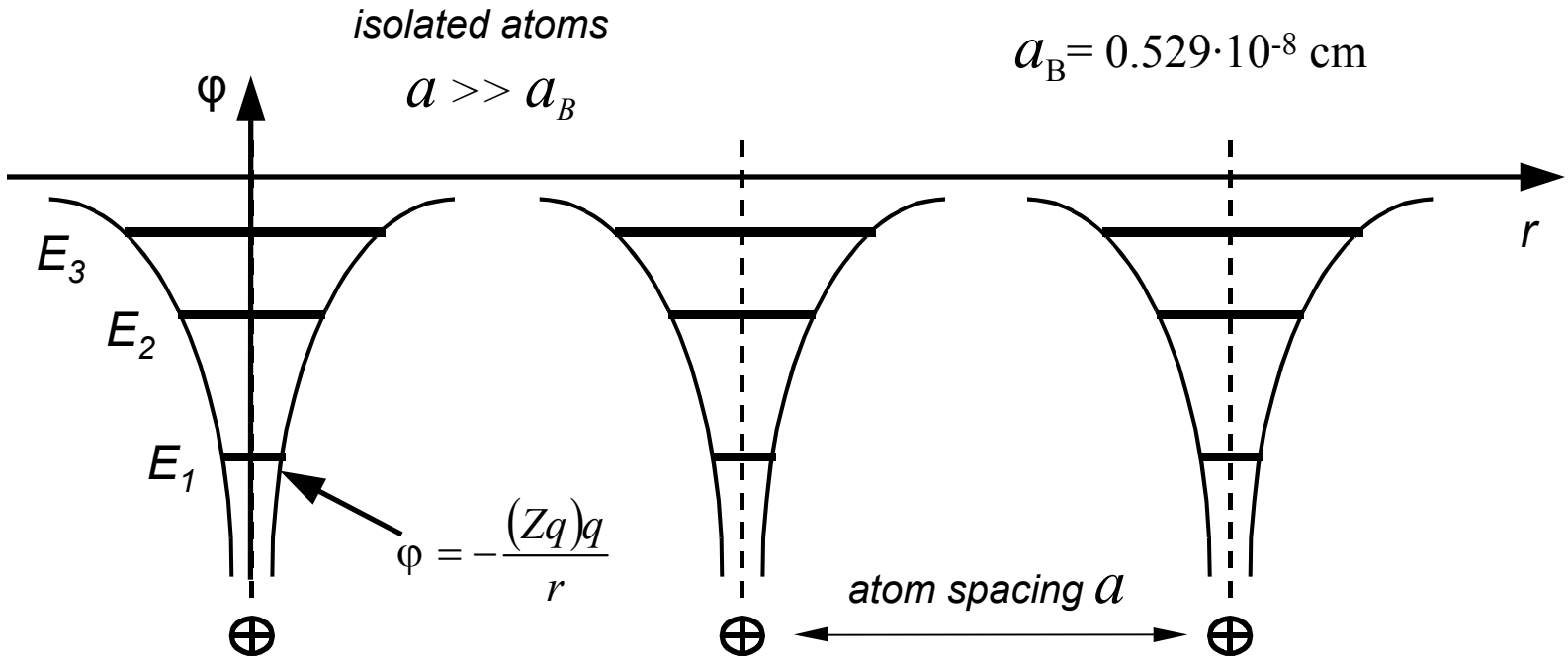
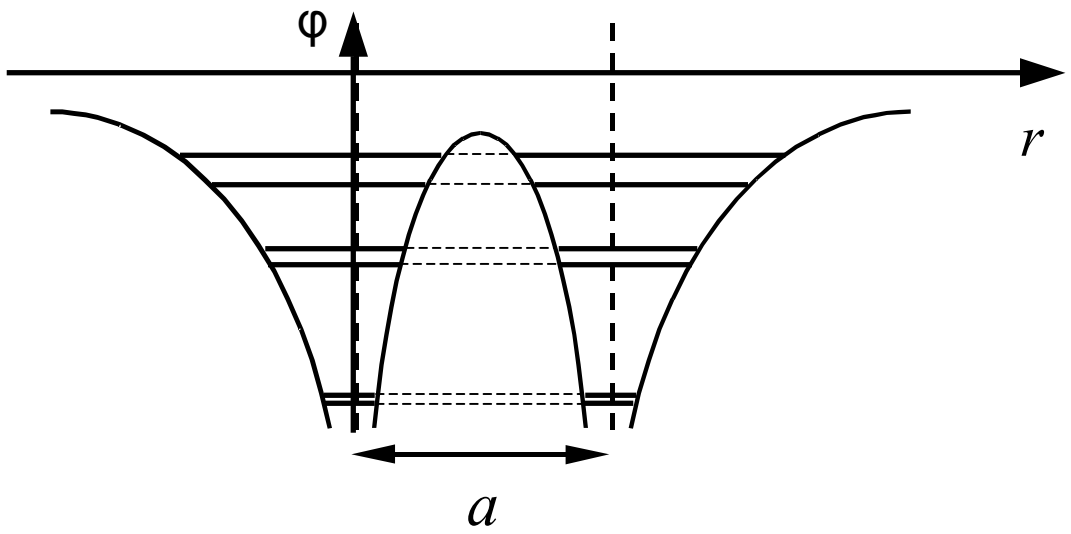
Free carriers in materials

Metals	$n \sim 10^{22}$ cm^{-3}
Semiconductors	$n \sim 10^{8}...10^{19}$ cm^{-3}
Insulators	$n < 10^{8}$ cm^{-3}

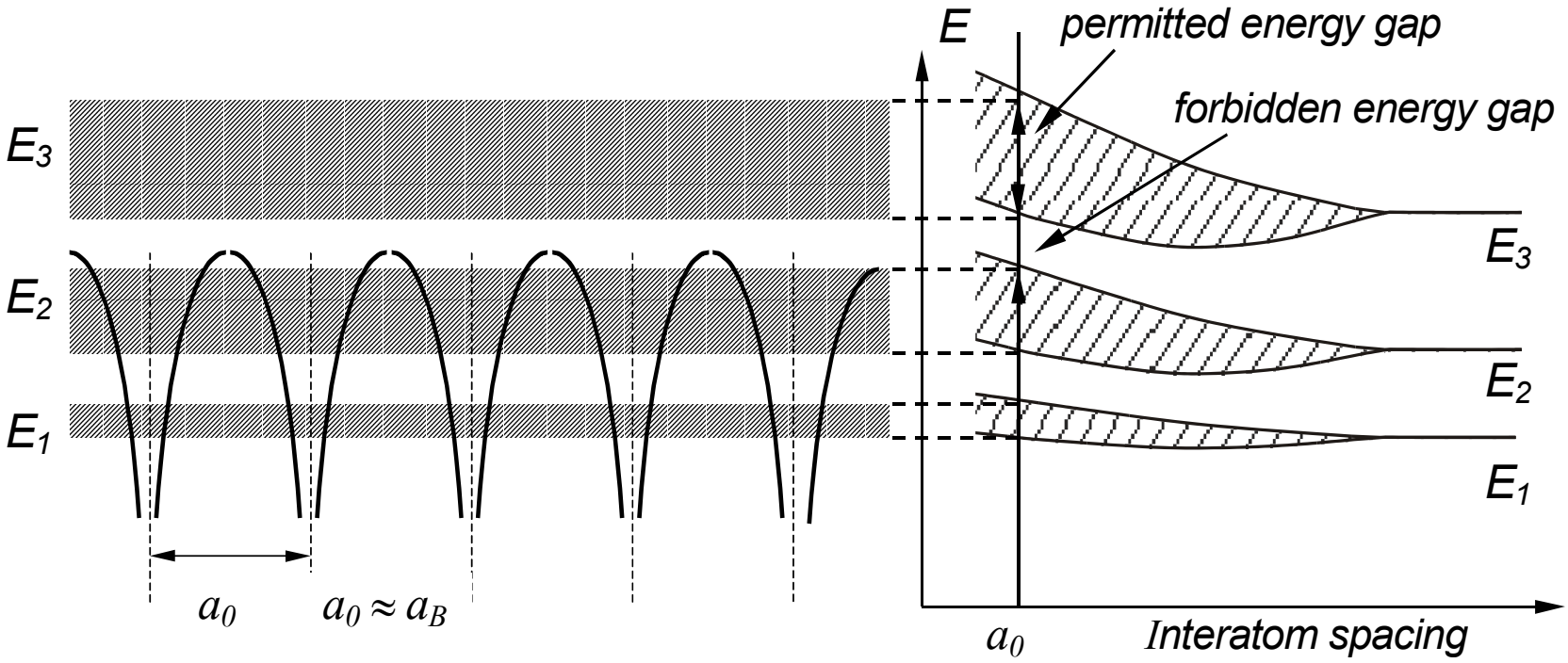


"Two atoms – two levels"



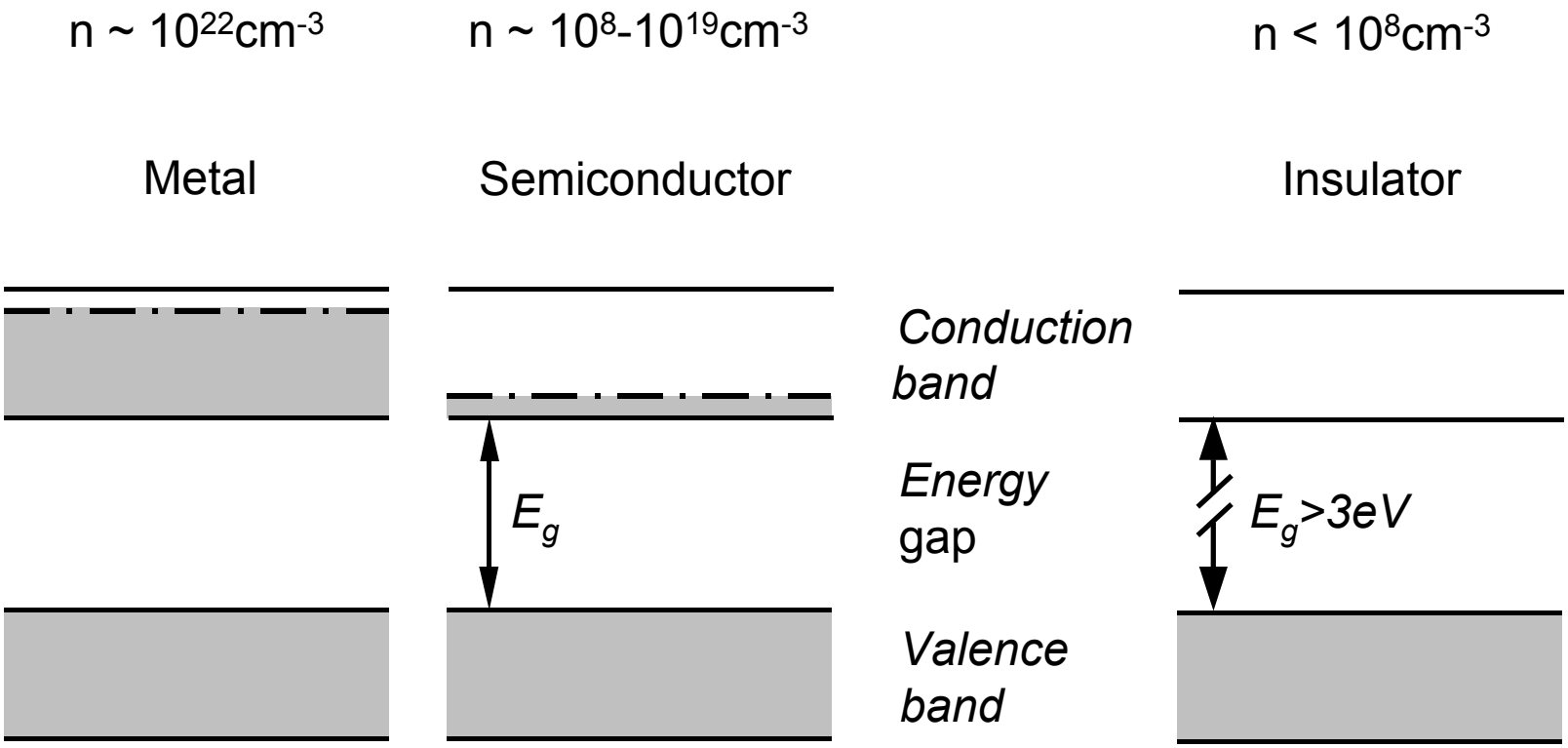
The splitting of every level on two levels due to interaction of atoms. The interaction is tunneling of electrons through potential barrier. The tunneling becomes considerable when $a \approx a_B$

"N atoms – N levels"



Every level is split on N levels. Every electron in permitted energy band belong to all atoms.

Metals, Semiconductors, Insulators



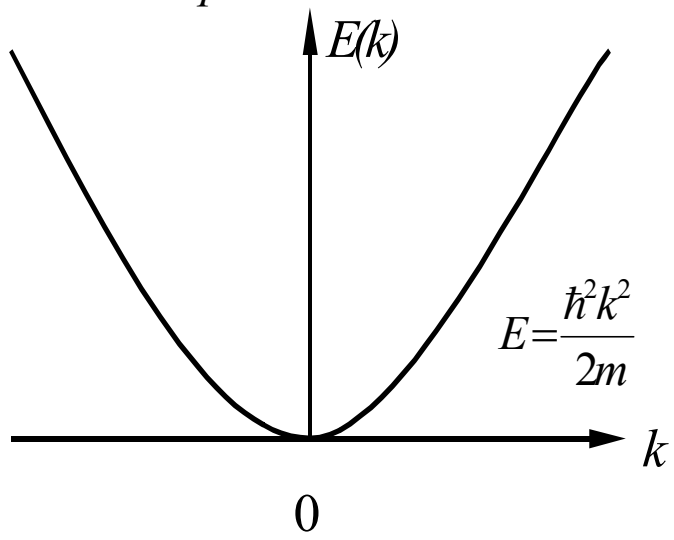
Dispersion law for free electron in vacuum

$$E = \frac{p^2}{2m}$$

**de Broil 1925* : $p = m\mathrm{v}$ $\lambda = \frac{2\pi\hbar}{m\mathrm{v}} = \frac{2\pi\hbar}{p}$ $p = \hbar\frac{2\pi}{\lambda} = \hbar k$

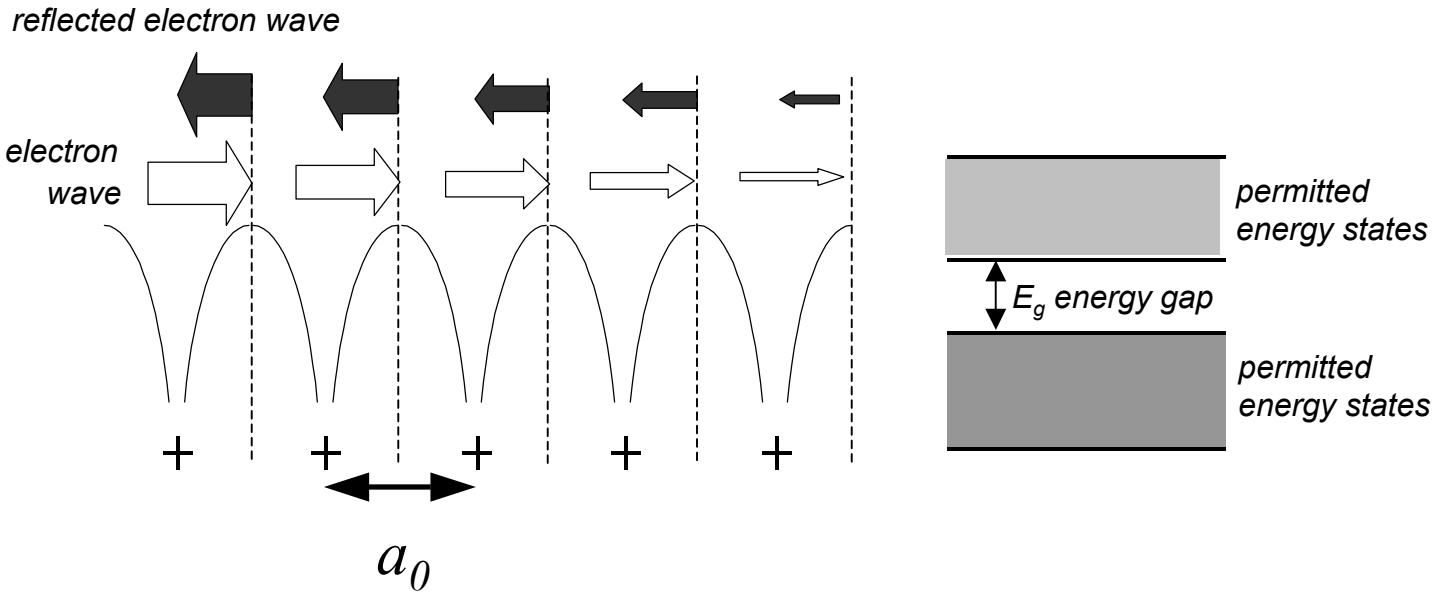
$k = \frac{2\pi}{\lambda}$ electron wave vector
like one for light wave

$$E = \frac{\hbar^2 k^2}{2m}$$



According to wave-particle dualism concept the electron possess simultaneously both particle and wave properties and can be characterized by wavelength λ, wave vector ***k*** and impulse ***p***

Electron in semiconductor



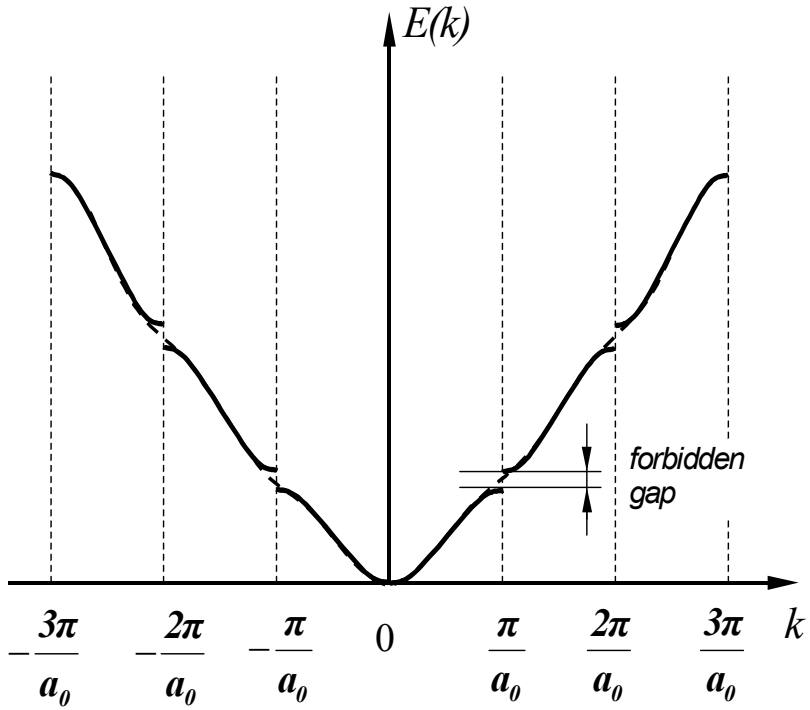
As soon as electron possess both particle and wave properties it can be reflected and diffracted exactly like light wave. In a periodic lattice with period a_0, electron wave with wavelength satisfying Bragg condition ($m\lambda=2a_0$, m-integer) can not propagate due to strong reflection from the energy barrier, i.e. electron with the energy in certain interval (energy gap) can not freely move in crystal.

Electron in semiconductor

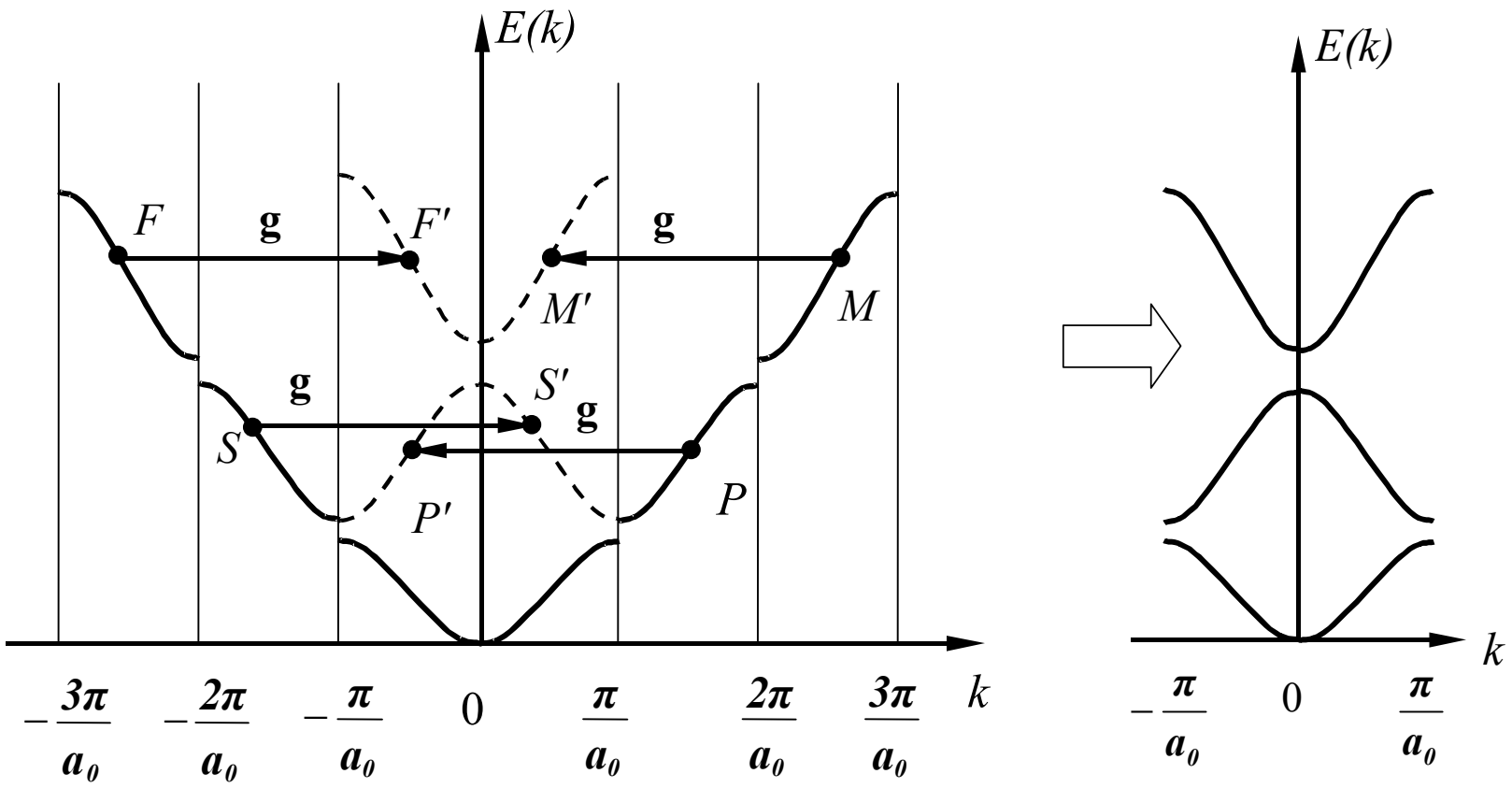
Condition of strong reflection of electron wave

$$\frac{2a_0}{\lambda} = \mathrm{m}, \qquad \mathrm{m} = 1, 2, 3... \qquad \mathrm{k} = \frac{2\pi}{\lambda} = \frac{\pi}{a_0}\mathrm{m}$$

Forbidden band gaps have to exist at definite wavevectors of electron.

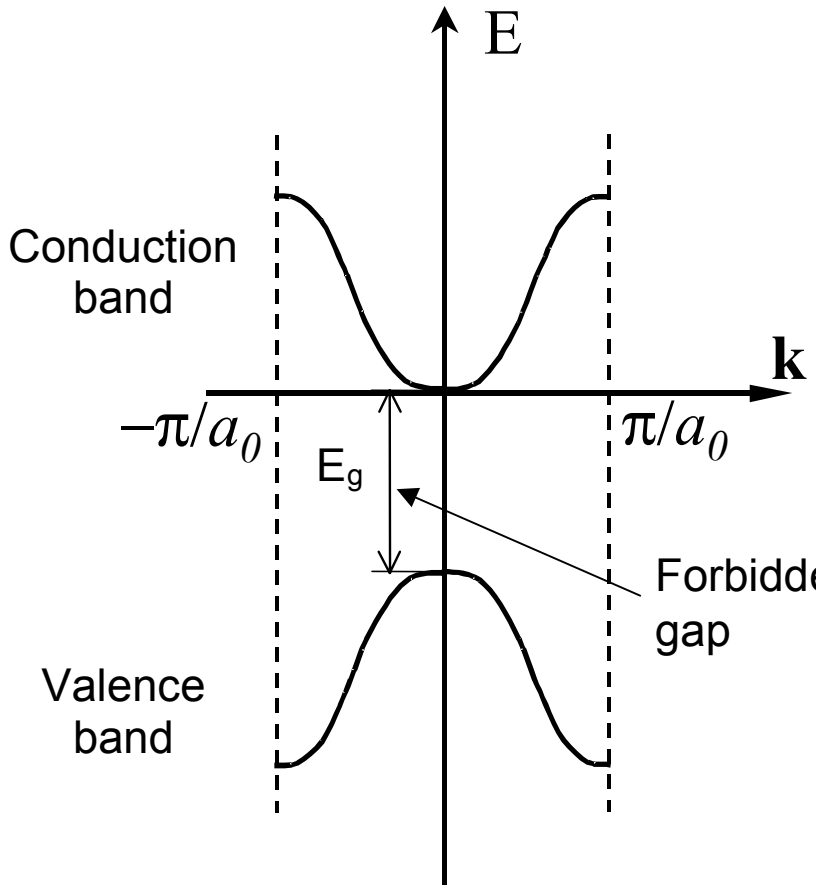


Brillouin zones



The wavefunctions and electron states are equivalent for $\mathbf{k}$ and $\mathbf{k} \pm m\mathbf{g}$ ($\mathbf{g}=2\pi/a_0$, m-integer): the states *M* and *M′* ; *P* and *P′* , *S* and *S′*, *F* and *F′* are equivalent. It is not necessary to use values of $|\mathbf{k}|$ larger than π/a in describing any states. This means, it is enough to plot the electron energy $E(\mathbf{k})$ vs $\mathbf{k}$ only within first Brillouin zone.

The effective mass of electron



For $k << \pi/a_0$

$$E(\vec{k}) = E_0 + \left.\frac{\partial E}{\partial \vec{k}}\right|_{k=0} \cdot \vec{k} + \frac{1}{2} \cdot \left.\frac{\partial^2 E}{\partial k^2}\right|_{k=0} \cdot k^2$$

$$E(\vec{k}) = E(-\vec{k}), \quad \left.\frac{\partial E}{\partial \vec{k}}\right|_{k=0} = 0$$

$$E(\vec{k}) = E_0 + \frac{1}{2} \cdot \frac{\partial^2 E}{\partial k^2} \cdot k^2$$

Let's make E_0 an origin in new coordinates: $E(\vec{k}) = \frac{1}{2} \cdot \left.\frac{\partial^2 E}{\partial k^2}\right|_{k=0} \cdot k^2$

Free electron: $E = \frac{\hbar^2 k^2}{2m}$

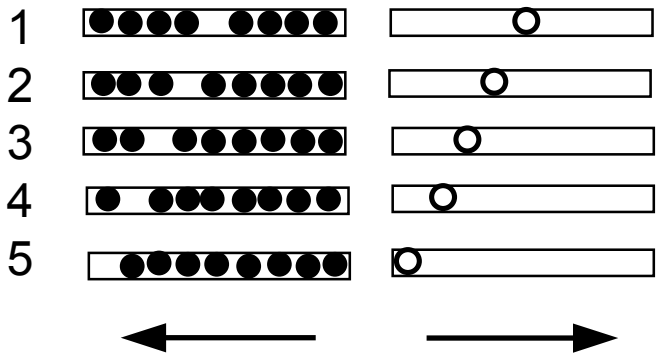
Electron in crystal:

for conduction band

$$E = \frac{\hbar^2 k^2}{2m_e^*} \qquad m_e^* = \left(\frac{1}{\hbar^2} \cdot \frac{\partial^2 E}{\partial k^2}\right)^{-1}$$

Holes in semiconductors

Hole concept
Real space

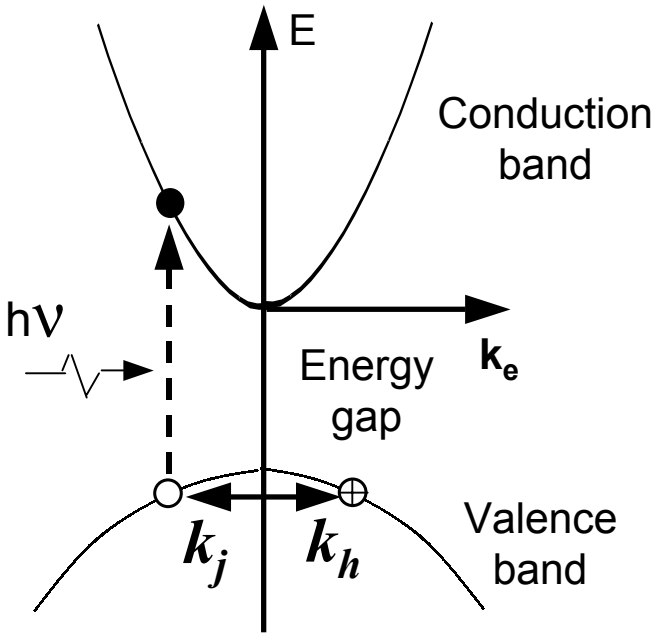


● negative electron
○ positive hole

Hole in k-space

The collective motion of negative electrons in k-space in valence band is equal to movement of few positively charge holes.

Holes in semiconductor



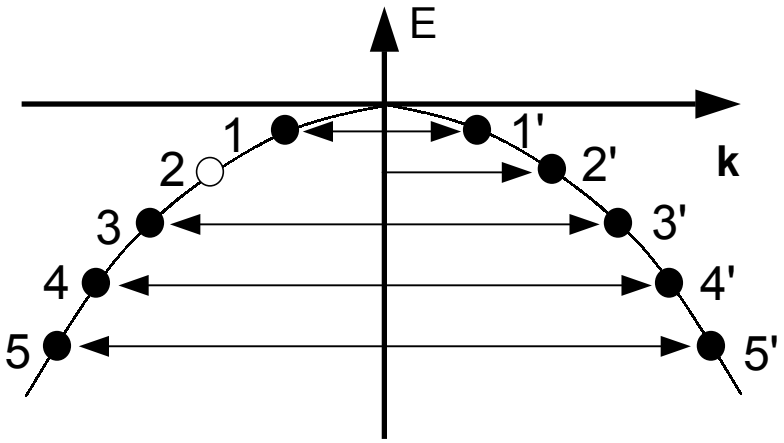
When valence band is filled by electrons

$$\sum_{i=1}^{N} \boldsymbol{k}_i = 0 \qquad (current = 0)$$

If one electron with $\boldsymbol{k}_j$ is removed, the remaining N-1 electrons are equivalent to the one positively charged particle with quasimomentum:

$$\boldsymbol{k}_h = \sum_{i=1, i\neq j}^{N} \boldsymbol{k}_i + (\boldsymbol{k}_j - \boldsymbol{k}_j) = \sum_{i=1}^{N} \boldsymbol{k}_i - \boldsymbol{k}_j = -\boldsymbol{k}_j$$

Holes in semiconductor



For N electrons (fully filled valence band) the current is zero. For N-1 there is one electron 2' which can contribute to the current density j.

$$j = -q \cdot \upsilon_{e2'}, \quad \upsilon_{e2'} = \frac{1}{\hbar} \cdot \left.\frac{\partial E}{\partial k}\right|_{k=k_{e2'}}$$

For electrons in conduction band with parabolic dispersion

$$E = \frac{\hbar^2 k^2}{2m_e^*}, \quad \upsilon_e = \frac{1}{\hbar} \cdot \frac{\partial E}{\partial k} = \frac{\hbar k}{m_e^*} = \frac{p}{m_e^*}$$

For electrons in valence band with parabolic dispersion

$$E = E_0 - \frac{\hbar^2 k^2}{2m_{eVB}^*}$$

Start from E_0: $\quad E = \dfrac{\hbar^2 k^2}{2(-m_{eVB}^*)}, \quad \upsilon_e = \dfrac{\hbar k_{e2'}}{-m_{eVB}^*} < 0$

The current of N-1 electrons in valence band

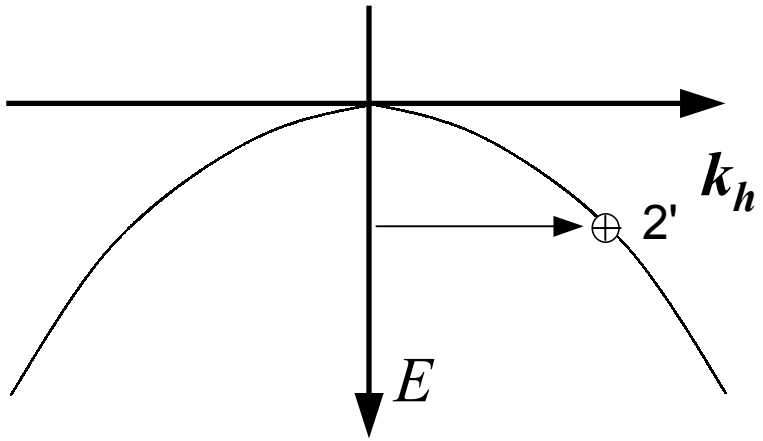
$$j = -q \cdot \frac{\hbar k_{e2'}}{-m_{eVB}^*}$$

Electron effective mass in valence band (VB) is negative ($-m_{eVB}^*$), i.e. electron energy decreases with quasimomentum ($\hbar k$) increase.

Holes in semiconductor

It is more convenient to reduce motion of the electrons with negative effective mass to motion of the quasiparticles with positive effective mass

$m_h^* = -m_{eVB}^* > 0$ and positive charge.

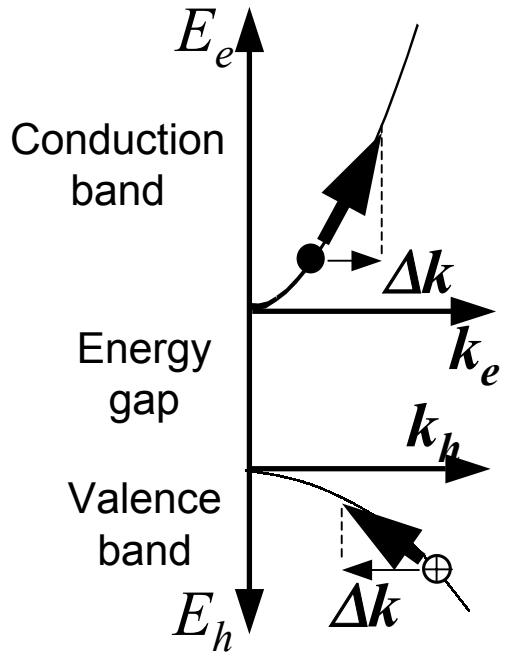


Current is equal to $j = +q \cdot \frac{\hbar k_{h2'}}{m_h^*}$

This current is equal to the one produced by N-1 electrons ($k_{h2'} = k_{e2'}$, $m_h^* = -m_{eVB}^*$)

When m electrons are exited from valence band to impurity levels or conduction band the rest of N-m electrons behave as m holes

Electrons and Holes



$\rightarrow$ $\boldsymbol{F = -qE}$ for electrons

$$E_e = \frac{p^2}{2m_e^*} = \frac{\hbar^2 k^2}{2m_e^*}$$

$\leftarrow$ E $\quad \Delta k = \frac{1}{\hbar} \cdot F \cdot \Delta t$

$\leftarrow$ $\boldsymbol{F = +qE}$ for holes

$$E_h = \frac{p^2}{2m_e^*} = \frac{\hbar^2 k^2}{2m_h^*}$$

Semiconductor	m_e^*	m_h^*
GaAs	0.063 m	0.52 m
InAs	0.023 m	0.41 m
InP	0.077 m	0.85 m