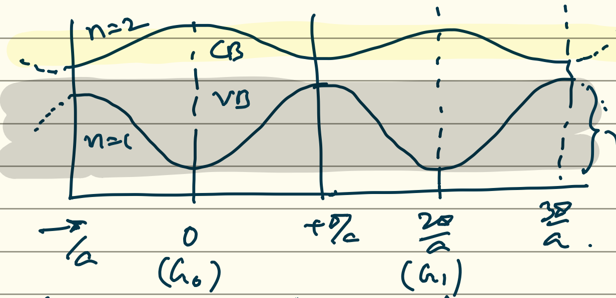
Effective mass of electron and concept of "hole".

Recall 1D band str: Consider a divalent system ⇒ fully filled lowest band ⇒ Insulator (or, Semiconductor if bandgap small)

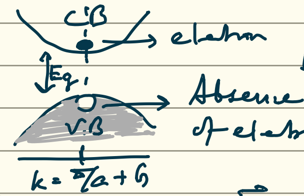


} Unoccupied band (conduction band (CB))

} Occupied band (Valence band (VB))

At room temperature: FD distribution: Small but nonzero probability to find electron at upper bands.

When an electron transits from VB to CB:



E_g → band gap

Let us consider application of an external force $\vec{F}$ over a time interval Δt such that the work done (W) on the system is a negligible fraction of the band gap E_g.

$$\frac{dW}{dt} = Fv = F\frac{1}{\hbar}\frac{dE(k)}{dk}.$$

Note that v is group velocity since the states of electron are Bloch states (or Wannier states) which are combinations of plane waves.

$$\Rightarrow \frac{dW}{dt} = \frac{dE(k)}{dk}\frac{dk}{dt} = \frac{F}{\hbar}\frac{dE(k)}{dk}$$

$E(k)$ → Band structure

$$\Rightarrow \boxed{\hbar\frac{dk}{dt} = F}$$

Since $\Delta W \ll E_g$ ⇒ $\Delta E \ll E_g$ ⇒ $\Delta k \to 0^+$ ⇒ k of electron and hole states will be close to $(\pi/a + G)$ or G if VB is n = odd or even

For electron near the CB minima;

$$E(k) = \underbrace{E_{CB}(k_0)}_{\text{Conduction band}} + \underbrace{\left.\frac{\partial E_{CB}}{\partial k}\right|_{k=k_0}(k-k_0)}_{\text{0 since band min}} + \frac{1}{2}\left.\frac{\partial^2 E_{CB}}{\partial k^2}\right|_{k=k_0}(k-k_0)^2 + \cdots$$

Let $k_0 = \frac{\pi}{a} + G$: n_{CB} is odd

$$\Rightarrow v_e = \frac{1}{\hbar}\left.\frac{\partial E(k)}{\partial k}\right|_{k=k_0} = \left.\frac{\partial^2 E_{CB}(k)}{\partial k^2}\right|_{k=k_0}(k-k_0) \Rightarrow \left.\frac{\partial^2 E_{CB}(k)}{\partial k^2}\right|_{k=k_0} \text{ has dimension } \hbar^2/m$$

$$\therefore \boxed{\hbar^2 \Big/ \left(\left.\frac{\partial^2 E_{VB}}{\partial k^2}\right|_{k=k_0}\right)}$$ can be interpreted as effective mass of electron: m_e^*

$$\Rightarrow E_e(k) = E_{CB}(k_0) + \frac{1}{2}\frac{\hbar^2(k-k_0)^2}{m_e^*}$$

(e → electron)

$$v_e(k) = \frac{1}{\hbar}\left.\frac{\partial E_e(k)}{\partial k}\right|_{k=k_0} = \frac{\hbar(k-k_0)}{m_e^*} \Rightarrow a_e(k) = \frac{\hbar}{m_e^*}\dot{k} = \frac{F}{m_e^*}$$

Note here that F is as felt by electron with −ve charge. Since we started with $\frac{dW}{dt} = Fv$ not $(-vF)$

In higher dimension effective mass is a tensor: $\boxed{M^{-1}_{e\,ij}(k) = \frac{1}{\hbar^2}\left.\frac{\partial^2 E_{VB}(\vec{k})}{\partial k_i \partial k_j}\right|_{k=k_0}}$

Similarly for the "hole" (h) near the VB maxima:

$$E_h(k) = E_{VB}(k_0) + \frac{1}{2}\left.\frac{\partial^2 E_{VB}}{\partial k^2}\right|_{k=k_0}(k-k_0)^2$$

$$= E_{VB}(k_0) - \frac{1}{2}A(k-k_0)^2,$$ since $E(k)$ is maxima $A > 0$

$$A = -\left.\frac{\partial^2 E_{VB}(k)}{\partial k^2}\right|_{k=k_0} \text{ has dimension } \frac{\hbar^2}{m} \Rightarrow m_h^* = -\hbar^2 \Big/ \left(\left.\frac{\partial^2 E_{VB}(k)}{\partial k^2}\right|_{k=k_0}\right)$$

which is > 0 as mass should classically be.

$$\Rightarrow v_h(k) = \frac{1}{\hbar}\left.\frac{\partial E_h(k)}{\partial k}\right|_{k=k_0} = -\frac{\hbar(k-k_0)}{m_h^*}$$

opposite to v_e ⇒ h must have opposite charge w.r.t electron.

$$\Rightarrow a_h(k) = -\frac{\hbar\dot{k}}{m_h^*} = -\frac{F}{m_h^*}$$

Since we started with as F is felt by electron.

Note that the VB maxima is always flatter than CB minima ⇒ $m_h^* > m_e^*$; $v_e > v_h$ ⇒ $\mu_e > \mu_h$ (μ → mobility)