✓ **Ans. Brillouin Zones (*i*) Linear lattice.** According to Kronig and Penney model the energy discontinuities in a one dimensional lattice occur when $k = \frac{n\pi}{a}$, where n is a positive or negative integer. In a one dimensional monatomic lattice a line representing the values of k is divided by energy discontinuities into segment of length $\frac{\pi}{a}$ as shown in **Fig. 6.3 (Q 6.2)**.

These line segments are known as Brillouin Zones. The first reflection and the first energy gap occurs at $k = \pm\frac{\pi}{a}$. The reflection at $k = \pm\frac{\pi}{a}$ arises because the wave reflected from one atom in a linear lattice interferes constructively with the wave from a *nearest neighbour* atom, the phase difference between the two reflected waves for the values of $k = +\frac{\pi}{a}$ and $k = -\frac{\pi}{a}$ being $\frac{2\pi}{a}$. The region in *k-space* between $-\frac{\pi}{a}$ and $+\frac{\pi}{a}$, *i.e.*, the segment $-\frac{\pi}{a} \leq k \leq +\frac{\pi}{a}$ is called the *first Brillouin Zone* of the lattice.

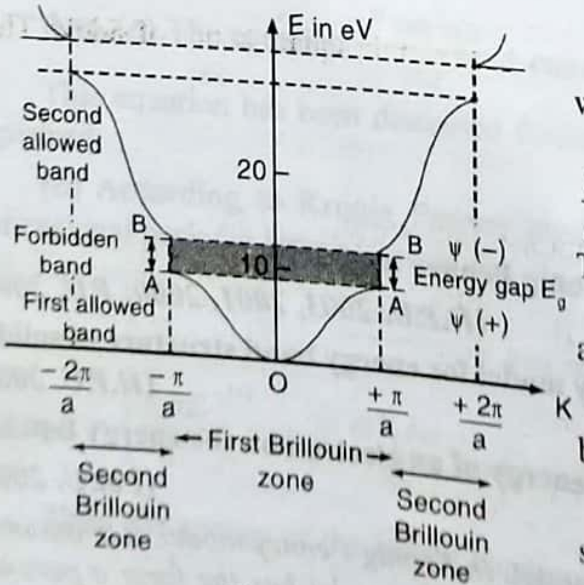

Fig. 6.11

The second Brillouin zone contains electrons with $k > \frac{\pi}{a}$, *i.e.*, electrons having k-values between $\frac{\pi}{a}$ and $\frac{2\pi}{a}$ for electrons moving in the $\pm x$ direction. The second reflection and second energy gap occurs at $k = \pm\frac{2\pi}{a}$ and, therefore, the region in the k space between $-\frac{2\pi}{a}$ to $-\frac{\pi}{a}$ and $+\frac{\pi}{a}$ to $+\frac{2\pi}{a}$, *i.e.*, the segment $-\frac{2\pi}{a} \leq k \leq -\frac{\pi}{a}$ and $+\frac{\pi}{a} \leq k \leq +\frac{2\pi}{a}$ forms the second Brillouin zone of the lattice. Similarly, we can discuss the formation of third etc., Brillouin zone.

The first and second Brillouin zones and the energy gaps are shown in Fig. 6.11 by plotting the value of E in eV corresponding to various values of $\vec{k}$.

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(*ii*) **Two dimensional lattice.** Proceeding as in the case of a linear lattice, the first zone for a two dimensional lattice in the *X-Y* plane is the square *ABCD* the boundaries of which are given by the relation $k_x = +\frac{\pi}{a}$ and $k_x = -\frac{\pi}{a}$ and $k_y = +\frac{\pi}{a}$ and $k_y = -\frac{\pi}{a}$.

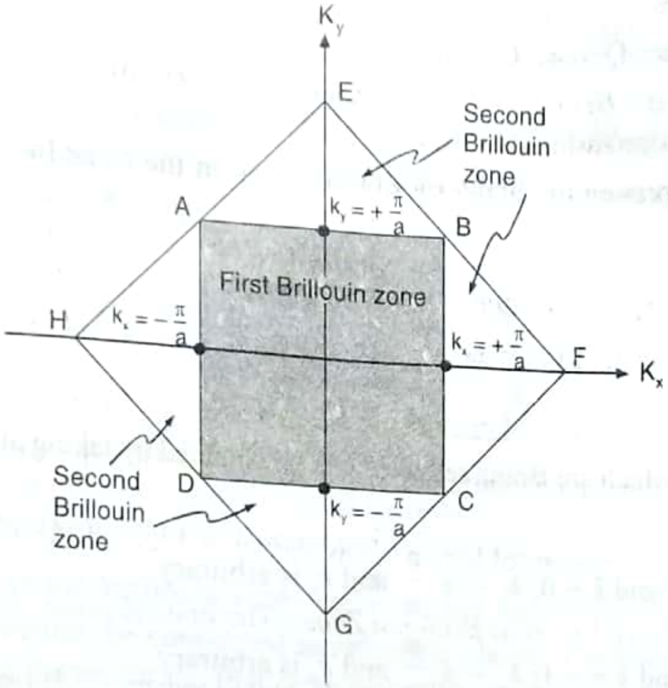

Fig. 6.12

The second Brillouin zone for a two dimensional lattice in the *X-Y* plane is the square *EFGH* the boundaries of which are given by the relation

$$k_x = \pm\frac{2\pi}{a};\; k_y = \pm\frac{2\pi}{a}$$

Brillouin Zones in reciprocal lattice. *A Brillouin zone is the locus of all those $\vec{k}$-values in the reciprocal lattice which are Bragg reflected.*

As an example, we shall construct the Brillouin zones for a simple square lattice of side *a*. The primitive translation vectors of this lattice are

$$\vec{a} = a\hat{i};\; \vec{b} = a\hat{j}$$

The corresponding translation vectors of the reciprocal lattice are

$$\vec{A} = \left(\frac{2\pi}{a}\right)\hat{i} \text{ and } \vec{B} = \left(\frac{2\pi}{a}\right)\hat{j}$$

Therefore, the reciprocal lattice vector $\vec{G}$ is given by

$$\vec{G} = h\vec{A} + k\vec{B} = \left(\frac{2\pi}{a}\right)(h\hat{i} + k\hat{j})$$

where *h* and *k* are integers. The wave vector $\vec{k}$ can be written as

$$\vec{k} = k_x\hat{i} + k_y\hat{j}$$

According to Bragg's condition,

$$2\vec{k}\cdot\vec{G} + G^2 = 0$$

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or

$$2(k_x G_x + k_y G_y) + G_x^2 + G_y^2 = 0$$

or

$$2\left(k_x \frac{2\pi}{a} h + k_y \frac{2\pi}{a} k\right) + \left(\frac{2\pi}{a}\right)^2 h^2 + \left(\frac{2\pi}{a}\right)^2 k^2 = 0$$

or

$$\frac{4\pi}{a}(hk_x + kk_y) = -\left(\frac{2\pi}{a}\right)^2 (h^2 + k^2)$$

or

$$hk_x + kk_y = -\frac{\pi}{a}(h^2 + k^2)$$

This equation represents a family of straight lines in the k_x and k_y plane. Their k_x and k_y intercepts are

$$k_x = -\frac{\pi}{a}\frac{(h^2 + k^2)}{h}$$

and

$$k_y = -\frac{\pi}{a}\frac{(h^2 + k^2)}{k}$$

The values of $\vec{k}$ which are Bragg reflected can be obtained by taking all possible combinations of h and k

For $h = \pm 1$ and $k = 0$; $k_x = \pm \frac{\pi}{a}$ and k_y is arbitrary

For $h = 0$ and $k = \pm 1$; $k_y = \pm \frac{\pi}{a}$ and k_x is arbitrary

These four lines $k_x = +\frac{\pi}{a}$, $k_x = -\frac{\pi}{a}$, $k_y = +\frac{\pi}{a}$ and $k_y = -\frac{\pi}{a}$ are plotted in Fig. 6.13

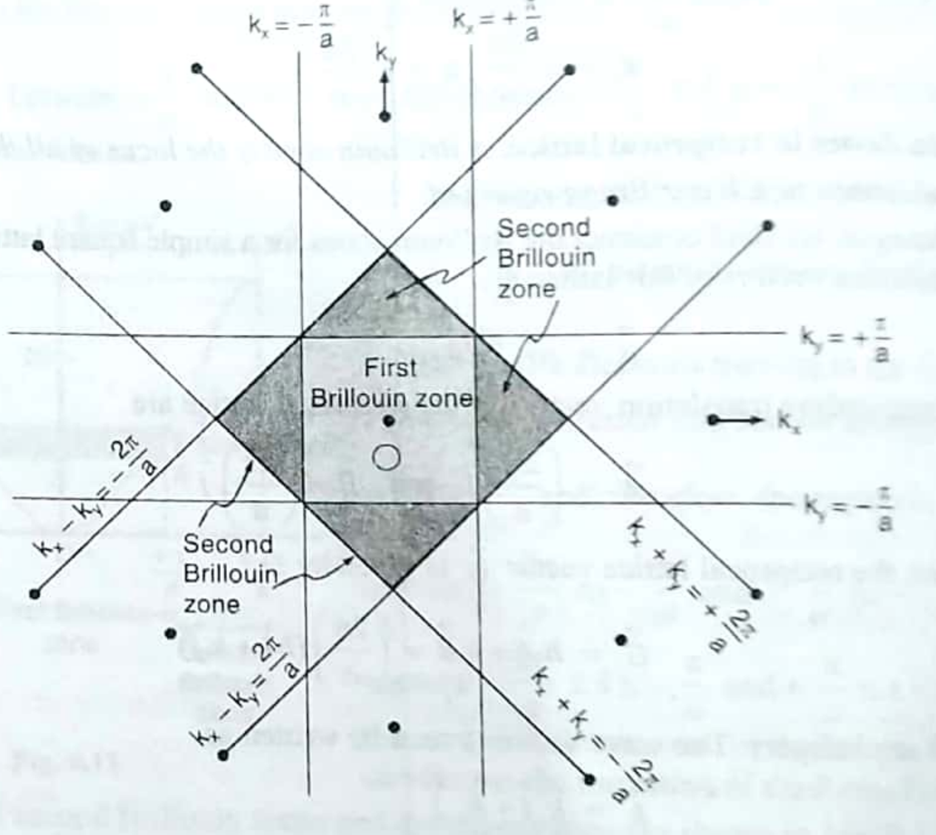

Fig. 6.13

Taking origin as shown at O, all the $\vec{k}$ vectors originating from it and terminating on these lines

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