Symmetry property of the energy function:

(i) Translational symmetry :

$$E_n(k+G) = E_n(k)$$

This shows that $E_n(k)$ is periodic with a period equal to reciprocal lattice vector $\left(G = \frac{2\pi}{a}\right)$

If our propagation vector (number of allowed k-values) lies outside the first Brillioun-zone, we can always reduce it to the first Brillioun-zone by subtracting a reciprocal lattice vector $\left(G = \frac{2\pi}{a}\right)$. Hence, the first zone contains all the necessary information about higher zones.

(ii) Inversion symmetry :

$$E_n(-k) = E_n(k)$$

This indicates that the bound is symmetric with respect to the inversion around the origin $k = 0$

(iii) Rotational symmetry:

The energy band $E_n(k)$ has the same rotational symmetry as that of a real lattice.

Fermi Surface:

Fermi Surface (FS) is defined as the surface of constant energy E_F in k-space inside which all the states are occupied by the valence electrons, while all the states lying outside are empty. It is also defined as the boundary between the filled and empty states (in k-space) in the ground state of crystal at absolute zero. The shape of fermi surface is determined by the geometry of energy contains in a zone. Temperature has a very slight effect on FS, however surface remains sharp even at room temperature or high temperature.

For a free electrons, the fermi surface is just a line in 1-dimension, a circle in 2-dimension and a sphere in 3-dimension. However, a distortion in the shape of fermi surface is observed under the effect of pseudopotential $V_{eff}(r)$. Hence, the information about the shape of fermi surface is very important in knowing the various properties of solids such as heat capacity, Pauli's paramagnetism, electrical conductivity, etc.

Effect of valence electron on the shape of FS:

The kinetic energy of free electron in *k*-space is given by the parabolic equation,

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

The centre of first $BZ(k=0)$ is a minimum energy position, $E = 0$, this implies that for $k = 0$, all the states are empty inside the BZ.

As the number of valence electrons starts increasing, the states lying near the bottom of the band are filled and occupied volume is a sphere (circle in 2-dimensions) of radius k_F. As the number of valence electrons are increased, more and more states are occupied and so the Fermi volume gradually expands. The FS begins to deform and loses its spherical shape near the zone boundary.

The degree of distortion depends on

(i) How near is the FS to the zone boundary

(ii) Magnitude of effective pseudopotential

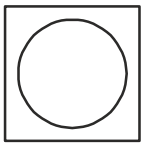
Fermi surfaces in two dimensions:

Consider a square lattice of peridocity a.

Area of Bz of square lattice.

$$A = \frac{4\pi^2}{a^2}$$

For monovalent metal: Only half the area of Bz is occupied



$$\therefore \qquad \pi k_F^2 = \frac{1}{2}\frac{4\pi^2}{a^2}$$

$$\Rightarrow \qquad k_F = \sqrt{\frac{2}{\pi}}\frac{\pi}{a} = 0.798\frac{\pi}{a}$$

where $\frac{\pi}{a}$ is the distance of the zone boundary from the centre of the zone.

$$0 < k_F < \frac{\pi}{a}$$

Therefore, FS lies well within first Bz and hence remains undistorted.

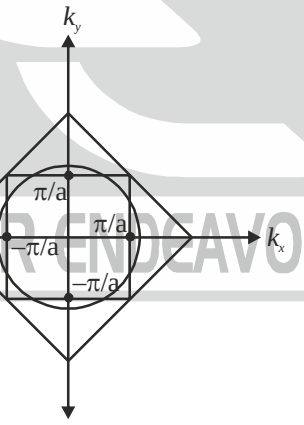
Divalent metal:

$$\pi k_F^2 = \frac{2}{2}\frac{4\pi^2}{a^2};\ k_F = 1.228\frac{\pi}{a}$$

The distance of a corner of first zone from centre is

$$\sqrt{2}\frac{\pi}{a} = 1.414\frac{\pi}{a} \quad \Rightarrow \qquad \frac{\pi}{a} < k_F < 1.414\frac{\pi}{a}$$

The circle of radius k_F will go beyond the first zone boundary but will remain inside the corner of first Bz.



Example: An electron of mass *m* moves in a square lattice of lattice spacing *a*. Assume that the nearly free electron approximation holds good. If there are two electrons per site, then which of the following is correct?

(a) system behaves as a metal (b) system behaves as an insulator

(c) both (a) and (b) (d) none of these

Soln. With two electrons per site, assuming that the constant energy lines are circles, we obtain

$$\pi k_F^2 = \left(\frac{2\pi}{a}\right)^2 \Rightarrow \boxed{k_F = \frac{2\sqrt{\pi}}{a}}$$

This value is larger than π/a. Therefore, we need to consider the two bands. There will be two fermi surfaces, one in the upper band and other in the lower band. Each of the bands is partially filled, with two electrons per site the NFE approximation leads to a metal.

Correct option is (a)

Tetravalent metals:

$$\pi k_F^2 = \frac{4}{2}\frac{4\pi^2}{a^2} \Rightarrow k_F = 1.596\frac{\pi}{a} \Rightarrow \frac{\pi}{a} < 1.414\frac{\pi}{a} < k_F$$

This shows that Fermi circle for tetravalent case completely enclose the first BZ and passes through the second, third and fourth.

Steps for construction of fermi surfaces in metals:

(1) For a given metal lattice, construct the corresponding reciprocal lattice

(2) Near each receiprocal lattice point, construct a unit cell (known as BZ) by Weigner-Seitz method.

(3) For the given parameters of the BZ and valency of the metal, determine the radius of fermi sphere k_F.

Simple cubic lattice:

Consider a simple cube of unit cell whose lattice parameter is *a*

Reciprocal lattice point = $\frac{2\pi}{a}$

The first BZ will again be a cube of side $\frac{2\pi}{a}$

Radius of fermi sphere can be determined as follows

$\left(\frac{2\pi}{a}\right)^3$ volume contains 1 allowed k-values

Unit volume contains $\frac{1}{(2\pi/a)^3}$ allowed k-values

$\frac{4}{3}\pi k_F^3$ volume contains $\frac{\frac{4}{3}\pi k_F^3}{(2\pi/a)^3}$ allowed k-value

Each k-value constitutes two electrons because of polarization

Therefore, total number of electrons inside Fermi sphere

$$N = \frac{2\times\frac{4}{3}\pi k_F^3}{(2\pi/a)^3} \qquad \{\because\ a^3 = V\}$$

$$N = \frac{2\times V\times\frac{4}{3}\pi k_F^3}{8\pi^3} \Rightarrow k_F^3 = \frac{3\pi^2 N}{V} \Rightarrow k_F = \left(\frac{3\pi^2 N}{a^3}\right)^{1/3}$$

For $N = 1$,

$$k_F = 0.985\frac{\pi}{a}$$

$$0 < k_F < \frac{\pi}{a}$$

$\Rightarrow$ k_F is very close to zone boundaries

Body centred cubic lattice:

$$k_F = \left(3\pi^2 \frac{N}{a^3}\right)^{1/3} = \left(3\pi^2 \times \frac{2}{a}\right)^{1/3} \Rightarrow k_F = 1.24\frac{\pi}{a}$$

N = 2 (since, there are two atoms per unit cell)

Face-centred cubic lattice:

$$k_F = \left(3\pi^2 \frac{N}{a^3}\right)^{1/3}$$

{N = 4, because there are four atoms in FCC unit cell}

$$\Rightarrow \qquad k_F = \left(3\pi^2 \times \frac{4}{a^3}\right)^{1/3} \Rightarrow k_F = 1.563\frac{\pi}{a}$$

Characteristics of Fermi surfaces:

(1) The volume of FS represents the number of conduction electrons

(2) FS has spherical shape within the first BZ and non-spherical shape in higher zones

(3) For a spherical fermi surface velocity of an electron is

$$V = \frac{\hbar k}{m_0}$$

For non-spherical, $V = \frac{1}{\hbar}\nabla_k E(k)$

Effect of electric field on FS:

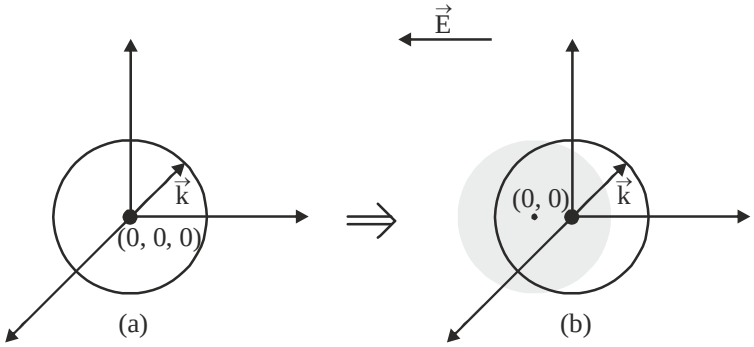
When an external electric field is applied, the equation of motion in the absence of electron collision with imperfection, phonons or any other impurities is given as

$$\frac{d}{dt}(\hbar k) = -eE$$

Or, $$\hbar\frac{dk}{dt} = -eE$$

Therefore, velocity of electrons in k-space is constant

Therefore, entire FS moves through Δk in k-space opposite to the field direction



(a) without electric field (b) with electric field

Effect of magnetic field on FS:

Equation of motion is given as

$$\hbar\frac{dk}{dt} = e(V \times B)$$