

## Module 6 : PHYSICS OF SEMICONDUCTOR DEVICES

### Lecture 31 : Electron in a Potential Well

#### Objectives

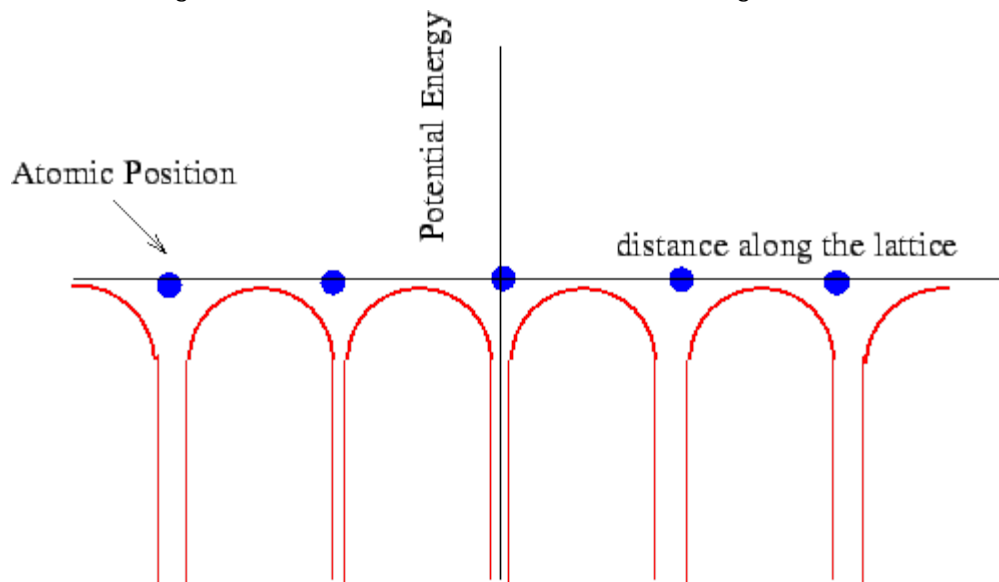
In this course you will learn the following

- Motion of electrons in a potential well.
- Electron in a periodic potential - Kronig Penny model.
- Concept of Brillouin zone.
- Origin of gap in the energy spectrum at the zone boundary.

#### Electron in a Potential Well

A simplified model of an electron inside a crystal is to consider the electron to move in a periodic potential well structure.

The essential features of the problem is brought out by considering the crystal lattice to be a regular arrangement of atoms along a straight line with inter-atomic separation  $a$ . The variation of potential energy with distance on a line along the centre of the atoms is as shown in the figure.

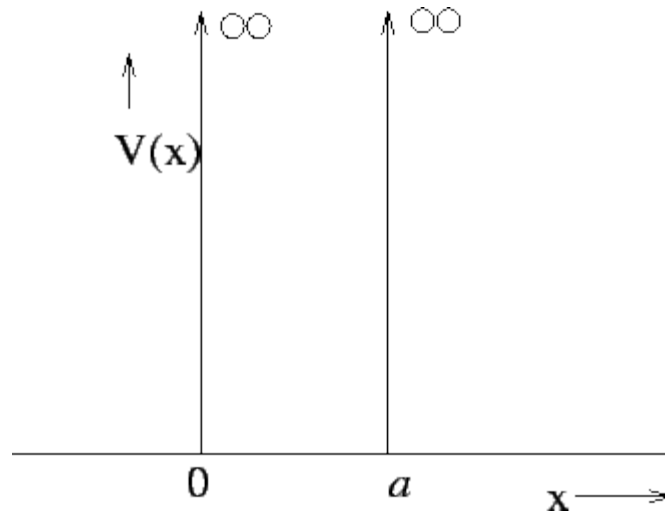


[See the animation](#)

Before discussing this problem, let us consider the motion of an electron in a single **square well potential**.

The potential is given by

$$V(x) = \begin{cases} 0, & \text{for } 0 \leq x \leq a \\ \infty & \text{otherwise} \end{cases}$$



Having a finite total energy the electron cannot be in the region  $x < 0$  or  $x > a$ . Thus the electron wavefunction in these regions vanishes. For the region  $0 \leq x \leq a$ , the one dimensional Schrödinger equation is

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

which has a solution

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

where  $A$  and  $B$  are constants and the wave number  $k$  is given by

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

By continuity of wavefunction at the boundaries

$$\psi(x) = 0 \text{ at } x = 0 \text{ which gives } B = 0, \text{ and}$$

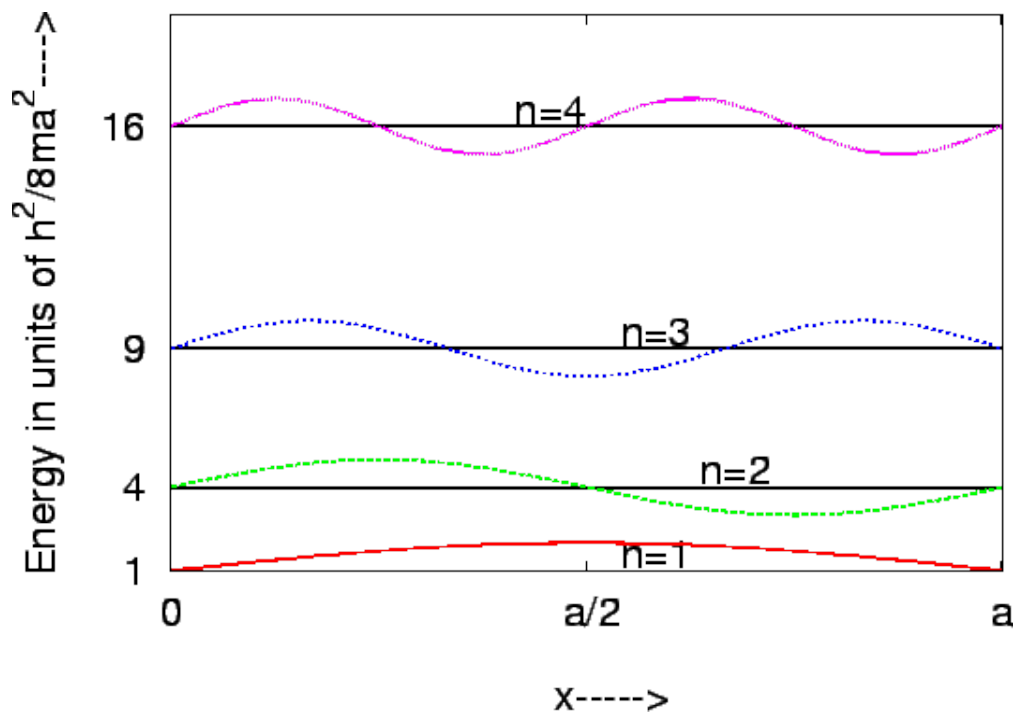
$$\psi(x) = 0 \text{ at } x = a \text{ which gives}$$

$$\sin ka = 0 \text{ so that } k = \frac{n\pi}{a}$$

where  $n$  is an integer  $1, 2, 3, \dots$  ( $n = 0$  is not possible because it would make the wavefunction inside the well vanish; negative values of  $n$  does not give new solution as it amounts to multiplying the whole wavefunction by  $-1$ .) Thus the electron energy in the potential well are

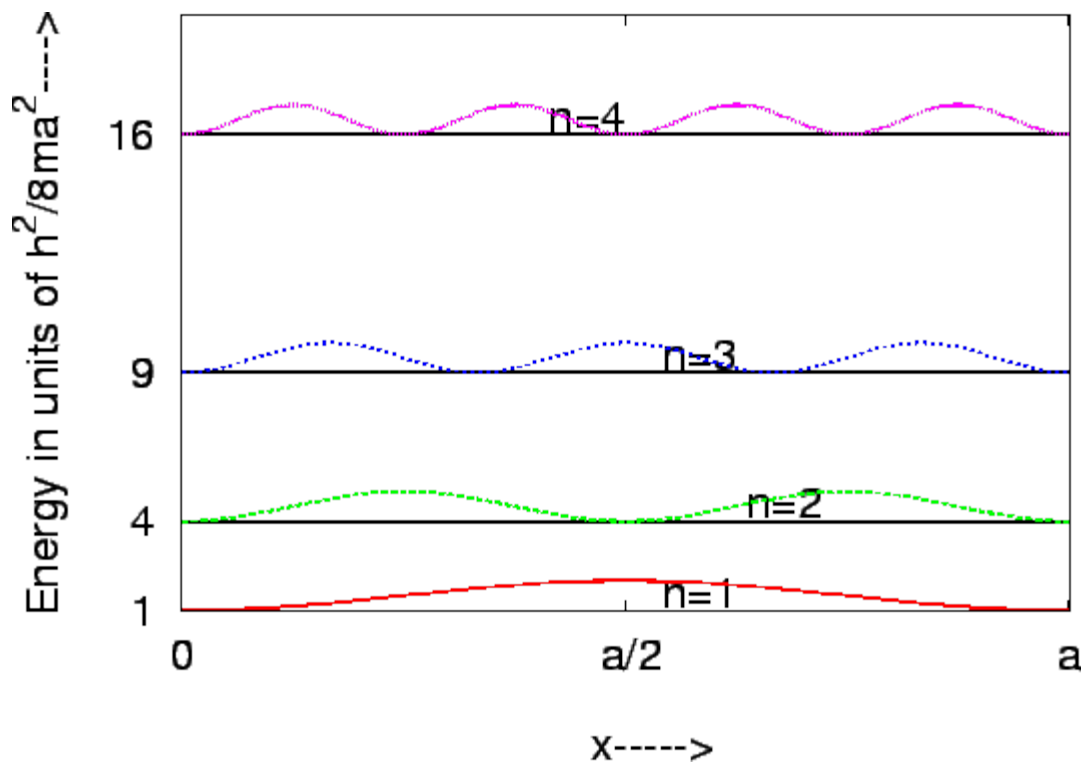
$$E = \frac{\hbar^2 k^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

The energy levels corresponding wave functions are shown in the figure.



[See the animation](#)

The figure below shows the probability densities corresponding to various states.



### Exercise 1

Verify that the normalization factor  $k$  — for the wavefunction for a particle in a potential well is  $\sqrt{2/a}$ .

### Electron in a Periodic Potential

Inside a lattice the electron is subjected to a periodic potential, i.e., the form potential repeats itself in space. Thus if  $a$  is the inter-atomic distance in a one dimensional lattice, we have

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

For potentials that are periodic, the wavefunction satisfies **Bloch theorem** which states that the form of the wavefunction is

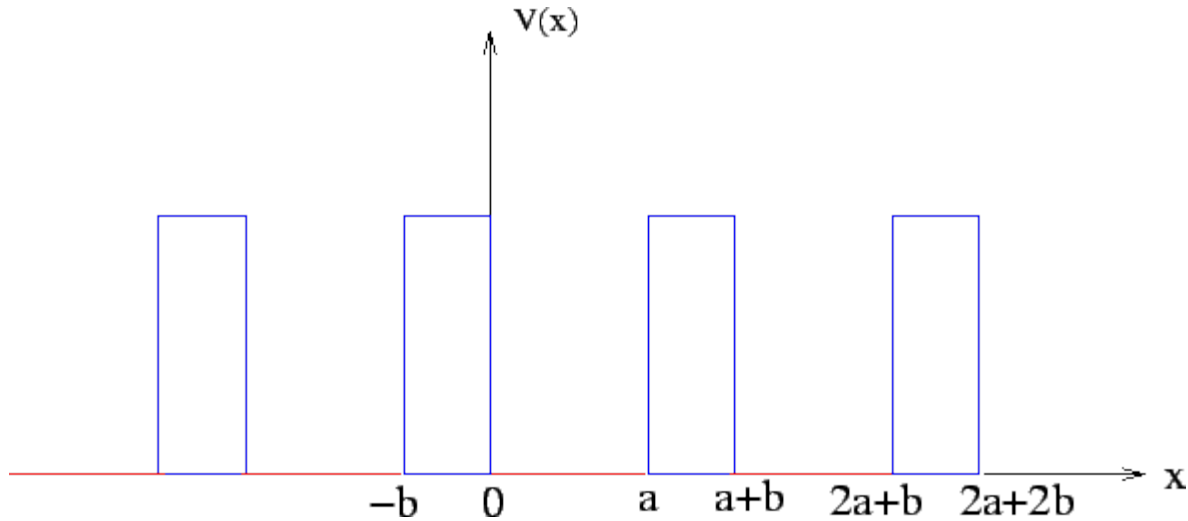
$$\psi(x) = u(x)e^{ikx}$$

where  $u(x)$  is a periodic function with the same periodicity as that of the lattice, i.e.,

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

Substituting this in Schrödinger equation for  $\psi(x)$ , we would obtain an equation for  $u(x)$  which must be solved.

A simple model often used to mimic the periodic potential is known as the **Krönig-Penny model**, the form of which is shown in the figure.



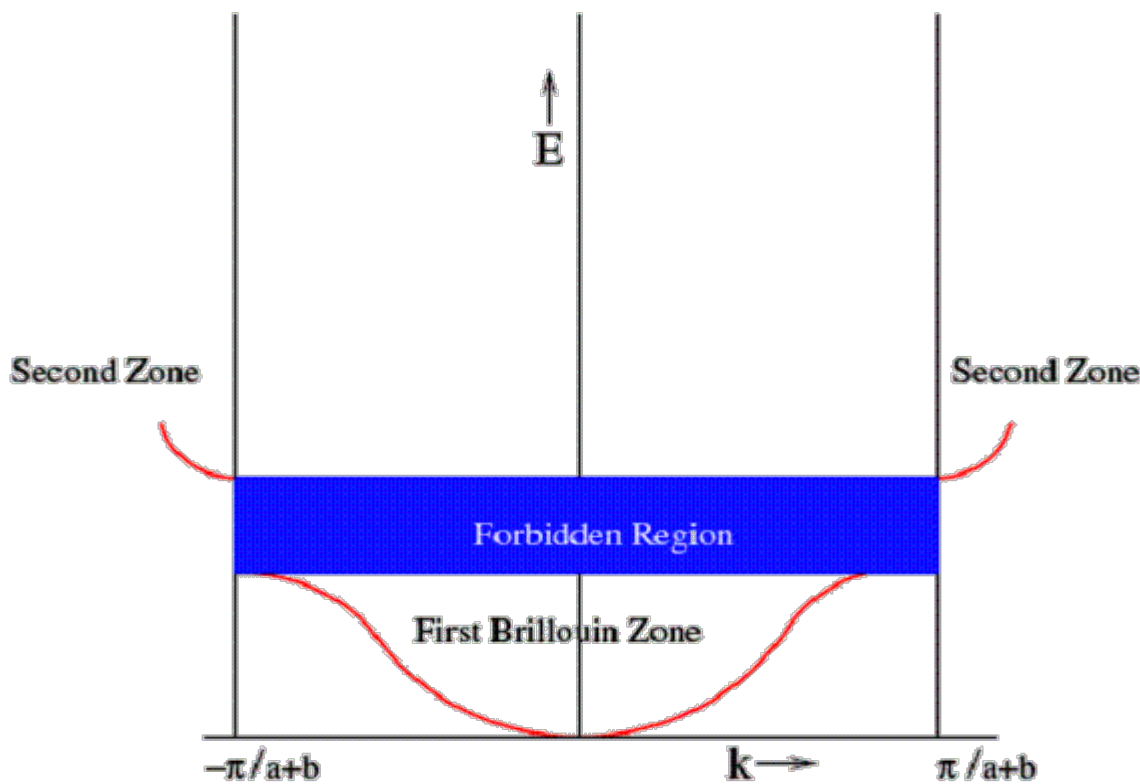
The potential is periodic with a period  $a + b$ . In this case the electrons diffract from the periodic lattice resulting in some values of  $k$  for which no solution exists. The reason can be traced to formation of standing waves for such values of  $k$ . For a crystal with periodicity  $a + b$ , as shown above, standing waves would form if the electron wavelength  $\lambda$  is an integral multiple of  $2(a + b)$ . Thus the condition for formation of standing waves is

$$2(a + b) = n\lambda = n \frac{2\pi}{k}$$

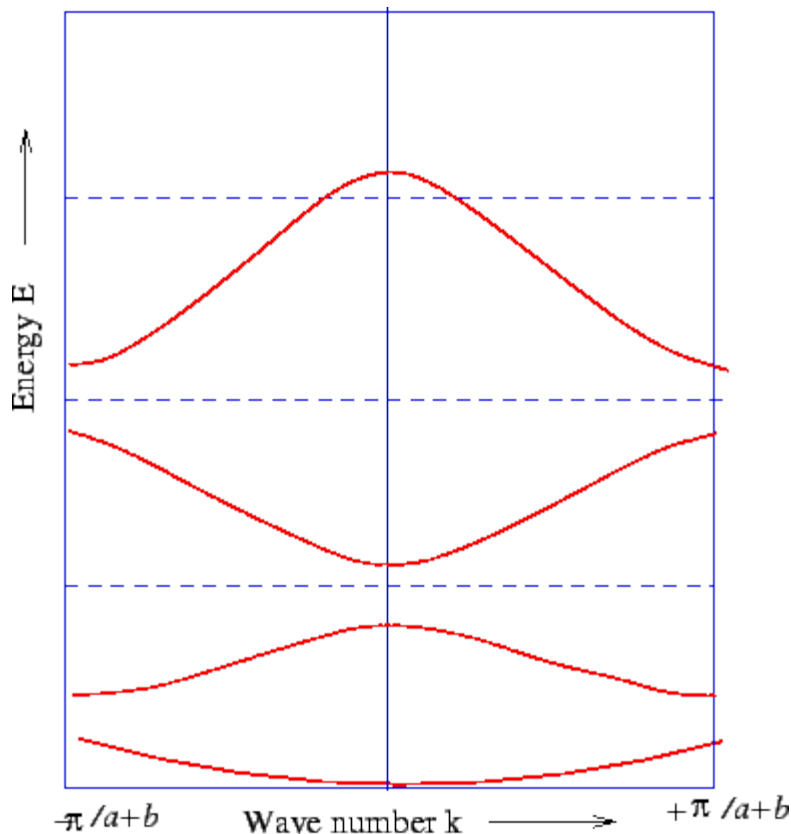
so that

$$k = \frac{n\pi}{a + b}$$

For each region of k-space in which the energy is continuous is said to be a **Brillouin Zone**. Thus the **First Brillouin Zone** is for  $k$  values running from  $-\pi/(a + b)$  to  $+\pi/(a + b)$ , the second Brillouin zone from  $-\pi/(a + b)$  to  $-2\pi/(a + b)$  and from  $\pi/(a + b)$  to  $2\pi/(a + b)$  and so on. The  $E - k$  diagram where the values of  $k$  extends from  $-\infty$  to  $+\infty$  is called an **extended zone scheme**.



One can present  $E - k$  diagram in a scheme known as the **reduced zone scheme** in which  $k$  values are restricted to their values in the first Brillouin zone. The energy band structure in such a scheme is discontinuous as the bands in the picture are folded back to the first zone using periodicity.



The parameter  $k$  in these diagram does not have the interpretation of momentum; however, in analogy with the case of free particle  $\hbar k$  is known as **crystal momentum**". When an electron in a crystal is subjected to an external force  $F_{ext}$ , it is this crystal momentum which satisfies the Newton's laws

$$F_{ext} = \frac{d}{dt}(\hbar k)$$

### Origin of Gap in Energy Spectrum

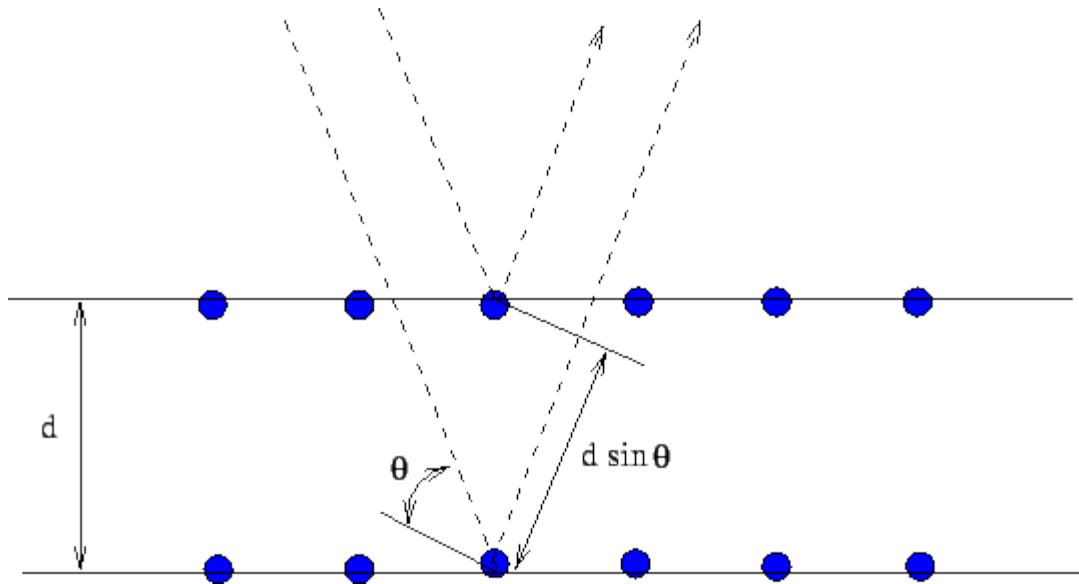
From the energy diagram shown, it can be seen that there are discontinuities that arise at certain values of  $k$ . Such gaps occur when the wavelength of electron is such that the condition for Bragg diffraction by the periodic lattice structure is satisfied.

We know that an electron wave incident on such a lattice undergoes reflection if Bragg condition

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

is satisfied. For waves travelling along the line of atoms in the crystal, the angle of incidence is  $90^\circ$ , so that the wave vector of the electron for which Bragg condition is satisfied is

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

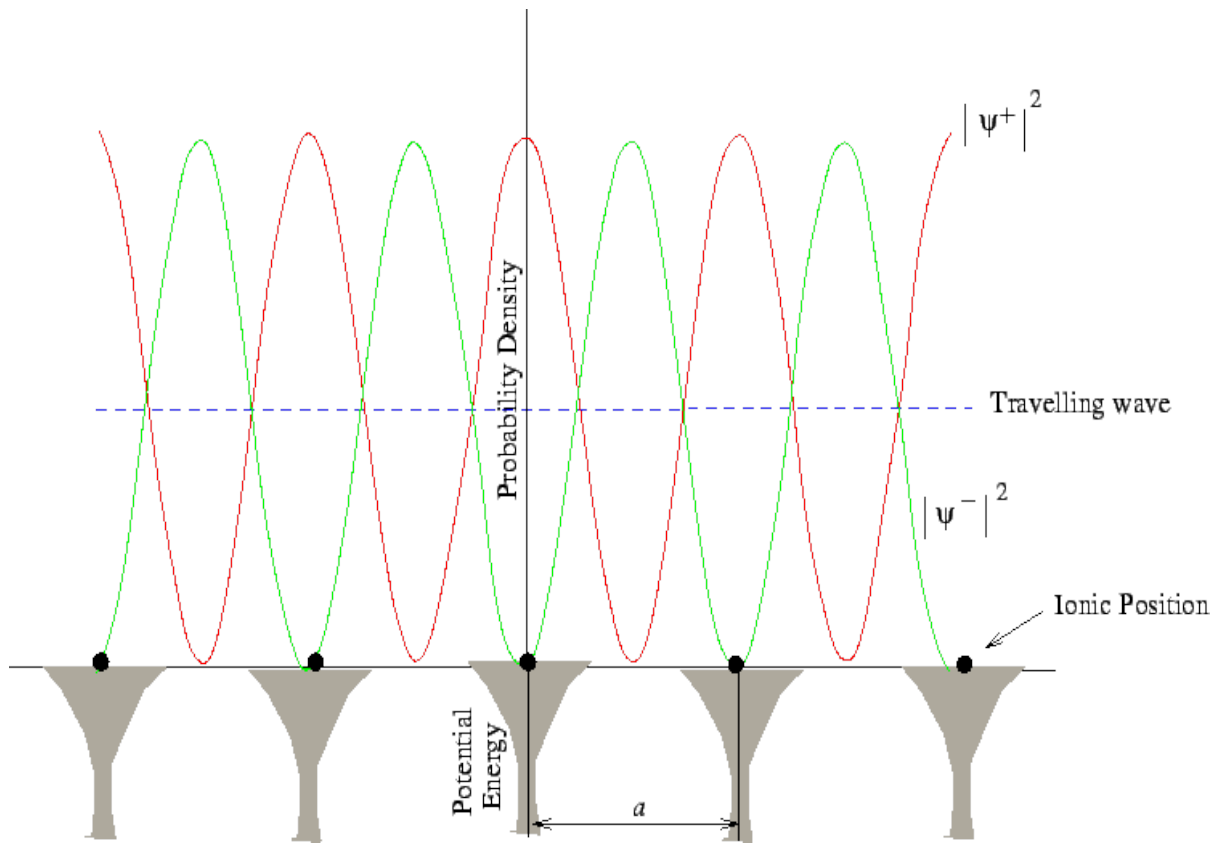


Thus energy is continuous in the region  $-\pi/d < k < +\pi/d$ . At  $k = \pm\pi/d$  there is a discontinuity.

The region between  $-\pi/d$  and  $+\pi/d$  is the first Brillouin zone.

We have seen that the solution of the Schrödinger equation for an arbitrary value of  $k$  is a plane wave  $e^{ikx}$ . This, however, is not true at the zone boundary where Bragg reflection takes place. At such a boundary the wave function has two components, viz.,  $e^{ikx}$  and  $e^{-ikx}$ . One can form two standing waves using these two wavefunctions, viz.,  $\psi^+ = \cos(\pi x/d)$  and  $\psi^- = \sin(\pi x/d)$ . The corresponding

electron densities are proportional to  $\cos^2(\pi x/d)$  and  $\sin^2(\pi x/d)$ . These two densities have their maxima respectively at the locations of the atoms and midway between atoms, as shown.



For wave vectors other than at the zone boundaries, the wavefunction being a travelling wave, the probability density has uniform value. When we calculate the average of the potential energy for the three probability densities, i.e.  $\int V(x)\rho^\pm$ , the potential energy is the largest for the cosine wave and the

smallest for the sine wave, the case of uniform density falling in between. The difference between the two energies is the energy gap at the zone boundary.

### Reciprocal Lattice

We have seen that Bragg diffraction occurs for values of  $\vec{k}$ — vectors which are multiples of  $\pi/d$ . Bragg

diffraction is a consequence of periodicity of the lattice and diffraction pattern forms a geometric image which bears an inverse relationship with lattice periodicity. Because the scale associated with the points at which Bragg condition is satisfied has the dimensions of inverse length (as seen in the one dimensional relation  $\vec{k} = \pi/d$ ), the geometrical structure defined by diffraction peaks is called the **reciprocal lattice**

corresponding to the real space lattice which is also referred to as the **direct lattice**.

An equivalent way of describing diffraction in crystal is known as von-Laue formulation, according to which the condition of constructive interference is satisfied if

$$\vec{R} \cdot (\vec{k} - \vec{k}') = 2\pi n$$

where  $\vec{R}$  is a direct lattice vector,  $\vec{k}$  is the wave vector of the incoming wave,  $\vec{k}'$  that of outgoing wave and  $n$  is any integer.

One can define **reciprocal lattice vector**  $\vec{G}$

$$\vec{G} \cdot \vec{R} = 2\pi n$$

where  $n$  is an integer.

Another way of stating Laue condition is

$$\vec{k} - \vec{k}' = \vec{G}$$

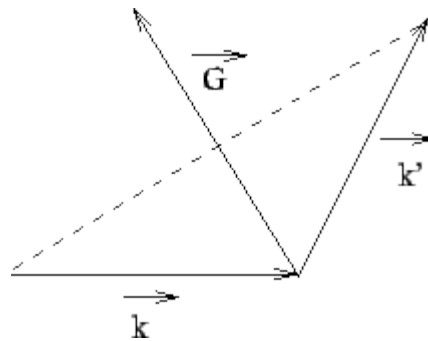
Squaring both sides and using  $|\vec{k}| = |\vec{k}'|$ , we get

$$\vec{k} \cdot \vec{G} = -\frac{1}{2}G^2$$

Since  $-\vec{G}$  is also a reciprocal lattice vector, one can rewrite the above equation as

$$\vec{k} \cdot \vec{G} = \frac{1}{2}G^2$$

Geometrically, this implies that Laue condition is satisfied if  $\vec{k}$  lies in a plane that bisects  $\vec{G}$  perpendicularly.



### Example-1

The density of free electrons in silver is  $6 \times 10^{28}$  per cubic meter. Calculate the Fermi energy of silver in eV.

#### Solution

The Fermi momentum is given by

$$k_F = (3\pi^2 n)^{1/3} = 1.21 \times 10^{10} \text{ m}^{-1}$$

The Fermi energy

$$E_F = \frac{\hbar^2 k_F^2}{2m} = 9.053 \times 10^{-19} \text{ J}$$

Dividing by electronic charge, the Fermi energy is 5.65 eV.

### Exercise 2

Taking the density of state of silver to be of the free electron form, calculate the number of free electrons per unit volume in silver having energy between 4 eV and 4.1 eV.

(Ans.  $1.36 \times 10^{27}$  )

### Exercise 3

Obtain an expression for the free electron density of states in (i) one dimension and in (ii) two dimensions.



(Ans. (i)  $(1/\pi)(m/E\hbar^2)^{1/2}$  (ii)  $m/\pi\hbar^2$  )

## Fermi Function

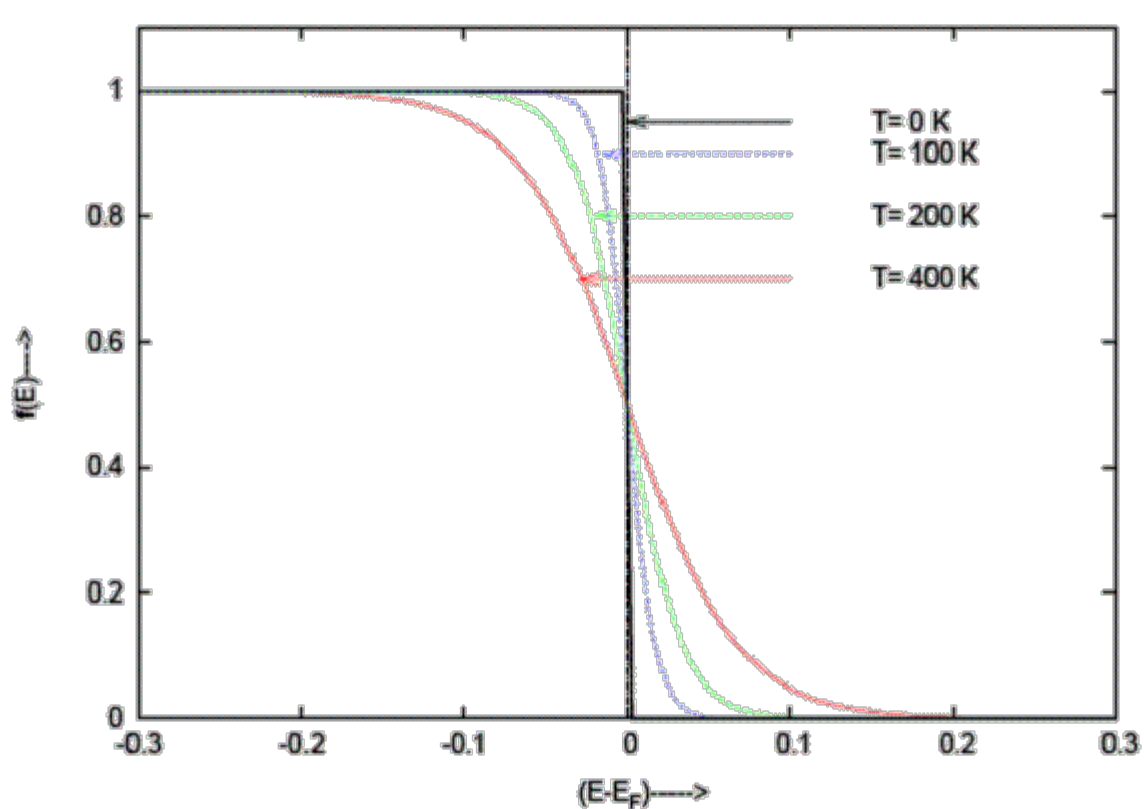
At a finite temperature, the electron states are filled by a probability density function  $f(E)$  given by

$$f(E) = \frac{1}{1 + e^{(E-E_F)/kT}}$$

where  $f(E)$  is the probability of a particular energy state  $E$  being occupied. Electrons and other particles which follow the above distribution function are called **fermions** . At  $T = 0$ ,  $f(E)$  is a step function

$$f(E) = 1 \text{ for } E < E_F$$

$$= 0 \text{ otherwise}$$



At all non-zero temperatures, the value of  $f(E)$  at  $E = E_F$  is  $1/2$ . Thus one of the ways in which Fermi energy can be defined is the energy level where half of the available energy states are filled.

### Exercise 4

Show that  $f(x) + f(-x) = 1$ .

### Recap

In this course you have learnt the following

- Motion of an electron in a one dimensional potential well was studied. The energy levels are discrete and the wavefunctions are standing waves with nodes at the wall boundaries.

- Motion of an electron in a periodic potential was discussed. The wavefunction satisfies Bloch theorem according to which the solution is a product of a free electron function and another function having the periodicity of the lattice.
- An electron wave moving in a periodic lattice undergoes Bragg diffraction at points in  $k$ -space where Bragg condition is satisfied. This leads to creation of a forbidden gap in the energy spectrum inside which no physical state exists.