6.730 Physics for Solid State Applications

Lecture 23: Electrons and Holes

Outline

- Effective Mass
- Semiclassical Equations of Motion in an Electric Field
  - Bloch Oscillations
  - Ohm's Law
  - Holes

April 2, 2004

Semiclassical Equations of Motion

$$\boxed{\langle \mathbf{v_n(k)} \rangle = \frac{\langle \mathbf{p} \rangle}{\mathbf{m}} = \frac{\mathbf{1}}{\hbar}\nabla_{\mathbf{k}}\mathbf{E_n(k)}} \qquad \boxed{\mathbf{F_{ext}} = \hbar\frac{\mathbf{dk}}{\mathbf{dt}}}$$

Lets try to put these equations together....

$$a(t) = \frac{dv}{dt} = \frac{1}{\hbar}\frac{\partial}{\partial t}\frac{\partial E_N(k)}{\partial k} = \frac{1}{\hbar}\frac{\partial^2 E_N(k)}{\partial k^2}\frac{dk}{dt}$$

$$= \left[\frac{1}{\hbar^2}\frac{\partial^2 E_N(k)}{\partial k^2}\right] F_{\text{ext}}$$

Looks like Newton's Law if we define the mass as follows...

$$m^*(k) = \hbar^2 \left(\frac{\partial^2 E_N(k)}{\partial k^2}\right)^{-1}$$ dynamical effective mass

→ mass changes with k...so it changes with time according to k

Dynamical Effective Mass (3D)

Extension to 3-D requires some care,
F and a don't necessarily point in the same direction

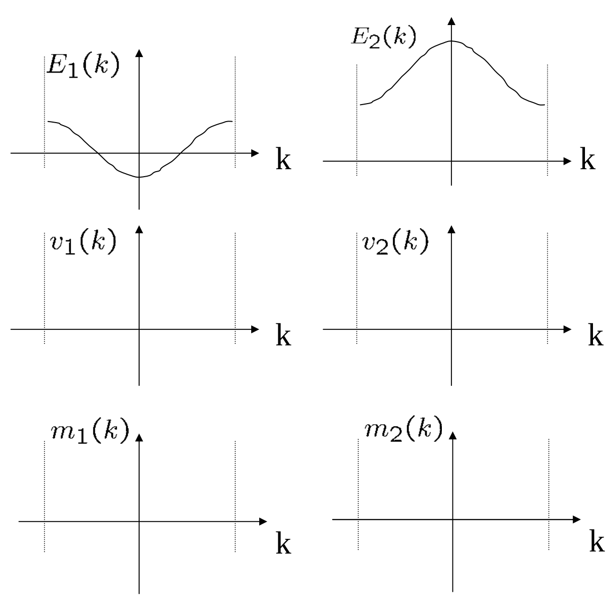
$$\mathbf{a} = \overline{\overline{\mathbf{M}}}^{-1}\mathbf{F}_{\text{ext}} \quad \text{where} \quad \overline{\overline{\mathbf{M}}}^{-1}_{i;j} = \frac{1}{\hbar^2}\frac{\partial^2 E_N}{\partial k_i \partial k_j}$$

$$\begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} = \frac{d}{dt}\begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = \begin{pmatrix} \frac{1}{m_{xx}} & \frac{1}{m_{xy}} & \frac{1}{m_{xz}} \\ \frac{1}{m_{yx}} & \frac{1}{m_{yy}} & \frac{1}{m_{yz}} \\ \frac{1}{m_{zx}} & \frac{1}{m_{zy}} & \frac{1}{m_{zz}} \end{pmatrix}\begin{pmatrix} F_x \\ F_y \\ F_z \end{pmatrix}$$

Bandstructure, Velocity, and Effective Mass

$$v(k) = \frac{1}{\hbar}\frac{\partial E_N(k)}{\partial k}$$

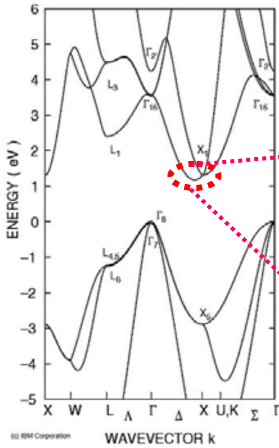
$$m^*(k) = \hbar^2\left(\frac{\partial^2 E_N(k)}{\partial k^2}\right)^{-1}$$



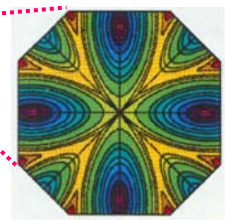
Dynamical Effective Mass (3D)
Ellipsoidal Energy Surfaces

Fortunately, energy surfaces can often be approximate as...

$$E_N(k) = E_c + \frac{\hbar^2}{2}\left(\frac{(k_x - k_x^0)^2}{m_t} + \frac{(k_y - k_y^0)^2}{m_t} + \frac{(k_z - k_z^0)^2}{m_l}\right)$$



Silicon

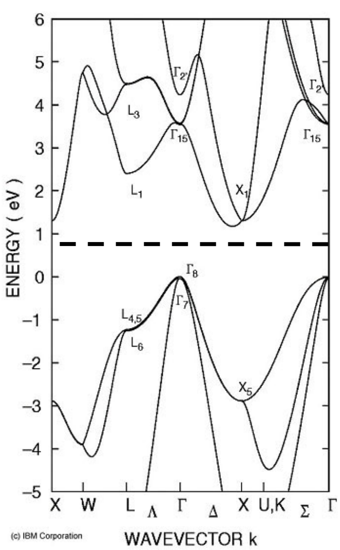


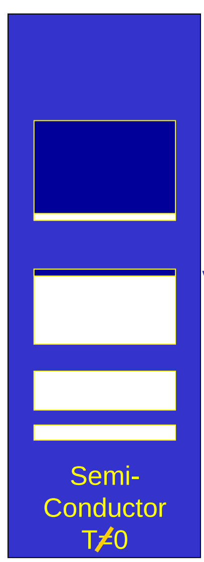
$$\overline{\overline{\mathrm{M}}}^{-1} = \begin{pmatrix} \frac{1}{m_t} & 0 & 0 \\ 0 & \frac{1}{m_t} & 0 \\ 0 & 0 & \frac{1}{m_l} \end{pmatrix}$$

$$\overline{\overline{\mathrm{M}}} = \begin{pmatrix} m_t & 0 & 0 \\ 0 & m_t & 0 \\ 0 & 0 & m_l \end{pmatrix}$$

http://csmr.ca.sandia.gov/workshops/nacdm2002/viewgraphs/Conor_Rafferty_NACDM2002.pdf

Electron and Vacancies



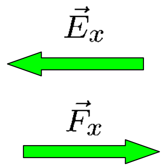


Thermal excitations cause

Electrons in conduction band n(T)

vacanies in valence band p(T)

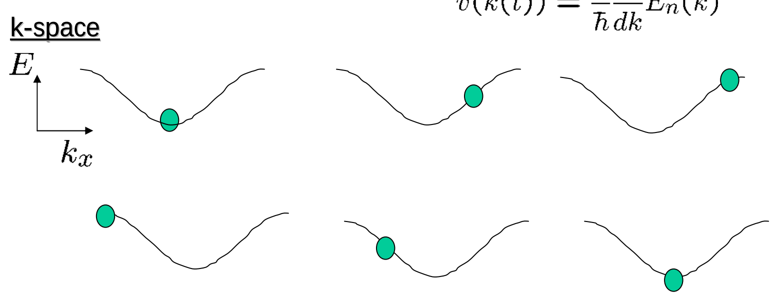
Semiclassical Motion of Electron Wave packet in a band



$$F_x = \hbar \frac{dk_x}{dt}$$ electrons have negative charge

$$k(t) = k(0) + eE_{DC}t/\hbar$$

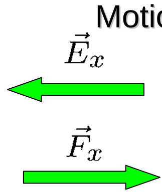
$$v(k(t)) = \frac{1}{\hbar}\frac{d}{dk}E_n(k)$$



"Electrons" move in the positive k_x direction and undergo periodic motion with period $T_{\text{Bloch}} = \dfrac{2\pi\hbar}{eE_{\text{DC}}a}$

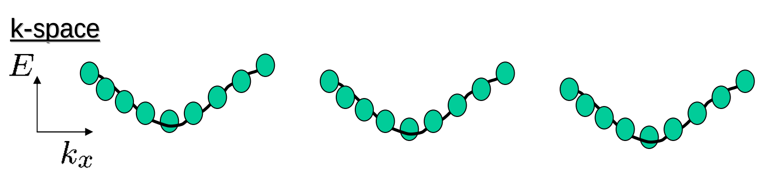
For a = 1nm, E=1volt, T = 10^4 seconds. Why don't we observe in Si devices?

Motion of Electrons in a Full band



$$F_x = \hbar \frac{dk_x}{dt} \qquad v(k(t)) = \frac{1}{\hbar}\frac{d}{dk}E_n(k)$$

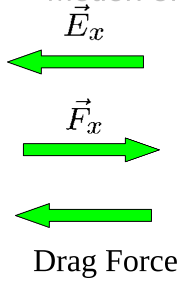
$$k(t) = k(0) + eE_{DC}t/\hbar$$



Electrons all move in the positive k_x direction and undergo periodic motion with period but all the states are filled so that there is no net current.

A filled band carries no current

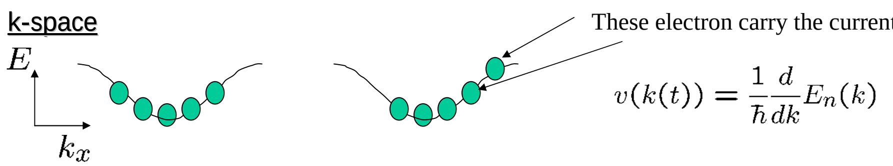
Motion of Electrons in a band: Ohms law



$$\hbar\frac{dk_x}{dt} = \mathbf{F}_{ext} - \underbrace{\frac{\hbar(\mathbf{k}-\mathbf{k}(0))}{\tau}}_{\text{Drag Force}}$$

In steady state, each electron moves in *k-space* by

$$k(t) - k(0) = eE_{DC}\tau/\hbar \ll \frac{2\pi}{a}$$

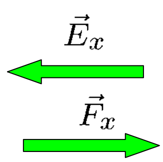


$$v(k(t)) = \frac{1}{\hbar}\frac{d}{dk}E_n(k)$$

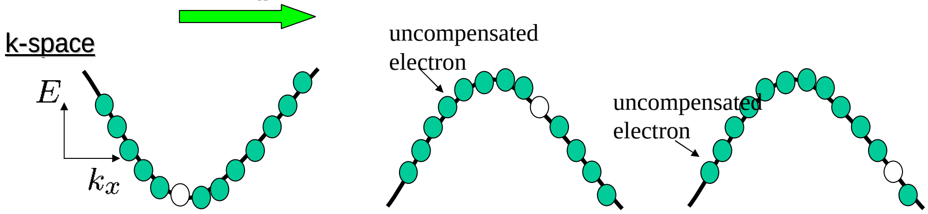
- Electrons move in the positive k_x direction by the same very small fraction of the Brillion zone, τ/T_{Bloch}.
- Uncompensated electrons carry the current
- Current is in the direction of the applied electric field.

Motion of Electrons in the valence band

$$F_x = \hbar\frac{dk_x}{dt}$$



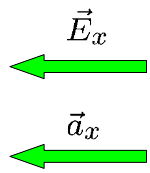
Valence electrons (and vacancy) all move in the positive k_x direction



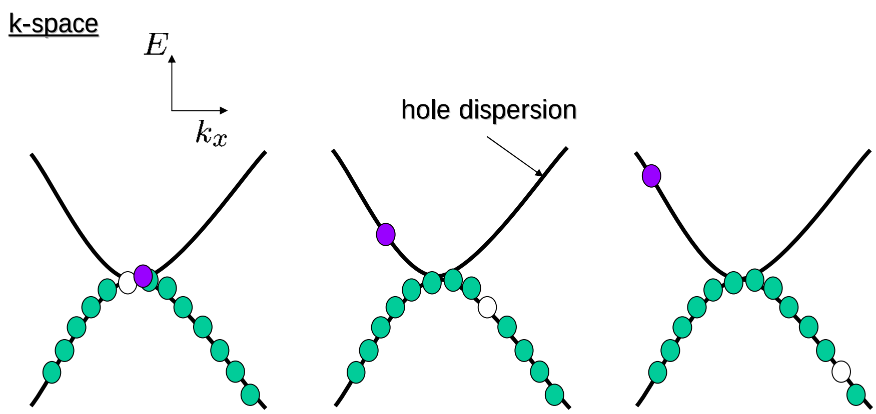
All the current (which is in the same direction of the field) is carried by the *uncompensated electron*

1. This uncompensated electron has the negative velocity of an electron if it were at the vacancy position.
2. It has a negative effective mass (same as an electron in the vacancy.
3. Invent a new particle to describe the current carried by the whole band with a vacancy, which has a positive charge and positive mass which carries the correct current.
4. The “Hole is Born”

Motion of Valence Electrons



Hole is a quasi-particle with positive charge and positive mass...



	Electrons	Holes
Charge	-e	e
Velocity	$v = \frac{1}{\hbar}\frac{d}{dk}E_e(k)$	$v = \frac{1}{\hbar}\frac{d}{dk}E_h(k)$
Current	- e $v_e(k)$	+ e $v_h(k)$
Crystal Momenta	$k = k_e$	$k = k_h = -k_v$
m*	$\frac{1}{m_e^*} = \frac{1}{\hbar^2}\frac{d^2}{dk^2}E_e(k)$	$\frac{1}{m_h^*} = \frac{1}{\hbar^2}\frac{d^2}{dk^2}E_h(k) = -\frac{1}{m_v}$
Eqn of Motion	$\frac{d}{dt}\hbar k = -eE_{\text{dc}} - \hbar(k - k(0))/\tau_e$	$\frac{d}{dt}\hbar k = eE_{\text{dc}} - \hbar(k - k(0))/\tau_h$
	Wave packet	"Quasiparticle" of collective motions of a nearly full band of electrons

Summary

- An "electron" in a solid is a wavepacket which extends over many lattice sites.
- The motion of electrons is governed by the Semiclassical Equations of Motion which gives k(t), the velocity is then read off E(k) band diagram, and then the real space motion can be found.
- A Hole is a fictional quasiparticle which describes the current due to electrons in a nearly filled valence band.
- When in doubt: Think about "electrons"
- The scattering time is phenomenological. Want to be able to calculate it: Future Lectures.