"Complementi di Fisica"
Lecture 16

Livio Lanceri
Università di Trieste

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In this lecture

- **Contents**
  - Introduction to the semi-classical approximation:
    - orders of magnitude for "internal" and "external" electric fields in crystals;
    - use of "effective mass" in a classical example
  - Semi-classical equations of motion for electrons in crystals ("Bloch wave-packets")
  - Effective mass of electrons
  - Examples of electrons confined in energy bands and comparison with a free electron: "Bloch oscillations"
- **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. 231-235 ("9.1: Motion of Electrons in Bands and the Effective Mass")

Electric fields in materials

- "Internal", *microscopic* (atomic level) $q = 1.6 \times 10^{-19} C, \quad r \approx 10^{-10} m$

$$E_x = \frac{1}{4\pi\varepsilon_0}\frac{q}{r^2} \approx 9\times 10^{9}\frac{Vm}{C}\times\frac{1.6\times 10^{-19}}{\left(10^{-10}\right)^2}\frac{C}{m^2} \approx 1.4\times 10^{11}\, V/m$$

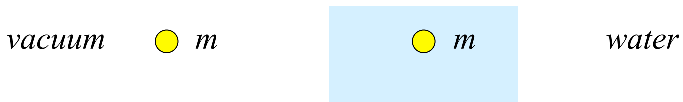
- "External", *macroscopic* (for instance, the potential difference set by an external electric circuit over a junction)

$$|E_x| = \frac{dV}{dx} \approx \frac{1}{10^{-4}}\frac{V}{m} \approx 10^{4}\, V/m$$

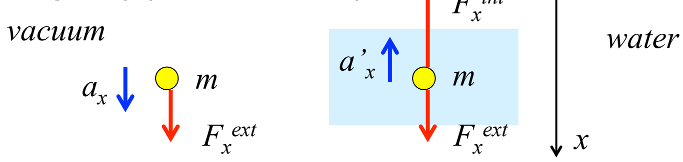
- Different by many orders of magnitude: can be treated separately!
  - *Microscopic*: quantum mechanical description, periodic potential
  - *Macroscopic*: semi-classical description, in terms of (group) velocity, acceleration, inertia (effective mass, that may be negative!!!)

"Effective mass": classical example

- Tennis ball in a vacuum, or immersed in a fluid (water)
  - without gravity ("external" force)



  - With gravity ("external" force)



$$F_x^{ext} = ma_x > 0 \qquad F_x^{ext} + F_x^{\text{int}} = ma'_x < 0$$

  - "effective mass" (consider only the external force) $m^* = F_x^{ext}/a_x$

$$m^* = m > 0 \qquad m^* = \frac{F_x^{ext}}{a'_x} < 0 \qquad \left(m^* \neq m\right)$$

"Effective mass": classical example

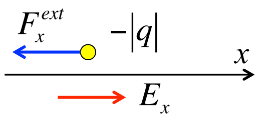
- In this example:
  the "effective mass", defined as $m^* = F_x^{ext} / a_x$
  is *negative* in water, because:
  Gravity ("external force") pulls the ball downwards, ***but:***
  Archimede's force ("internal", interaction with the fluid), pushes upwards;
  The net force and the acceleration are directed upwards

- Similar effects may be expected for electrons in crystals, if we consider separately
  - "external" forces (macroscopic electric or magnetic fields)
  - "internal" interactions with the periodic crystal fields

Semi-classical equation of motion

- Electron in a crystal with an external field:
  - The "quantum" interaction with the crystal periodic potential:
    - Separable wave functions and energy *E* eigenvalues
    - Dispersion relation *E(k)* with *k* "crystal wave number"
    - Bloch wave packets, propagating with group velocity *dE/dk*
  - The "semi-classical" interaction with the external field changes:
    - the electron energy E and wave number k (quantum description)
    - the group velocity (acceleration: classical description)
  - Example in real space, electric field E_x>0

$$F_x^{ext} = -|q| E_x$$



In other words:

- **An electron, partially localised in a crystal:**
  - **is described by a Bloch wave packet:**

$$\Psi(x,t) = \int_{k_0-\Delta k}^{k_0+\Delta k} a(k) u_k(x) e^{i\left(kx - \frac{E(k)}{\hbar}t\right)} dk \qquad v_g = \frac{1}{\hbar}\frac{dE}{dk}$$

  - **The net force on the electron has 2 contributions:**
    - **"internal" interaction with the crystal, described by *dE/dk***
    - **"external" interaction with a macroscopic field, that determines changes in *E*, *k*, and in v_g**

Interaction with the external field

- **Work theorem: variation of (kinetic …!) energy *E***

$$F_x^{ext} dx = \delta E$$

$$dx = v_g dt = \frac{1}{\hbar}\frac{dE}{dk} \qquad \delta E = \frac{dE}{dk} dk$$

$$\Rightarrow F_x^{ext} \frac{1}{\hbar}\frac{dE}{dk} dt = \frac{dE}{dk} dk$$

$$\Rightarrow \hbar \frac{dk}{dt} = F_x^{ext}$$

- **Kinematics: acceleration as derivative of group velocity**

$$a_x = \frac{dv_g}{dt} = \frac{d}{dt}\left(\frac{1}{\hbar}\frac{dE}{dk}\right) = \frac{1}{\hbar}\frac{d}{dk}\left(\frac{dE}{dk}\right)\frac{dk}{dt} = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}\hbar\frac{dk}{dt} = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}F_x^{ext}$$

$$\Rightarrow m^* = \frac{F_x^{ext}}{a_x} = \hbar^2 \Big/ \left(\frac{d^2E}{dk^2}\right)$$

"effective mass"

Semi-classical equation of motion

- **Summary: we should remember, for an electron in a crystal interacting also with an external field:**

Semi-classical equation of motion: time-evolution of *k*

$$\hbar \dot{k}_x \equiv \hbar \frac{dk_x}{dt} = F_x^{ext}$$

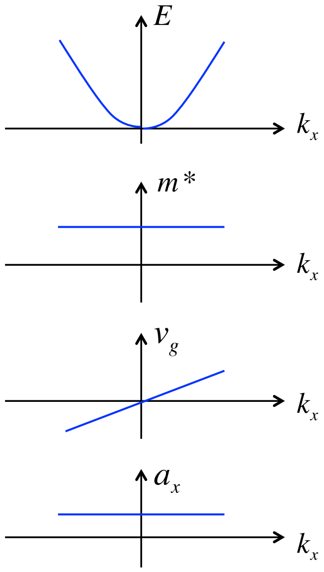
$$m^* = \hbar^2 \Big/ \left(\frac{d^2 E}{dk^2} \right)$$

similar to $\dfrac{dp_x}{dt} = F_x^{ext}$

Effective mass (may be negative!)

Exercise: application to three different dispersion relations *E(k)*: "free particle", "valence band", "conduction band"

Free electron in uniform electric field



$$E(k) = \frac{\hbar^2 k_x^2}{2m} = \frac{p_x^2}{2m} \qquad k_x = \frac{p_x}{\hbar}$$

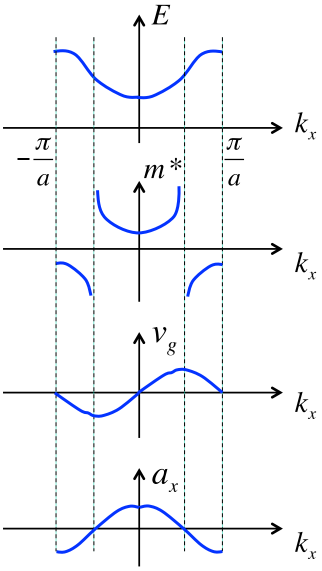
$$m^* = \hbar^2 \Big/ \left(\frac{d^2 E}{dk_x^2} \right) = m = \text{const.}$$

$$v_g = \frac{1}{\hbar}\frac{dE}{dk_x} = \frac{\hbar k_x}{m} = \frac{p_x}{m}$$

$$a_x = \frac{dv_g}{dt} = \frac{\hbar \dot{k}_x}{m} = \frac{F_x^{ext}}{m} = \text{const.}$$

$$\text{if:} \quad F_x^{ext} = -|q_e| E_x = \text{const.}$$

Electron in "conduction band"



$E(k)$

$$m^* = \hbar^2 \Big/ \left(\frac{d^2E}{dk_x^2} \right)$$

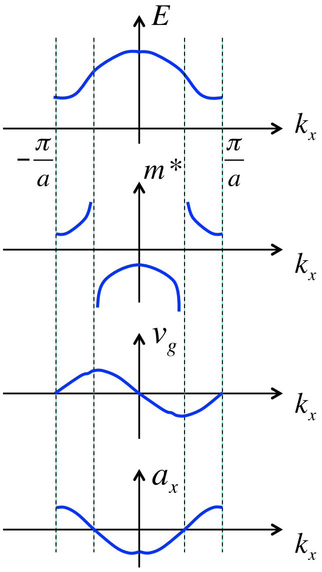
$$v_g = \frac{1}{\hbar}\frac{dE}{dk_x}$$

$$a_x = \frac{dv_g}{dt} = \frac{F_x^{ext}}{m^*}$$

even if: $F_x^{ext} = -|q_e|E_x = \text{const.}$

a_x is NOT constant!

Electron in "valence band"



$E(k)$

$$m^* = \hbar^2 \Big/ \left(\frac{d^2E}{dk_x^2} \right)$$

$$v_g = \frac{1}{\hbar}\frac{dE}{dk_x}$$

$$a_x = \frac{dv_g}{dt} = \frac{F_x^{ext}}{m^*}$$

even if: $F_x^{ext} = -|q_e|E_x = \text{const.}$

a_x is NOT constant!

Consequences

- "Bottom" of conduction band
  - Positive effective mass
  - Acceleration: follows the external force, as usual
  - The electron energy increases
- "Top" of valence band
  - *Negative* effective mass!
  - Acceleration *contrary* to the external force!
  - The electron energy *decreases*!
  - Who takes the energy? The crystal…
- "Bloch oscillations" in a band in an ideal crystal
  - Experimentally observed in a periodic "potential"

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