"Complementi di Fisica" Lecture 17

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In this lecture

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  - Contributions from electrons in a band to the electrical current in an external electric field
  - The "hole" concept; properties:
    - Wavevector, energy, velocity, effective mass
    - equation of motion
  - Insulators, conductors, semiconductors
- Reference textbooks
  - D.A. Neamen, Semiconductor Physics and Devices, McGraw-Hill, 3rd ed., 2003, p.71-78
  - Ch.Kittel, Introduction to Solid State Physics, J.Wiley & Sons, 7th ed., p.203-212 ("equations of motion, effective mass")
  - W.Ibach & H.Luth, Solid-State Physics, Springer, 3rd ed., p. 235-237 ("9.2: Currents in Band and Holes")

Electrical current density

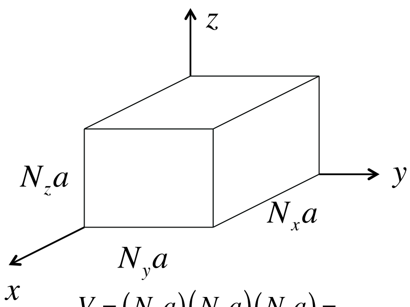
- **Contribution from electrons in a band**
  - Neglect the very weak interaction among electrons (screening)
  - Pauli exclusion principle:
    - In each state (k_x, E) two electrons with opposite spin
  - Contribution to the electrical current density by electrons in the states in an interval dk_x around k_x:

Electron charge — Group velocity

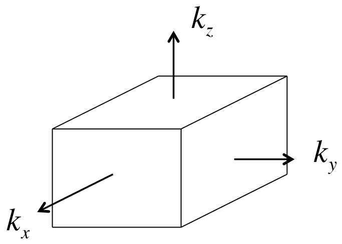
$$dj_{n,x} = \frac{-|q_e|}{8\pi^3} v_{g,x}(k_x)\,dk_x = \frac{-|q_e|}{8\pi^3\hbar}\frac{\partial E}{\partial k_x}dk_x$$

Density of states in k-space, per unit volume of real space

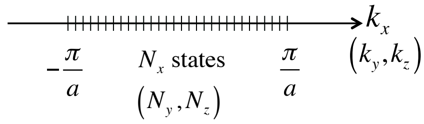
Density of states in k-space



$$V = (N_x a)(N_y a)(N_z a) = (N_x N_y N_z)a^3 = Na^3$$



1st Brillouin zone



Density of states in k-space, per unit volume of real space (x, y, z):

$$\frac{N_x}{\frac{2\pi}{a}}\frac{N_y}{\frac{2\pi}{a}}\frac{N_z}{\frac{2\pi}{a}} = N\frac{a^3}{(2\pi)^3} = N\frac{V}{(2\pi)^3} \quad \Rightarrow \quad N\frac{V}{(2\pi)^3}\frac{1}{V} = \frac{N}{(2\pi)^3}$$

Current density, fully occupied band

- **x-component (similar for y- and z-components)**

$$j_{n,x} = \frac{-|q_e|}{8\pi^3}\int_{Bz} v_{g,x}(k_x)\,dk_x = \frac{-|q_e|}{8\pi^3\hbar}\int_{Bz}\frac{\partial E}{\partial k_x}dk_x = 0$$

Integral over the 1st Brillouin zone

Odd function, see previous lecture: $v_{g,x}(-k_x) = -v_{g,x}(k_x)$

- **The electrons of fully occupied band do not contribute to the electrical current !**

$$\vec{j}_n = 0$$

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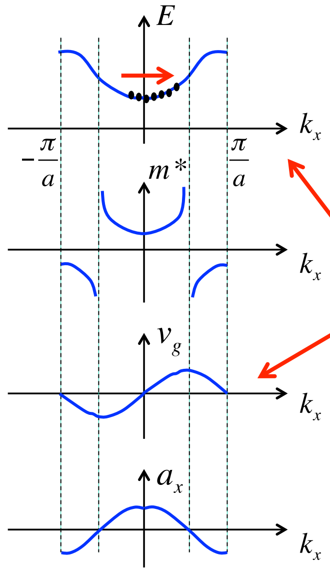
Partially filled bands



- **For instance, at the bottom of the conduction band of semiconductors:**

No external force: symmetric distributions of electrons in the available states; the net current density is *zero*:

$$j_{n,x} = \frac{-|q_e|}{8\pi^3}\int_{Bz} v_{g,x}(k_x)\,dk_x = 0$$

A positive x-component of external force induces a migration towards positive k_x, contrasted by dissipative interactions with phonons; result: asymmetric population of states, therefore current density is *not zero*:

$$j_{n,x} = \frac{-|q_e|}{8\pi^3}\int_{Bz} v_{g,x}(k_x)\,dk_x = 0$$

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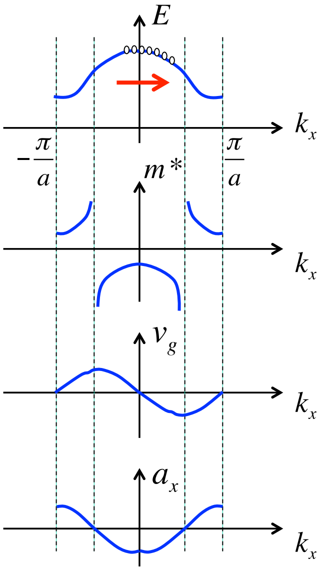
Almost full bands: "holes"



- **valence band, top:**

External force, asymmetric distribution:

$$j_{n,x} = \frac{-|q_e|}{8\pi^3}\int_{Bz,\text{ full states}} v_{g,x}(k_x)\,dk_x =$$

$$= \frac{-|q_e|}{8\pi^3}\int_{Bz} v_{g,x}(k_x)\,dk_x -$$

$$-\frac{-|q_e|}{8\pi^3}\int_{Bz,\text{ empty states}} v_{g,x}(k_x)\,dk_x =$$

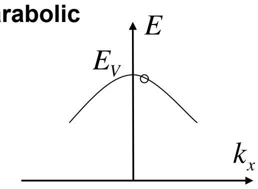
$$= \frac{+|q_e|}{8\pi^3}\int_{Bz,\text{ empty states}} v_{g,x}(k_x)\,dk_x$$

Convenient description: few empty states ("holes"), *positive charge !*

Holes: effective mass?

- **Empty electron states in the valence band: *negative* effective mass - $|m_e^*| < 0$ *for electrons*… what about missing electrons?**

Holes are found at the top of the band, where the parabolic approximation of $E(k_x)$ is valid:



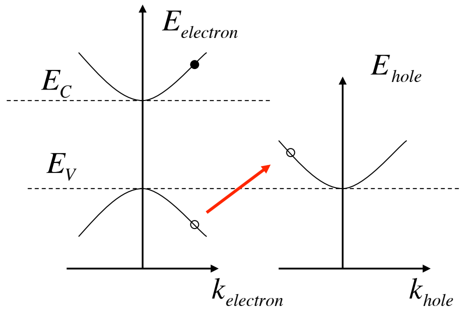
$$E(k_x) = E_V + \frac{\hbar^2 k_x^2}{2\left(-|m_e^*|\right)} = E_V - \frac{\hbar^2 k_x^2}{2|m_e^*|}$$

The acceleration of a hole in one of these states under the influence of an external electric field ε_x is that of a positive charge with positive mass!

$$a_x = \dot{v}_g = \frac{d}{dt}\left(\frac{1}{\hbar}\frac{\partial E}{\partial k_x}\right) = \frac{d}{dk_x}\left(\frac{1}{\hbar}\frac{\partial E}{\partial k_x}\right)\frac{dk_x}{dt} = \frac{1}{\hbar}\frac{\partial^2 E}{\partial k_x^2}\frac{dk_x}{dt} =$$

$$= \frac{1}{-|m_e^*|}\left(\hbar\dot{k}_x\right) = \frac{-|q_e|\varepsilon_x}{-|m_e^*|} = \frac{|q_e|\varepsilon_x}{|m_e^*|}$$

Hole properties: summary



mass

$$m_h^* = -m_e^* = \left| m_e^* \right| > 0$$

charge

$$q_h = -q_e = \left| q_e \right| > 0$$

momentum, wave number

$$p_h = \hbar k_h = -\hbar k_e = -p_e$$

energy

$$\left(E - E_V\right)_h = -\left(E - E_V\right)_e > 0$$

A missing momentum (or energy) contribution in a band is equivalent to a contribution with opposite sign!

group velocity:

$$v_{g,h} = \frac{1}{\hbar}\frac{dE_h}{dk_h} = \frac{1}{\hbar}\frac{-dE_e}{-dk_e} = \frac{1}{\hbar}\frac{dE_e}{dk_e} = v_{g,e}$$

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