B. Sc. (H) SEM - VI

PHYSICS - C XIII, Solid State Physics.

Effective mass of electrons: Holes (m_e^*)

According to kronning Penney Model electrons are passing through wells and barriers, i.e. rectangular Potential Barriers. So when the electron is passing through these periodic rectangular potential barriers the mass aquired by these electrons is known as effective mass of electrons. Since the electron is moving through the periodic potential it was considered it might aquire an effective mass. In order to derive an expression for the effective let us consider an electron having mass $\underline{m}$ and charge $\underline{e}$ passing through rectangular periodic potential wells and barriers.

The electron can be accelarated either by electric Potential (field) or magnetic fields. The force ~~can~~ acting on the charge carrier will be

$$F = m_e^* a \qquad \text{—— (1)}$$

where m_e^* is the effective mass of electron not the ~~restma~~ restmass and a is the accelaration produced.

From the wave mechanics we know that when a charged particle is accelarated by Electric or magnetic field the velocity aquired by the particle is equal to the group velocity of the wave representing the particle and is given by

$$v = \frac{d\omega}{dk} = \frac{d\omega}{dE} \cdot \frac{dE}{dk} \qquad \text{—— (2)}$$

where ω is the angular frequency of the de Broglie waves.

Then the energy of the particle is

$$E = \hbar\omega \quad \text{— (3)}$$

or $$\frac{dE}{d\omega} = \hbar$$

or $$\frac{d\omega}{dE} = \frac{1}{\hbar} \quad \text{— (4)}$$

Using eq. (4) in eq (2) we get.

$$v = \frac{1}{\hbar}\left(\frac{dE}{dk}\right) \quad \text{— (5)}$$

$$\Rightarrow v \propto \left(\frac{dE}{dk}\right) \quad \text{— (5)}$$

Eq (5) is the most important relation in band theory for describing the motion of an electron can be completely defined only if the energy - wave vector curve is available. For a free electron, however, we have,

$$\cancel{E = \frac{p^2}{2m} = \left(\frac{h}{\lambda}\right)^2 \frac{1}{2m} = \left(\frac{\hbar}{2\pi/k}\right)^2 \frac{1}{2m}} \text{ ~~as~~ ~~and~~}$$

$$E = \frac{p^2}{2m} = \left(\frac{h}{\lambda}\right)^2 \cdot \frac{1}{2m} = \left(\frac{h}{2\pi/k}\right)^2 \cdot \frac{1}{2m} \quad \text{as } \lambda = \frac{h}{p} \text{ and } k = \frac{2\pi}{\lambda}$$

$$E = \frac{\hbar^2 k^2}{2m} \text{ — (6)} \quad \text{or} \quad E \propto k^2 \quad \text{— (7)}$$

so that the energy is directly proportional to k^2 is

Let us consider E-k curve as shown in the fig (a) for the first Brillouin zone where $-\pi/a \leq k \leq \pi/a$. We see that the velocity of varies with slope of E-k curve. To explain further let us combine E-k curve from equation (7) and v-k curve from eq (5) in fig. (b)

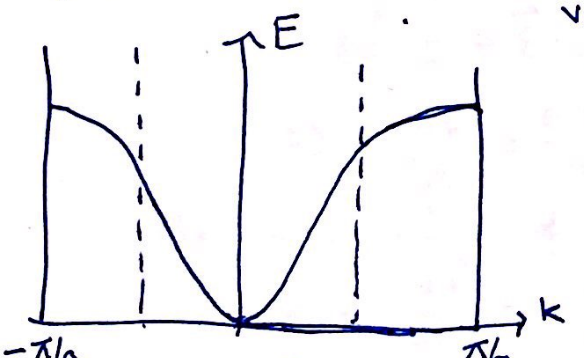
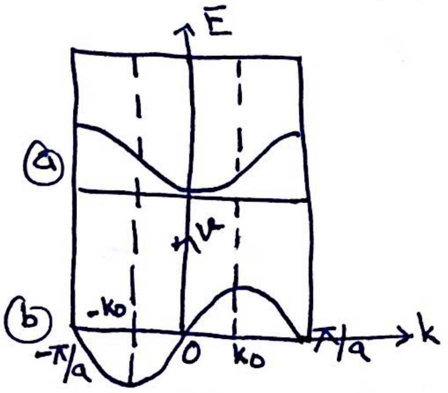


fig (a)

fig (b)



Plot of energy and velocity as a function of k.

From the expression (5) we observe that the velocity of e^- varies with the slope of E–k curve. The slope is zero for $k=0$ and $k=\pm\pi/a$. here velocity of e^- is zero at the bottom as well as at the top of the first Brillouin zone or band. At the intermediate regions of the band the velocity reaches the free electron velocity. The absolute value of the velocity reaches a maximum for $k=k_0$, where k corresponds to the inflection point (wher curvature changes) of the E(k) curve. Beyond this point the velocity decreases with increasing energy. This is a very different result from that of the behaviours of free electrons.

Now let us consider an external electric field $\vec{\mathcal{E}}$ be applied to the electrons in a solid for a time dt. If $\vec{v}$ be the velocity of electrons, then the distance travelled by it in time dt is $\vec{v}dt$. so that the gain in the energy of electron is

$$d\vec{E} = \text{force acting on } \bar{e}\,(e\vec{\mathcal{E}}) \times \text{distance travelled } (vdt)$$

$$d\vec{E} = e\vec{\mathcal{E}}\cdot v dt = \text{work done on the electron}$$

$$d\vec{E} = e\vec{\mathcal{E}}\cdot\frac{1}{\hbar}\left(\frac{dE}{dk}\right)dt$$

$$\Rightarrow \frac{d\vec{k}}{dt} = \frac{e\vec{\mathcal{E}}}{\hbar} \quad \text{—} (8)$$

The accelaration of the electron is given by

$$\vec{\alpha} = \frac{d\vec{v}}{dt} = \frac{d}{dt}\left[\frac{1}{\hbar}\left(\frac{dE}{d\vec{k}}\right)\right] = \frac{1}{\hbar}\frac{d}{d\vec{k}}\left[\frac{dE}{d\vec{k}}\right]\cdot\frac{d\vec{k}}{dt}$$

Using eq (8)

$$\Rightarrow \vec{\alpha} = \frac{1}{\hbar}\left(\frac{d^2E}{dk^2}\right)\cdot\frac{e\vec{\mathcal{E}}}{\hbar} = \frac{e\vec{\mathcal{E}}}{\hbar^2}\left(\frac{d^2E}{dk^2}\right) \quad \text{—} (9)$$

Comparing eq (9) with the acceleration of free e^- of mass m, ~~we find that~~ from eq (6)

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

$$\frac{dE}{dk} = \frac{\hbar^2 k}{m} \Rightarrow \frac{d^2E}{dk^2} = \frac{\hbar^2}{m}$$

$$\text{or} \quad m = \frac{\hbar^2}{(d^2E/dk^2)} \quad \text{--- (10)}$$

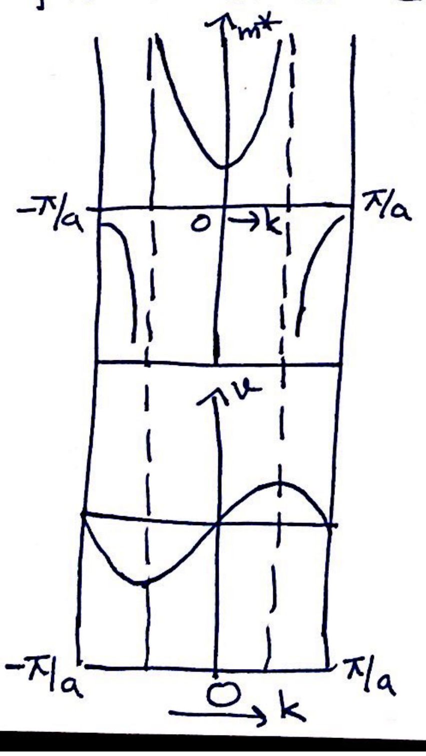
Also from equation (9) for accelaration we find that effective mass of electron in the band is ($F=ma$)

$$m^* = \frac{\hbar^2}{d^2E/dk^2)} \quad \text{--- (11)}$$

Thus for free electron $m = m^*$. But for an electron moving in a periodic potential, E does not vary with k in the manner given by eq (7) and (6), therefore,

$$\underline{m \neq m^*}$$

Moreover m^* will not be same for all energy values but it will vary due to complex form of E-k curve. In this way the electron in a crystal behaves dynamically just like a particle with variable effective mass due to the effect of periodicity of the potential. To explain further let us examine fig. (C) representing m^*-k curve along with v-k curve in first zone.



Near $k=0$, the effective mass approaches m. As the value of k increases, m^* increases reaching its maximum value at the point of inflection of the curve. Above this point of inflection, m^* is negative and as $k \to \pi/a$, it decreases to a small negative value. At point of inflection $\frac{d^2E}{dk^2} = 0$ (see fig (a)) and hence m^* becomes infinite and beyond this m^* is -ve. It means e^- has a negative mass this situation can be avoided if we introduce concept of hole, a particle which has all the properties of electron except that it has +ve charge. A hole thus represent absence of an electron. And instead of saying that top of the band in fig (c) is occupied by electron's having negative mass, we say that top band is occupied by holes. This way concept of holes came into picture so that motion of particles of positive mass can be visualised.

The same result can be arrived at, if we consider v-k curve in fig (c). When electric field is applied across the crystal, an e^- starts at $k = 0$; Its wave vector increases with time till is reaches max. velocity at inflection point. Beyond this, the same field produces a decrease in velocity, i.e. mass must become negative in the upper band.
