lower than that of the travelling wave whereas that of ρ_- is higher than that of the travelling wave.

$\rho_+ < \rho_{travellingwave} < \rho_-$.

Hence we have an energy gap of width E_g.

THE BLOCH THEOREM

It states that the solutions of the Schrödinger equation $-\frac{\hbar^2}{2m}\frac{\partial^2\psi(r)}{\partial x^2} + V(x)\psi(r) = E\psi(r)$.

$$\frac{\partial^2\psi(r)}{\partial x^2} + \frac{2m}{\hbar^2}[E - V(r)]\psi(r) = o \qquad (*)$$

are the plane waves modulated by the function $U_k(\vec{r})$ which has the same periodicity as the lattice $\psi_k(\vec{r}) = e^{i\vec{k}.\vec{r}}U_k(\vec{r})$.

The potential $V(r)$ includes interaction of electrons with all the atoms in the solid as well as its interaction with other electrons. Thus the potential is periodic. Let the potential of the electrons satisfy $V(\vec{r}) = V(\vec{r} + \vec{R})$, where $\vec{R}$ is the lattice vector or period.

According to Bloch theorem the solution to the equation (*) will be given by $\psi_k(\vec{r}) = e^{i\vec{k}.\vec{r}}U_k(\vec{r})$ for a periodic potential U, where the function U_k has the same translation symmetry as the lattice or period i.e $U_k(\vec{r} + \vec{R}) = U_k(\vec{r})$.

Since the potential $V(\vec{r})$ is periodic then all observable quantities associated with the electron must be periodic. This also includes the quantity $|\psi(r)|^2$ which gives the electron probability. The only function which satisfies this requirement for all $\vec{r}$ is one of the exponential form i.e $e^{i\vec{k}.vecr}$. Thus the solution to the Schrödinger equation has the Bloch form.

Wave functions of the form $\psi_k(\vec{r}) = e^{i\vec{k}.\vec{r}}U_k(\vec{r})$ are called Bloch functions where the function $\psi_k(\vec{r})$ has the following properties:

1. It has the form of the travelling wave represented by $e^{i\vec{k}.vecr}$ which implies that the electron

propagates through the crystal like a free particle.

2. The electron has a de Broglie wave length $\lambda = \frac{2\pi}{k}$ and hence momentum $\vec{p} = \hbar\vec{k}$ since it behaves as a wave of vector $\vec{k}$.

3. The bloch function ψ_k is a crystal orbital as it is delocalised throughout the solid. Thus the electron is shared by the whole crystal.

Read about: Extrinsic and Intrinsic semi conductors.

HOLES AND ELECTRONS

Vacant orbitals in a band are commonly called holes. Holes in the valence band can be treated as positively charged carriers.

INTRINSIC CARRIER CONCENTRATION

Here we shall be expressing the number of electrons excited to the conduction band at temperature T in terms of the chemical potential μ (of the fermi level) and the energy gap (E_g). We suppose for the conduction band of a semi conductor $E - \mu >> k_BT$ and thus the fermi dirac distribution function reduces to $f_e = e^{\frac{(\mu - E)}{k_BT}}$.

This defines the probability that the conduction electron of the orbital is occupied (valid $f_e << 1$). The density of states in the conduction band at energy E is $D_e(E) = \frac{1}{2\pi^2}(\frac{2m_e}{\hbar^2})^{\frac{3}{2}}(E - E_c)^{\frac{1}{2}}$ where E_c is the energy at the conduction band edge.

The concentration of electrons in the conduction band is given by

$n = \int_{E_c}^{\infty} D_e(E) f_e(E) dE$

$\Rightarrow n = \frac{1}{2\pi^2}(\frac{2m_e}{\hbar^2})^{\frac{3}{2}} e^{\frac{\mu}{k_BT}} \int_{E_c}^{\infty}(E - E_c)^{\frac{1}{2}} e^{\frac{-E}{k_BT}} dE$

$$n = 2(\frac{m_e k_B T}{2\pi\hbar^2})^{\frac{3}{2}} e^{\frac{(\mu - E_c)}{k_BT}} \tag{1}$$

Similarly we can also calculate the concentration of holes, P. Here the distribution function f_h for holes is given by $f_h = 1 - f_e$, where f_e is the probability distribution for the electron hole concentration i.e since a hole is the absence of an electron.

$f_h = 1 - \frac{1}{e^{\frac{(E-\mu)}{k_BT}}+1}$

$f_h = \frac{1}{e^{\frac{(\mu-E)}{k_BT}}+1} \approx e^{\frac{(E-\mu)}{k_BT}}$ provided $(\mu - E) >> k_BT$.

If the holes near the top of the valence band behave as particles with effective mass, m_h, then $D_h(E) = \frac{1}{2\pi^2}(\frac{2m_h}{\hbar^2})^{\frac{3}{2}}(E_v - E)^{\frac{1}{2}}$, where E_v is the energy of the valence band edge.

The hole concentration p in the valence band is given by $P = \int_{-\infty}^{E_v} D_h(E) f_h(E) dE$

$$p = 2(\frac{m_h k_B T}{2\pi\hbar^2})^{\frac{3}{2}} e^{\frac{(E_v - \mu)}{k_BT}} \tag{2}$$

Multiplying expressions for n and p, we obtain equilibrium relation,

$$np = 4(\frac{k_B T}{2\pi\hbar^2})^3 (m_e m_h)^{\frac{3}{2}} e^{\frac{-E_g}{k_BT}} \tag{3}$$

where $E_g = E_c - E_v$ is the energy gap.

We note from equation (3) that np is independent of the fermi level μ (temperature dependent). Thus at a given temperature, np is a constant. Since for an intrinsic semi conductor the number of electrons is equal to the number of holes (because the thermal excitation of an electron leaves behind a hole in the valence band) with a notation i refering to intrinsic, we then have from equation (3) that

$n_i = p_i = 2(\frac{k_BT}{2\pi\hbar^2})^{\frac{3}{2}}(m_e m_h)^{\frac{3}{4}} e^{\frac{-E_g}{2k_BT}}$ which implies that the intrinsic carrier depends exponentially on $\frac{E_g}{2k_BT}$.

Setting equations (1) and (2) to be equal, we obtain

$e^{\frac{2\mu}{k_BT}} = (\frac{m_h}{m_e})^{\frac{3}{2}} e^{\frac{E_g}{k_BT}}$

$\Rightarrow \mu = \frac{1}{2}E_g + \frac{3}{4}k_BTln(\frac{m_h}{m_e})$.

For $m_h = m_e$, $\mu = \frac{1}{2}E_g$ and thus the fermi level is in the middle of the forbidden energy gap.

THE EFFECTIVE MASS AND CURVATURE

When a free electron is subjected from electric field $\vec{E}$, it experiences an acceleration given by $a = \frac{-e\vec{E}}{m}$. However, when electric field is applied to a crystal, few electrons if any have $a = \frac{-e\vec{E}}{m}$. This is because the crystal electrons are so tightly bound to the atoms that they can not be accelerated at all. For an electron which is not bound to any atoms, Newton's second law gives $ma = -eE+$ Force due to neighbouring ion cores and the electrons.

The sum of these other forces is not known quantitatively and thus ignoring them, the initial expression can be written as $m^*\vec{a} = -eE$ where m^* is the effective mass.

Considering the wave energy relation $E = \frac{\hbar^2k^2}{2m}$, the curvature is defined as $\frac{d^2E}{dk^2} = \frac{1}{m}$. Then the coefficient of k^2 determines the curvature of E versus k. For an electron in a I-D lattice we assume that the electron moves with a group velocity given by $V_g = \frac{1}{\hbar}\frac{dE}{dk}$ and the external force acting on the electron is given as $F = \hbar\frac{dk}{dt}$.

Hence $\frac{dV_g}{dt} = \frac{1}{\hbar}\frac{d^2E}{dkdt}$.

$\frac{dV_g}{dt} = \frac{1}{\hbar}\frac{d^2E}{dk^2}\frac{dk}{dt}$

But $\frac{dk}{dt} = \frac{F}{\hbar}$.

$\Rightarrow \frac{dV_g}{dt} = \frac{1}{\hbar^2}(\frac{d^2E}{dk^2})F$.

$F = \frac{\hbar^2}{\frac{d^2E}{dk^2}}\frac{dV_g}{dt}$.

Identifying $\frac{\hbar^2}{\frac{d^2E}{dk^2}}$ as the mass, then the above equation is identical to Newton's second law.