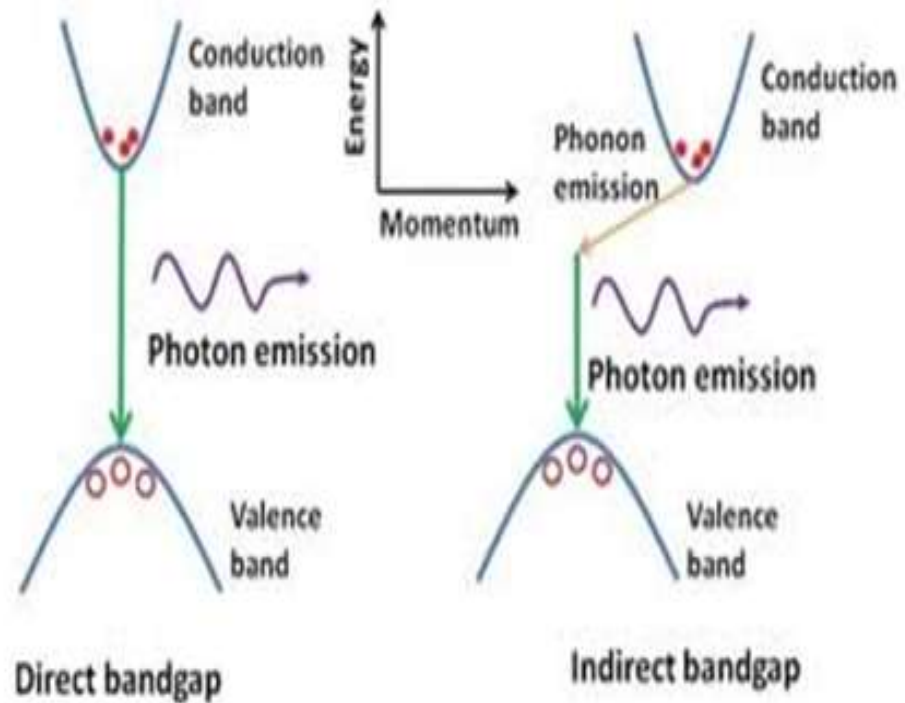
Where, symbols have usual meaning.

Now,

$$K = \frac{1}{2}mv^2 = \frac{1}{2}mv^2 \times \frac{m}{m} = \frac{1}{2} \frac{m^2 v^2}{m} = \frac{(mv)^2}{2m} = \frac{p^2}{2m}$$

therefore,

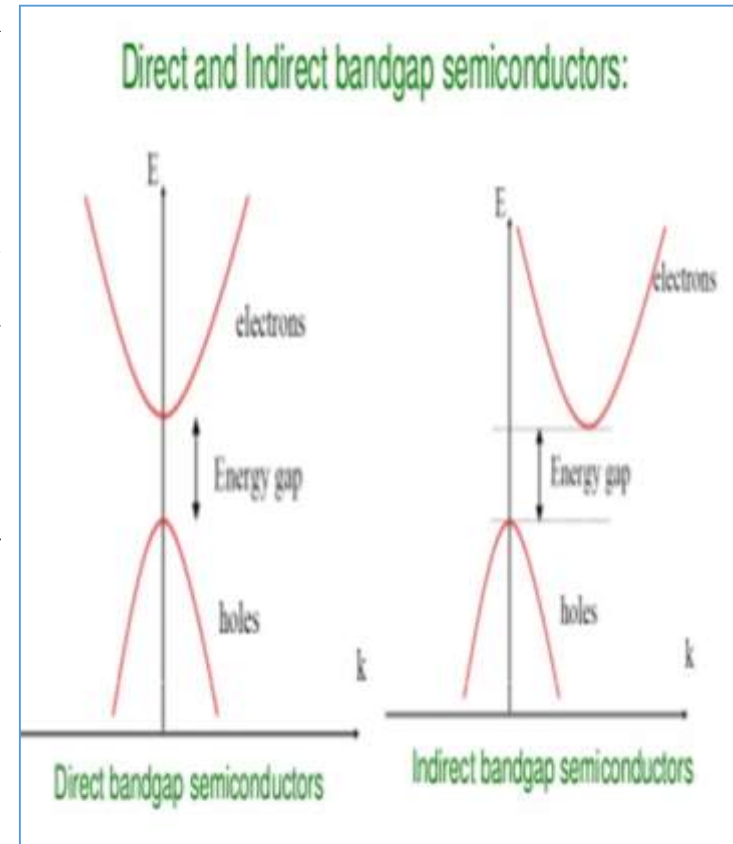
$$K = \frac{p^2}{2m}$$



A direct recombination occurs with the release of energy equals to energy difference between two levels such as  $E_g$ . The probability of radiative recombination is high and hence direct bandgap semiconductors are used in optical sources. Due to relative difference in momentum, first the momentum is conserved by release of energy only after both the Momentum align themselves. The probability of radiative recombination is comparatively low.

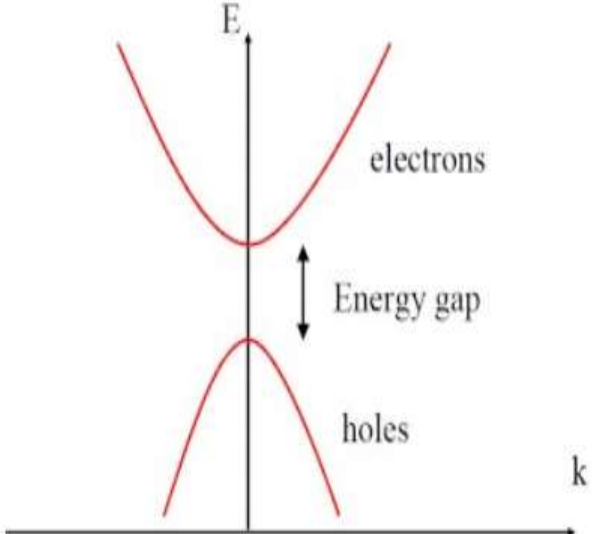
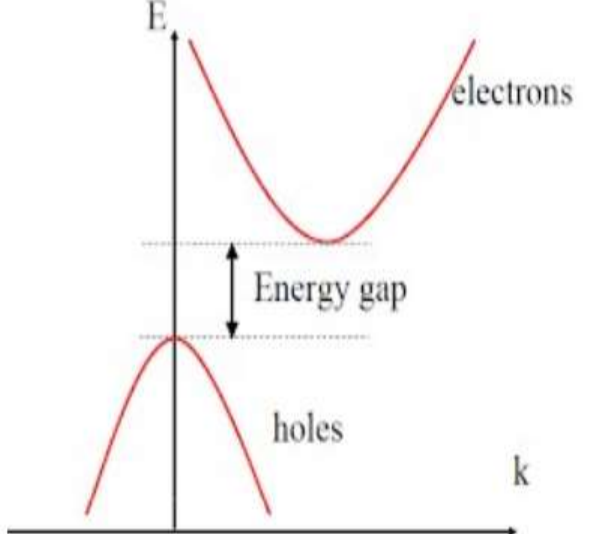
## Direct and Indirect band gap semiconductors

- We know the relation between energy and wave number for an one dimensional lattice. In real crystals the  $E - k$  relationship is much more complicated.
- In crystals the interatomic distances and internal potential energy distribution vary with direction of the crystal.
- Hence the  $E - K$  relationship and energy band formation depends on the orientation of the electron wave vector to the crystallographic axes.
- In few crystals like GaAs, the maximum of the valence band occurs at the same value of  $K$  as the minimum of the conduction band.
- This is called *direct band gap semiconductor*.





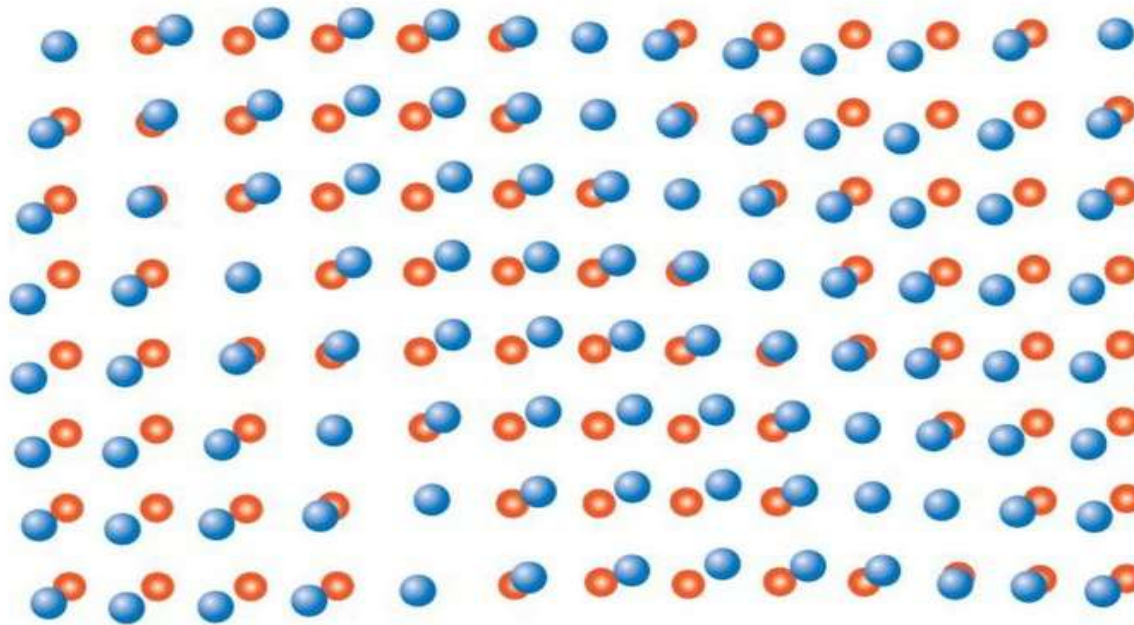
No	Direct Band gap semiconductor	Indirect band gap semiconductor
1	A direct band-gap (DBG) semiconductor is one in which the maximum energy level of the valence band aligns with the minimum energy level of the conduction band with respect to momentum.	A indirect band-gap (DBG) semiconductor is one in which the maximum energy level of the valence band are misaligned with the minimum energy level of the conduction band with respect to momentum.
2	In a DBG semiconductor, a direct recombination takes place with the release of the energy equal to the energy difference between the recombining particles.	Due to a relative difference in the momentum, first, momenta align themselves, a recombination occurs accompanied with the release of energy.
3	The efficiency factor of a DBG semiconductor is higher.	The efficiency factor of a IBG semiconductor is lower.
4	Example of DBG semiconductor material is Gallium Arsenide (GaAs).	Examples of IBG semiconductors are Silicon and Germanium.
5	DBG semiconductors are always preferred over IBG for making optical sources.	The IBG semiconductors cannot be used to manufacture optical sources.

No	Direct Band gap semiconductor	Indirect band gap semiconductor
6	The probability of a radiative recombination is high.	The probability of a radiative recombination is comparatively low.
7		

# Phonons

## Atomic Vibrations

Atomic vibrations are in the form of lattice waves or phonons



- Normal lattice positions for atoms
- Positions displaced because of vibrations

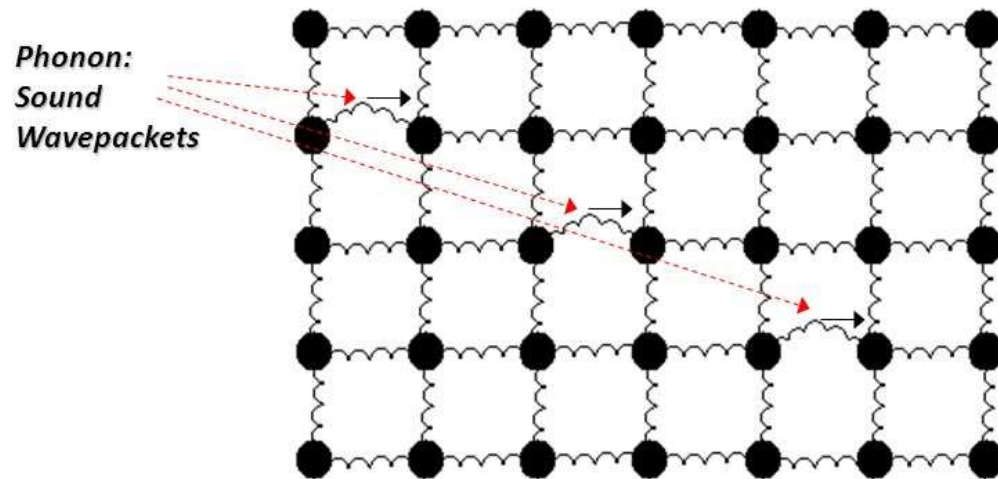
Adapted from Fig. 17.1

# CONCEPT OF PHONONS

- Any solid crystal consists of atoms bound into a specific repeating three-dimensional spatial pattern called a lattice.
- Here the atoms behave as if they are connected by tiny springs, their own thermal energy or outside forces make the lattice vibrate.
- This generates mechanical waves that carry heat and sound through the material.
- *A packet of these waves can travel throughout the crystal with a definite energy and momentum, so in quantum mechanical terms the waves can be treated as a particle, called a phonon.*
- A phonon is a definite discrete unit or *quantum* of vibrational mechanical energy, just as a photon is a quantum of electromagnetic or light energy.

# Phonon:

Propagating lattice vibrations can be considered to be sound waves, and their propagation speed is the speed of sound in the material.





## Phonon:

❖ A photon is the smallest unit of light. Similarly, for sound, the smallest unit is called phonon. In a lattice structure, vibrations are created by atoms. The quantized, lowest state energy of vibration is called phonon.

❖ Atoms were considered as rigid, with atoms stuck in their lattice. In reality, atoms can be considered as simple harmonic oscillators. The harmonic oscillator has a ground state energy and an associated vibrational mode even at  $0^\circ \text{ K}$ .

❖ It is named phonons because at high energy levels long wavelength phonons give rise to sound. According to quantum mechanics, similar particles have wave nature, waves must also have particle nature. So, phonon is also treated as quasi particle. Similar to particles, these waves can carry throughout the crystal, heat, energy and momentum.

# Comparison between Phonons and Photons

## PHONONS

- Quantized normal modes of lattice vibrations. The energies & momenta of phonons are quantized

$$E_{\text{phonon}} = \frac{h\nu}{\lambda}$$

$$p_{\text{phonon}} = \frac{h}{\lambda}$$

Phonon wavelength:

$$\lambda_{\text{phonon}} \approx 10^{-10} \text{ m}$$

## PHOTONS

- Quantized normal modes of electromagnetic waves. The energies & momenta of photons are quantized

$$E_{\text{photon}} = \frac{hc}{\lambda}$$

$$p_{\text{photon}} = \frac{h}{\lambda}$$

Photon wavelength (visible):

$$\lambda_{\text{photon}} \approx 10^{-6} \text{ m}$$

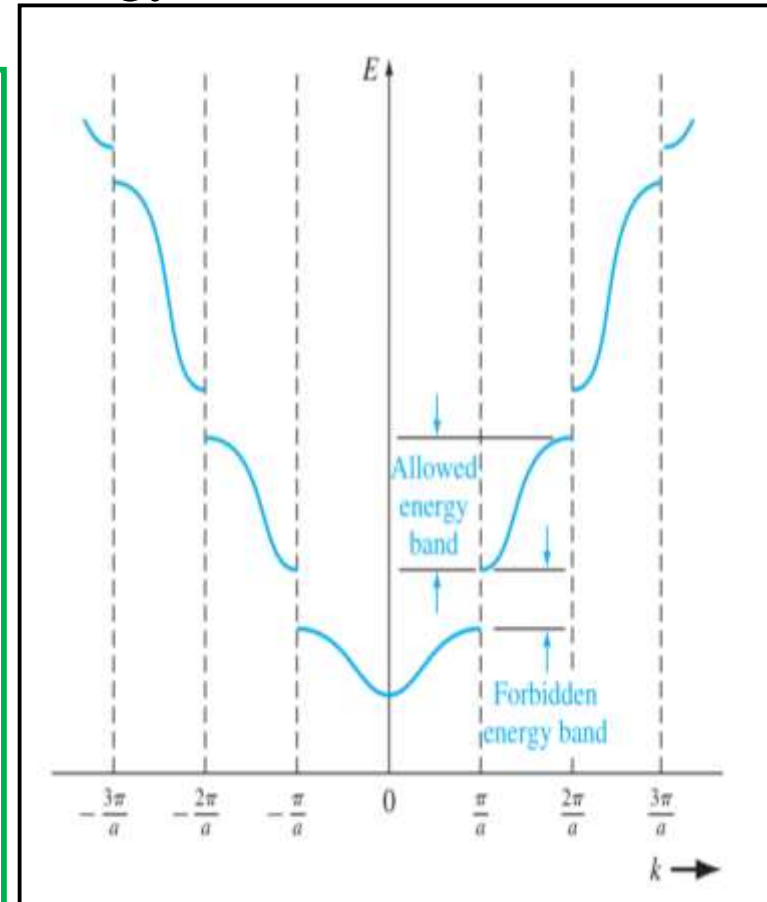
# Brillouin zones



Brillouin zones are the boundaries marked by the values of  $K$  in which electrons can have allowed energy values.

➤ In the fig. it is seen that the energy values increases continuously from 0 to  $\pm\pi/a$ . So the electrons is moving within region, so this region is called as first **Brillouin zones**.

➤ The second allowed energy values consists of two parts  $\pi/a$  to  $2\pi/a$  and  $-\pi/a$  to  $-2\pi/a$ . this is called second **Brillouin zones**.

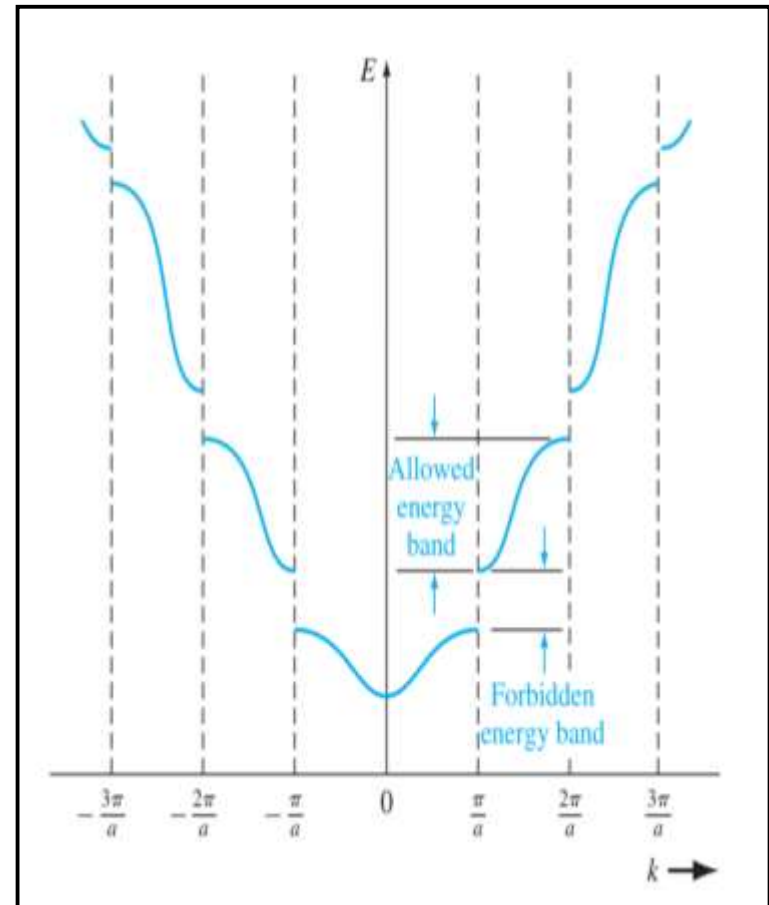




# Brillouin zones

➤ In the fig. it is noted that each Brillouin zone is separated by a forbidden zone. So the electron go from one Brillouin zone to other only if it is supplied with an energy equal to forbidden gap.

➤ So the forbidden gap is one which decides whether the solid is conductor/Insulator/semiconductor.

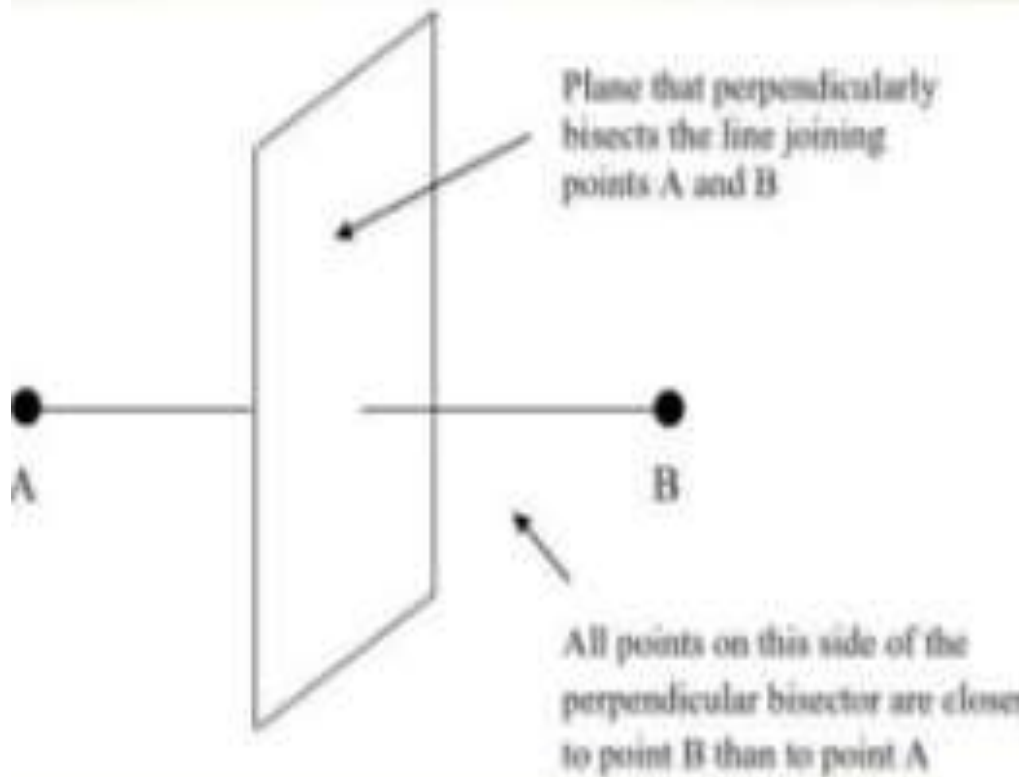


## Construction of Brillouin Zone

The first Brillouin zone is considered as the **Wigner-Seitz (WS) primitive cell** in the reciprocal lattice. In other words, the first Brillouin zone is a geometrical construction to the WS primitive cell in the  $k$ -space.

BZ is a primitive cell in reciprocal space (set of zones 1st, 2nd,.....), and can be described as an allowed energy - momentum region of electrons in reciprocal space. In that region of space the Bloch electrons will have traveling wave . At the boundaries of zones the electron waves will get Bragg diffracted and hence no traveling wave exist. The Bragg diffraction at the zone boundaries is the origin of forbidden gap in crystals.

## Bragg's Plane



$$2d \sin \theta = n \lambda$$

$$n = \text{integ..}$$

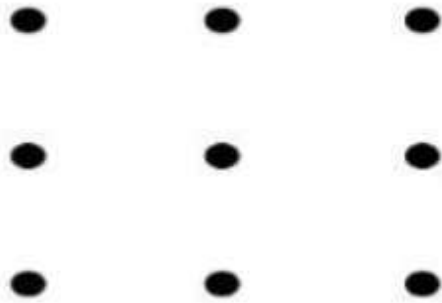
At normal incident

$$\theta = \frac{\pi}{2} \quad \& \quad d = a$$

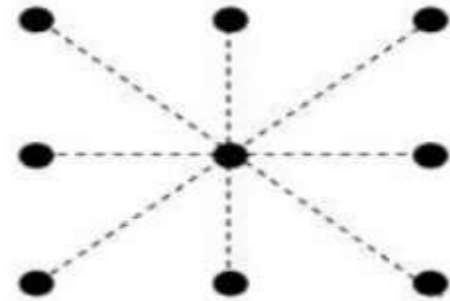
$$2a = n \lambda \rightarrow \lambda = \frac{2a}{n}$$

$$k = \frac{2\pi}{\lambda} = \frac{n 2\pi}{2a} = \frac{n\pi}{a}$$

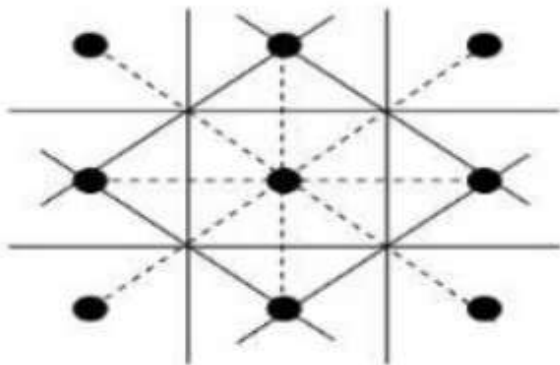
# Identifying a region closest to a given lattice point than to its neighbor in 2 Dimensional Space:



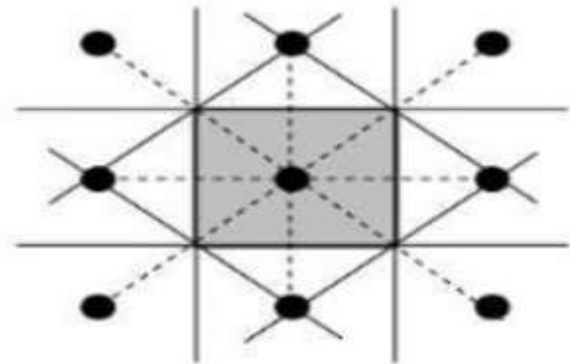
a) Two dimensional square lattice



b) Draw lines from a given lattice point to all of its nearest neighbors

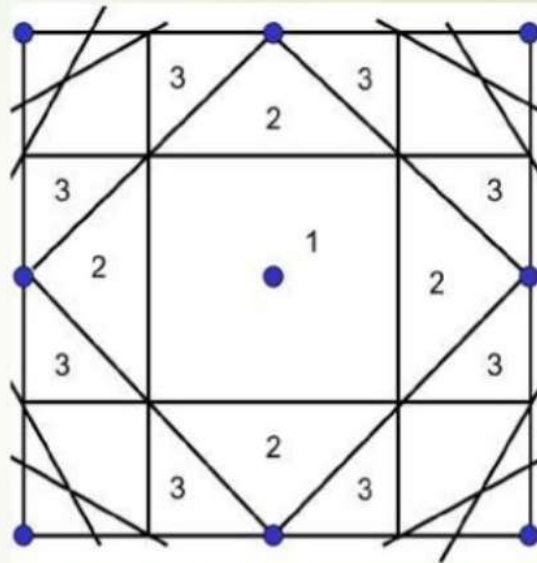


c) Draw perpendicular bisectors to the lines joining the point to its nearest neighbors

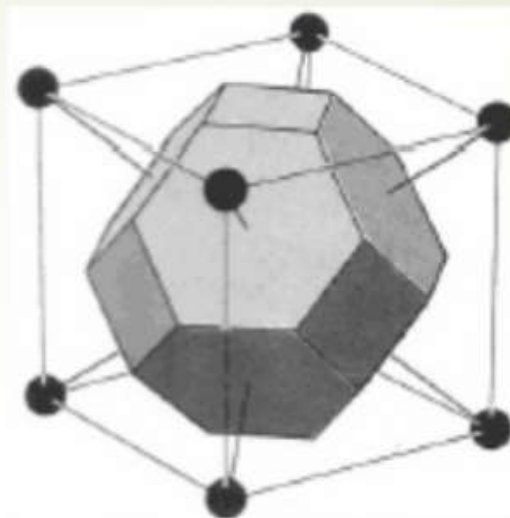
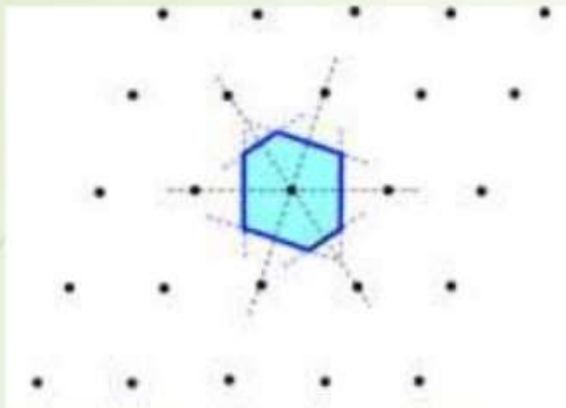


d) The Wigner-Seitz cell is identified as the innermost region bounded by the perpendicular bisectors. It is shown in the figure as the shaded region.

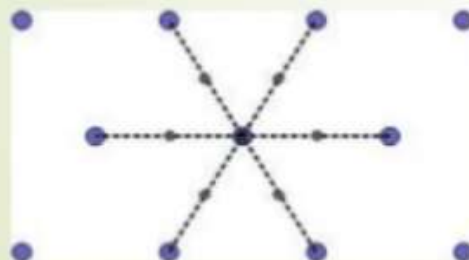
The numbers indicate the Brillouin zone to which each region belongs.



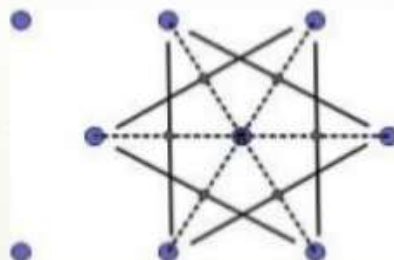
The Wigner-Seitz Cell can also be a unit cell



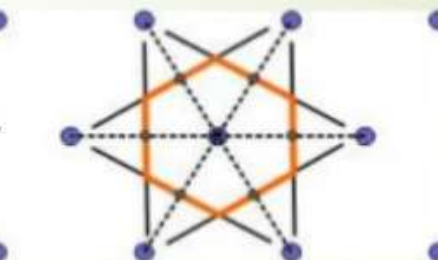
Wigner-Seitz cell for simple cubic in 3D



Select a lattice point and draw construction lines to the nearest neighbouring points



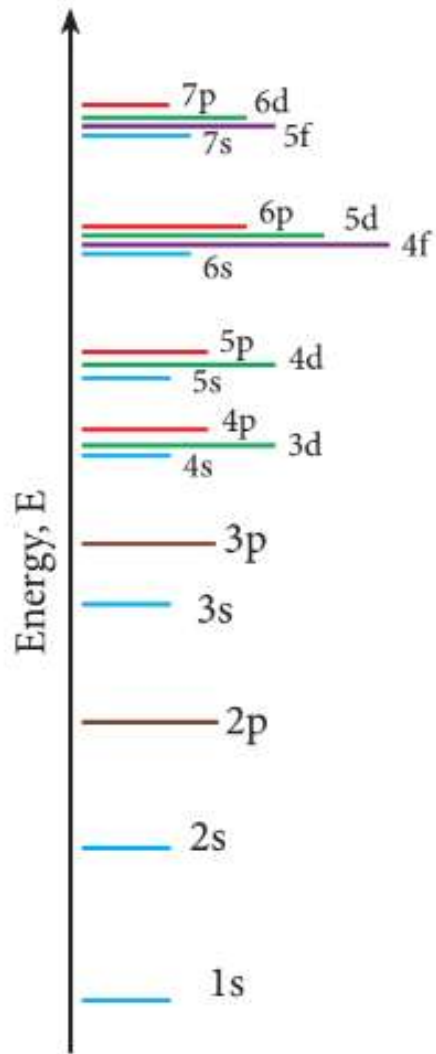
Draw lines that perpendicularly bisect the construction lines



The smallest enclosed area represents the Wigner-Seitz cell. Here shown in orange.

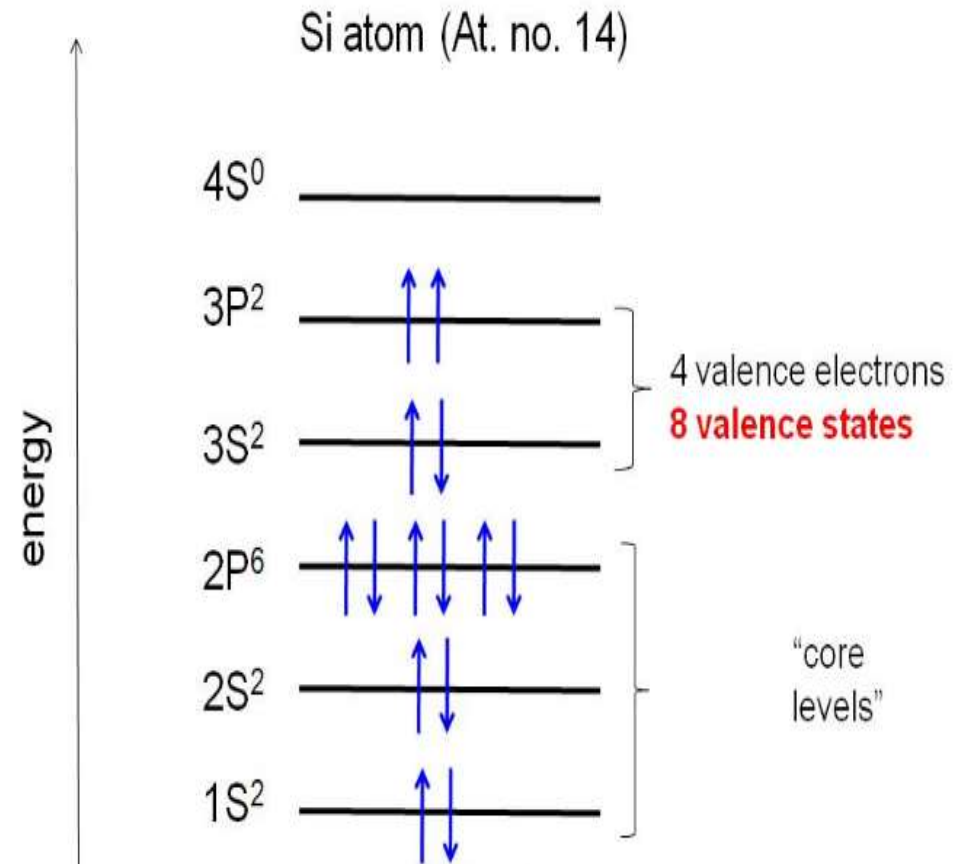
A Bragg “plane” for two points in lattice is the plane which is perpendicular to the line between the two points and passes through the bisector of that line. The first Brillouin zone for a point in a lattice is the set of points that are closer to the point than the Bragg plane of any point. In other words one can reach any of the points in the first Brillouin zone of a lattice point without crossing the Bragg plane of any other point in the lattice.

The second Brillouin zone is defined as the points which may be reached from the first Brillouin zone by crossing only one Bragg plane. This can be generalized to define the  $n$ -th Brillouin zone that can be reached from  $(n-1)$  Bragg plane.



Energy level of atomic orbit

## Silicon energy levels

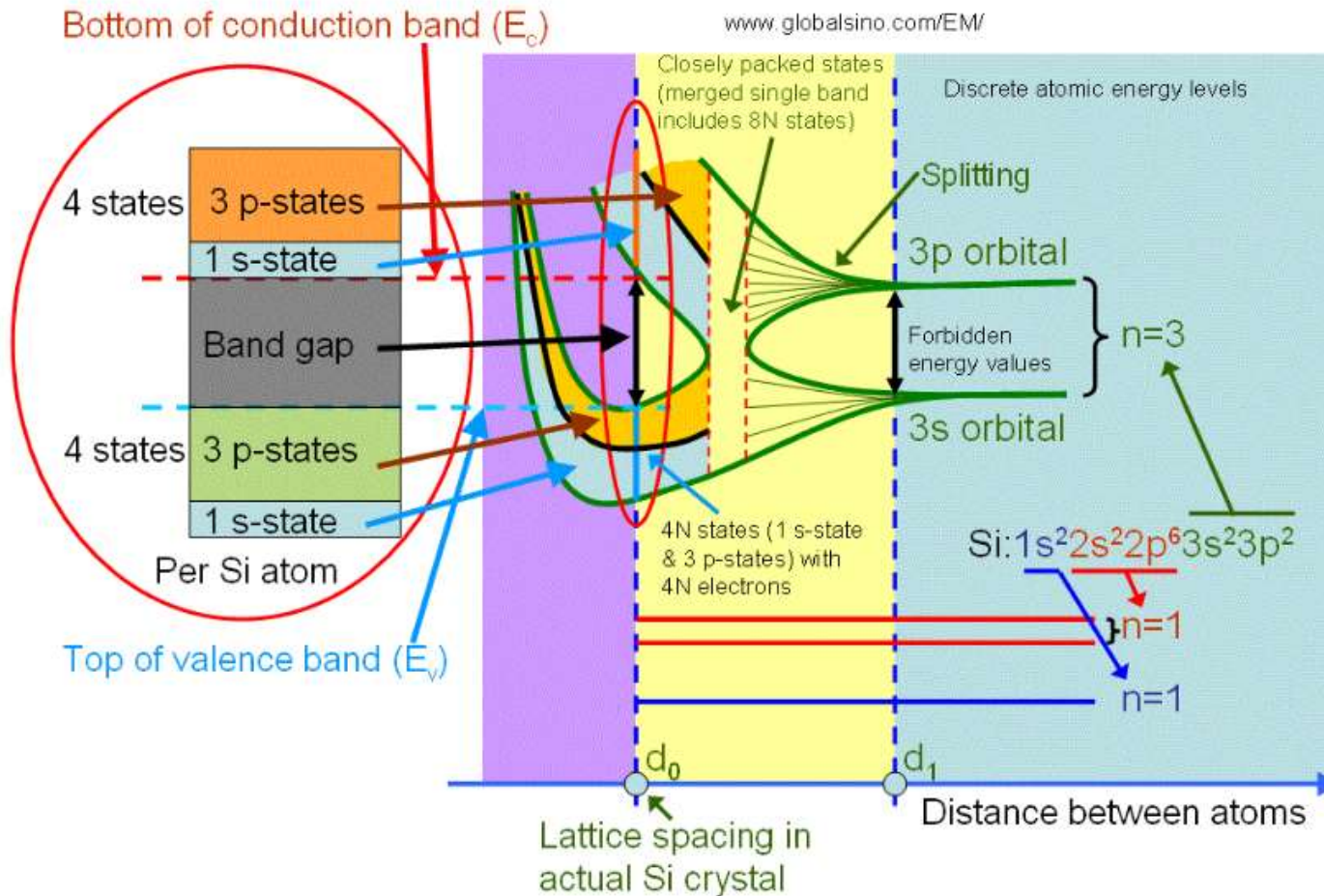




An isolated Si atom contains 14 electrons, which occupy 1s, 2s, 2p, 3s and 3p orbital in pairs. When atoms are far away from each other, the electrons in the out shell do not interact. As the distance between atoms is reduced to  $d_1$ , there is an overlap of electron wavefunctions across adjacent atoms. This leads to a splitting of the energy levels consistent with Pauli exclusion principle, and forming energy bands.

This splitting leads to  $2N$  states in the 3s band and  $6N$  states in the 3p band, where  $N$  is the number of Si atoms in the crystal. A further reduction of the lattice spacing causes the 3s and 3p energy bands to merge into a single band having  $8N$  available states, and then split again into two bands containing  $4N$  states each.

At the temperature of zero Kelvin, the lower band is completely filled with electrons and named as the valence band. The upper band is empty and named as the conduction band. Note that in crystal Si (with lattice spacing  $d_0$ ), the core level electrons do not start yet to interact.



**Detailed illustration of electronic structure of silicon as a function of distance between atoms. The left red circle is a zoom-in of the right red circle.**

