University of Anbar

College of Science – Dept. of Physics

Lectures of Semiconductors #1

for 3th level of physics students

Lecture 6 : Introduction to the Quantum Theory of Solids/2

by

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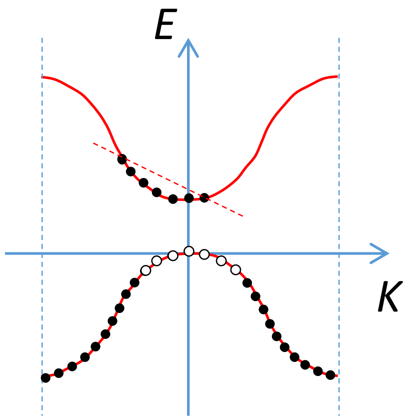
If a force is applied to a particle and the particle moves, it must gain energy. this effect is expressed as:

$$dE = F\,dx = F\,v\,dt \qquad \dots\dots\dots\dots (3)$$

where F is the applied force, dx is the differential distance the particle moves, v is the velocity, and dE is the increase in energy

If an external force is applied to the electrons in the conduction band, there are empty energy states into which the electrons can move: therefore, because of the external force, electrons can gain energy and a net momentum. The electron distribution in the conduction band may look like that shown in beside Figure, which implies that the electrons have gained a net momentum.



We may write the drift current density due to the motion of electrons as:

$$J = -e\sum_{i=1}^{n} v_i \qquad : q = -\,e \;\;(electron\ charge) \qquad \dots\dots \qquad (4)$$

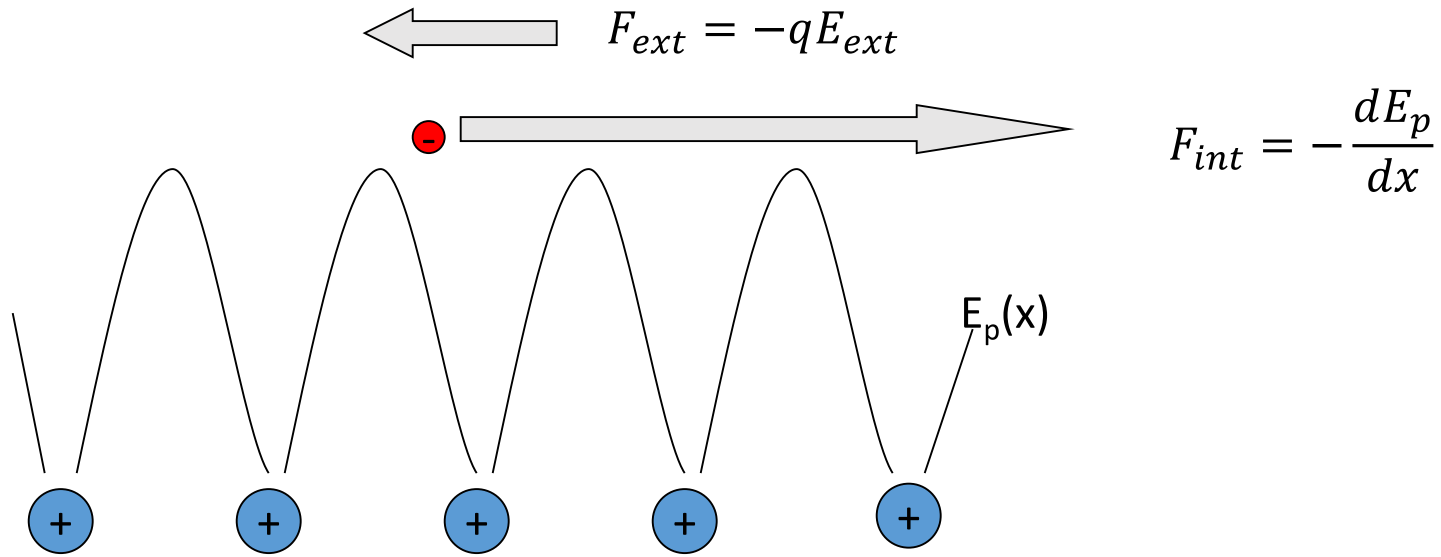
where e is the magnitude of the electronic charge and n is the number of electrons per unit volume in the conduction hand. Again, the summation is taken over a unit volume so the current density is A/cm^2

We may note from eq.(4) that the current is directly related to the electron velocity; that is, the current is related to how well the electron can move in the crystal.

3.2.3 Electron Effective Mass

In crystal the total force is caused from an externally applied force such as ***electric fields***, and the internal forces in the crystal due to positively charged ions or protons and negatively charged electrons (***ions and core electrons***) , which will influence the motion of electrons in the lattice.

- In a crystal lattice, the net force may be opposite the external force, however:



$$F_{total} = F_{xet} + F_{int} = m\,a \qquad \dots\dots\dots\dots\dots\dots (5)$$

where F_{total} , F_{xet}, and F_{int} , are the total force, the externally applied force, and the internal forces, respectively, acting on a particle in a crystal. The parameter $\boldsymbol{a}$ is the acceleration and m is the rest mass of the particle.

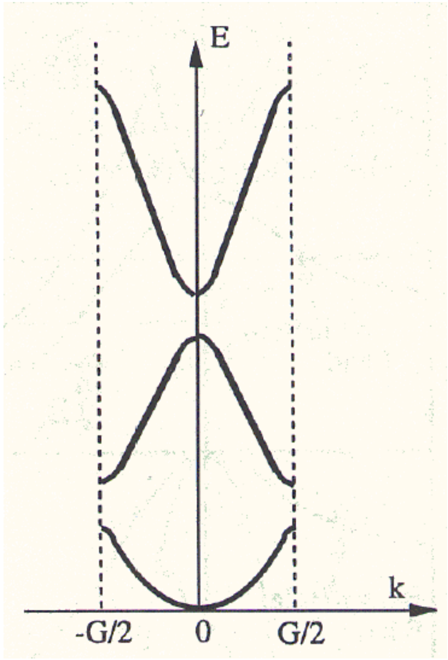
What is the expression for m*

Since it is difficult to take into account all of the internal forces, we will write the equation

$$F_{total} \approx F_{ext} = m^* a \qquad \dots\dots\dots\dots\dots\dots (6)$$

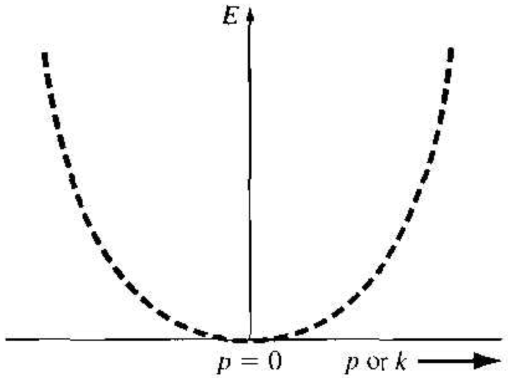
where the acceleration a is now directly related to the external force. The parameter m*. called the effective mass, takes into account the panicle mass and also takes into account the effect of the internal forces.

We can also relate the effective mass of an electron in a crystal to the E versus k curves, such as was shown in figure



➤ Mass of the free electron :

consider the case of a free electron whose $\boldsymbol{E}$ versus $\boldsymbol{k}$ curve was shown in Figure



Recalling Equation:

$$E = \frac{p^2}{2m} = \frac{k^2\hbar^2}{2m} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(7)$$

If we take the derivative of Equation (9) with respect to $\boldsymbol{k}$, we obtain :

$$\frac{dE}{dk} = \frac{d}{dk}\left(\frac{p^2}{2m}\right) = \frac{d}{dk}\left(\frac{k^2\hbar^2}{2m}\right)$$

$$\frac{dE}{dk} = \frac{k\hbar^2}{m} = \frac{\hbar\, p}{m}$$

$$\frac{1}{\hbar}\frac{dE}{dk} = \frac{p}{m} = \frac{mv}{m} = v \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.(8)$$

If we now take the second derivative of E with respect to k in eq. (7) , we have :

$$\frac{d^2E}{dk^2} = \frac{\hbar^2}{m} \quad \Rightarrow \quad \frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{1}{m} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.(9)$$

We may also note from above figure that $\frac{d^2E}{dk^2}$ is a positive quantity, which implies that the mass of the electron is also a positive quantity .

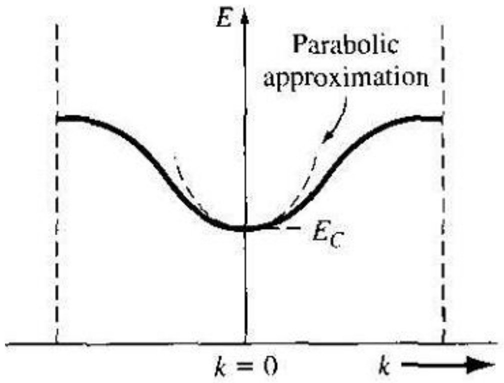
$F = m\,a$ ……………… (10) Newton's classical equation of motion

$\vec{F} = -q\vec{E} = -e\,\vec{E}$ ……………… (11) Faraday's classical equation of electric force

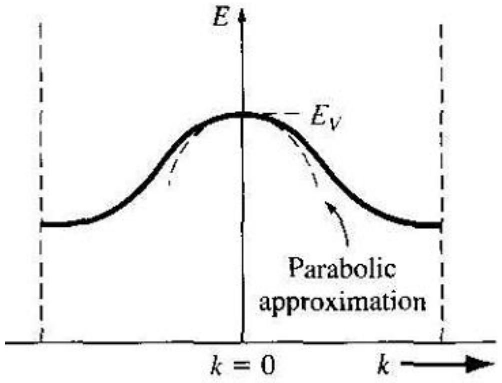
$$\vec{a} = -\frac{e\,\vec{E}}{m} \text{ ……………… } (12)$$

We note, the motion of the free electron is in the opposite direction to the applied electric field because of the negative charge.

We may now apply the results to the electron in the bottom of an allowed energy band. Consider the allowed energy band in beside figure (a) . The energy near the bottom of this energy band may be approximated by a parabola, just as that of a free particle. We may write :



(a)



(b)

$$E - E_c = C_1(k)^2 \text{ ……………… } (13)$$

The energy E, is the energy at the bottom of the band. Since $E > E_c$ the parameter $\boldsymbol{C_1}$ is a positive quantity.

$$E = C_1(k)^2 - E_c \text{ ……………… } (14)$$

$$\frac{d^2E}{dk^2} = 2C_1 \text{ ……………… } (15)$$

$$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{2C_1}{\hbar^2} \quad \dots\dots\dots\dots\dots\dots (16)$$

Multiply by $\frac{1}{\hbar^2}$

Comparing Equation (16) with Equation (9). We may equate $\frac{\hbar^2}{2C_1}$, to the mass of the particle.

However, the curvature of the curve in Figure 3.16a will not, in general, be the same as the curvature of the free-particle curve. We may write

$$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{2C_1}{\hbar^2} = \frac{1}{m^*} \quad \dots\dots\dots\dots\dots\dots (17)$$

$$m^* = \frac{\hbar^2}{2C_1} \quad \dots\dots\dots\dots\dots\dots (18)$$

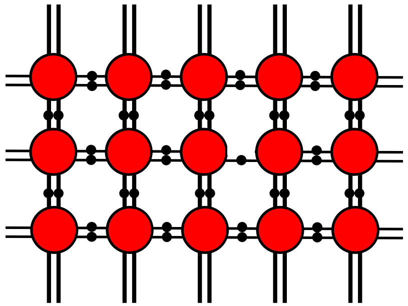
Where $\boldsymbol{m}^*$ is called the effective mass

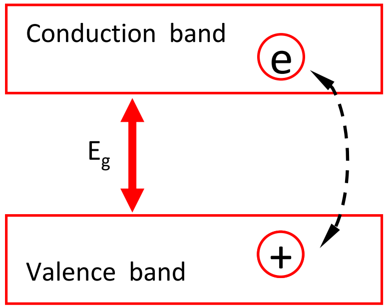
If we apply an electric field to the electron in the bottom of the allowed energy band, we may write the acceleration as :

$$a = -\frac{e\,E}{m^*} \quad \dots\dots\dots\dots\dots\dots (19)$$

The effective mass m: of the electron near the bottom of the conduction band is a constant.

3.2.4 Concept of the Hole





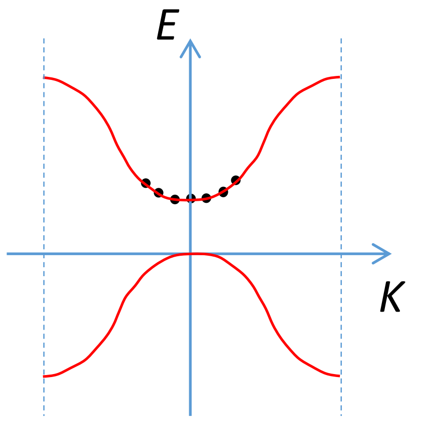
- In considering the two-dimensional representation of the covalent bonding shown in Figure , a positively charged "empty state" was created when a valence electron was elevated into the conduction band.

What is happen ?

- For T > 0 K, all valence electrons may gain thermal energy; if a valence electron gains a small amount of thermal energy, it may hop into the empty state
- The crystal now has a second equally important charge carrier that can give rise to a current
- This charge carrier is called a ***hole*** and, as we will see, can also be thought of as a classical particle whose motion can be modeled using Newtonian mechanics.

The drift current density due to electrons in the valence band, such as shown in below figure , can be written as

$$J = -e \sum_{i(filled)} v_i \quad \dots\dots\dots\dots\dots\dots\dots\dots (20)$$



where the summation extends over all filled states. This summation is inconvenient since it extends over a nearly full valence band and takes into account a very large number of states.

$$J = -e \sum_{i(total)} v_i + e \sum_{i(empty)} v_i \quad \dots\dots\dots\dots\dots\dots\dots\dots (21)$$

The distribution of electrons will respect to k cannot be changed with an externally applied force.

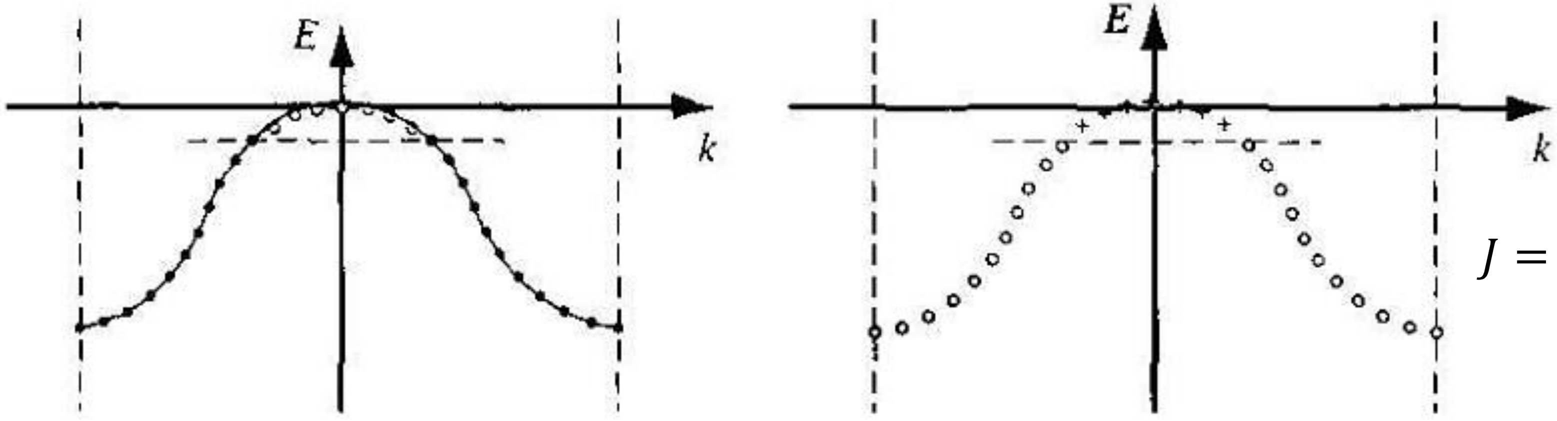
$$J = +e \sum_{i(empty)} v_i \qquad : -e \sum_{i(total)} v_i = 0 \quad \dots\dots\dots\dots\dots\dots\dots\dots (22)$$

If we consider a band that is totally full, all available states are occupied by electrons. The individual electrons can be thought of as moving with a velocity as given by

$$v(E) = \frac{1}{\hbar}\frac{dE}{dk} \quad \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots. (23)$$

where the v, in the summation is the associated with the empty state.

Equation (22) is entirely equivalent to placing a positively charged particle in the empty states and assuming all other states in the band are empty, or neutrally charged.



(a) (b)

$$J = +e \sum_{i(empty)} v_i$$

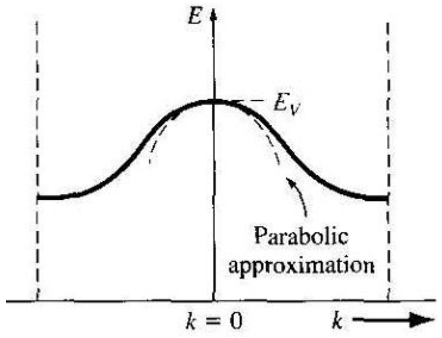
Valence band with conventional electron-filed sates and empty states

Concept of positive charges occupying the original empty states

Now consider an electron near the top of the allowed energy band shown in Figure

The energy near the top of the allowed energy band may again be approximated by a parabola so that we may write

$$(E - E_v) = -C_2 (k)^2 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (24)$$



The energy E_v is the energy at the top of the energy band

Since, $E < E_v$, for electrons in this band, then the parameter C_1 must be a positive quantity.

$$\frac{d^2E}{dk^2} = -2\,C_2 \;\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (25)$$

$$but \qquad \frac{d^2E}{dk^2} = \frac{\hbar^2}{m^*}$$

$$then\,, \frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{-2\,C_2}{\hbar^2} = \frac{1}{m^*} \ldots\ldots\ldots (26)$$

where $\boldsymbol{m}^*$ is again an effective mass. We have argued that C2 is a positive quantity, which now implies that C_2 is a positive quantity, which now implies that $\boldsymbol{m}^*$ is a negative quantity. An electron moving near the top of an allowed energy band behaves as if it has negative mass.

$$a = \frac{-e\,E}{-\,|m^*|} = \frac{e\,E}{|m^*|} \qquad \ldots\ldots.(27)$$

An electron moving near the top of an allowed energy band moves in the same direction as the applied electric field.

The net motion of electrons in a nearly full band can be described by considering just the empty states, provided that a positive electronic charge is associated with each state and that the negative of $\boldsymbol{m}^*$ from Equation (27) is associated with each state. We now can model this band as having particles with a positive electronic charge and a positive effective mass. The density of these particles in the valence band is the same as the density of empty electronic energy states. This new particle is the hole. The hole, then, has a positive effective mass denoted by $m_p{}^*$ and a positive electronic charge, so it will move in the same direction as an applied field.