Physics of Condensed Matter I

1100-4INZ`PC

"THAT, IN ITSELF, IS A BREAKTHROUGH."

Faculty of Physics UW
Jacek.Szczytko@fuw.edu.pl

Solid state 5

inżynieria nanostruktur

Periodic potential

Bloch theorem

Przykład:

Electron motion in a periodic potential.

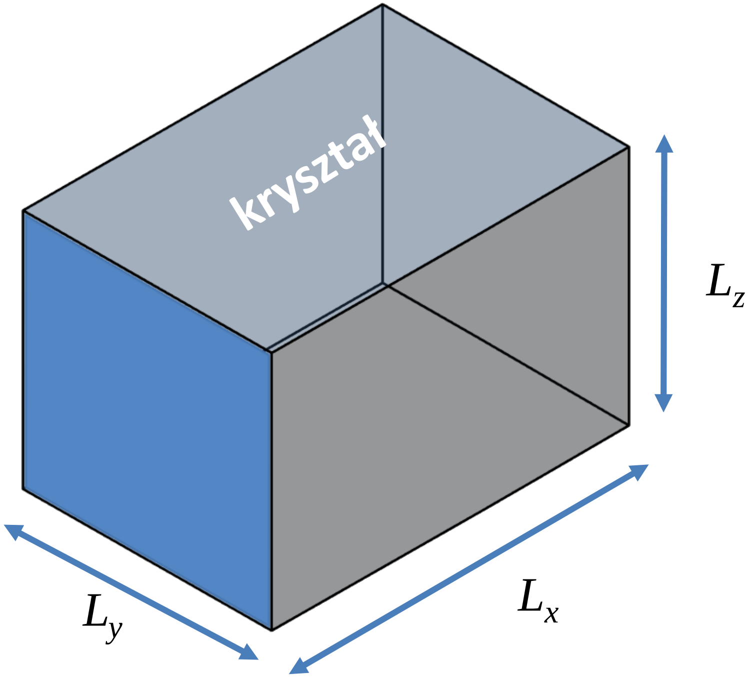
$$V(\vec{r}) = \sum_{\vec{G}} V_{\vec{G}} \exp\left(i\vec{G}\vec{r}\right)$$

The solution is:

$$\psi_{n,\vec{k}}(\vec{r}) = u_{n,\vec{k}}(\vec{r})\, e^{i\vec{k}\vec{r}}$$

Thus (see: Ibach, Luth *Solid-State Physics*):

$$u_{n,\vec{k}}(\vec{r}) = \sum_{\vec{G}} C_{\vec{k}-\vec{G}} e^{i\vec{G}\vec{r}}$$



If our crystal has a finite size set of vectors k is finite (though enormous!). for instance, we can assume periodic boundary conditions and then:

$$\vec{k}_i = 0, \pm\frac{2\pi}{L_i}, \pm\frac{4\pi}{L_i}, \pm\frac{6\pi}{L_i}, \dots, \pm\frac{2\pi n_i}{L_i}$$

Density of states

Density of states Number of states per unit energy $\rho^{nD}(E)$ depends on the dimension

If our crystal has a finite size the set of k –vectors is finite (though enormous!).
For example: we can assume periodic boundary conditions and then:

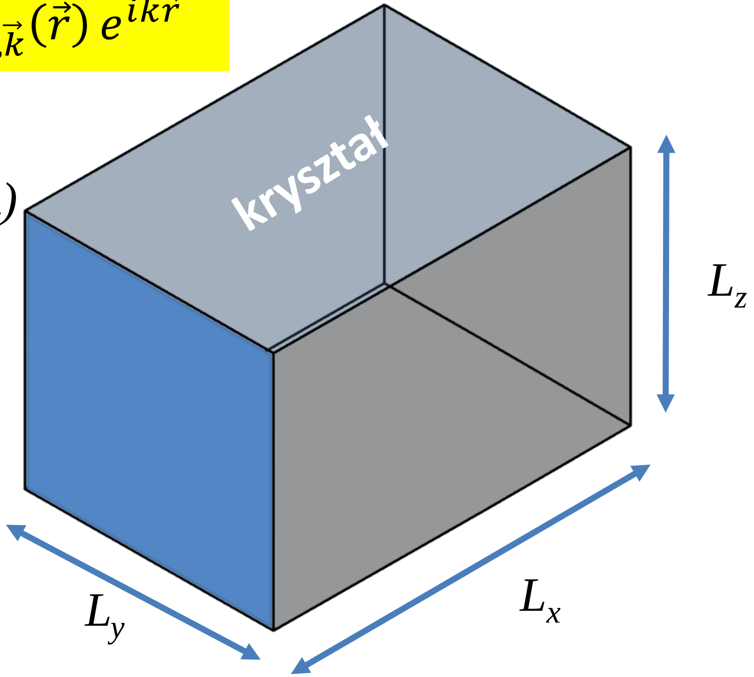
Born- von Karman boundary conditions

$$\psi_{n,\vec{k}}(\vec{r}) = u_{n,\vec{k}}(\vec{r})\, e^{i\vec{k}\vec{r}}$$

Finite size of the crystal L_x, L_y, L_z

$\psi_{n,\vec{k}}$ – the Bloch function

$$\psi_{n,\vec{k}}(x + L_x, y, z) = \psi_{n,\vec{k}}(x, y + L_y, z) = \psi_{n,\vec{k}}(x, y, z + L_z)$$



$$e^{ik_xL_x} = 1$$
$$e^{ik_yL_y} = 1$$
$$e^{ik_zL_z} = 1$$

$$\vec{k}_i = 0, \pm\frac{2\pi}{L_i}, \pm\frac{4\pi}{L_i}, \dots, \pm\frac{2\pi n_i}{L_i}$$

Number of states in the volume V $= \dfrac{2}{\frac{2\pi}{L_x}\times\frac{2\pi}{L_y}\times\frac{2\pi}{L_z}} = \dfrac{2V}{(2\pi)^3}$

Density of states

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If our crystal has a finite size the set of k −vectors is finite (though enormous!).
For example: we can assume periodic boundary conditions and then:

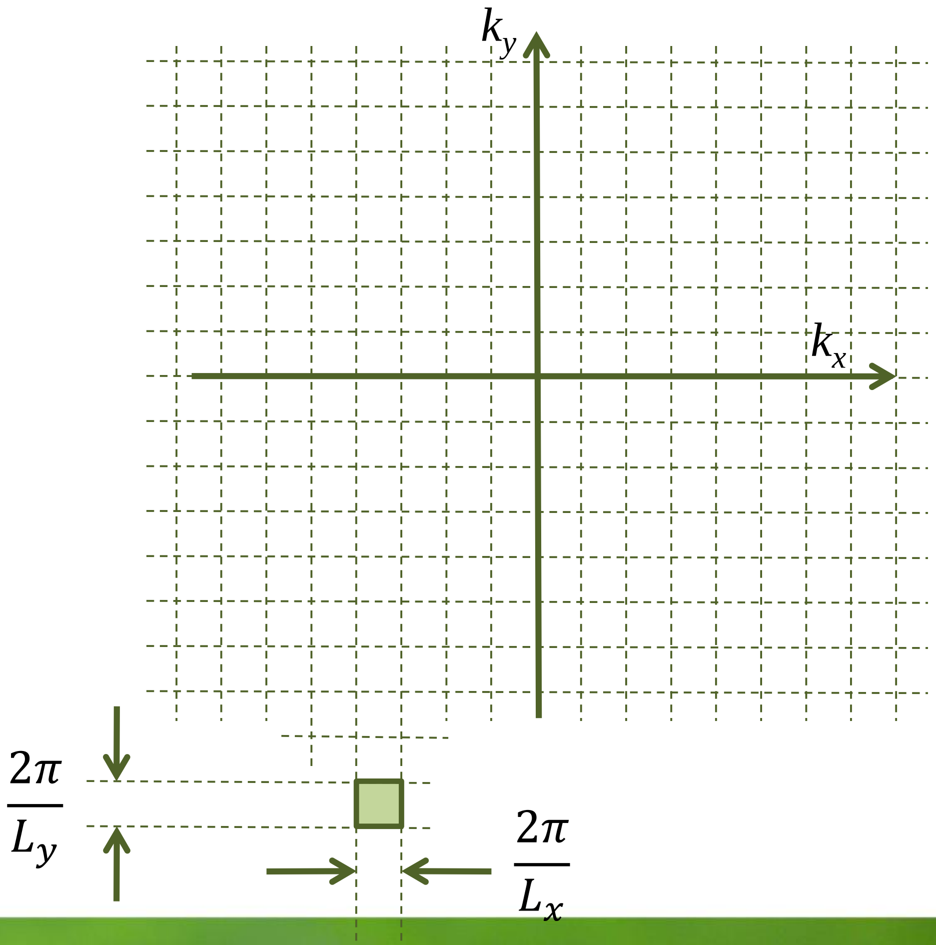
The density of states in k-space of n dimension (and the unite volume)

Case 3D: $$\rho_k^{nD} = 2\left(\frac{1}{2\pi}\right)^{3}$$

Case 2D: $$\rho_k^{nD} = 2\left(\frac{1}{2\pi}\right)^{2}$$

Case 1D: $$\rho_k^{nD} = 2\left(\frac{1}{2\pi}\right)^{1}$$

Number of states in the volume V $$= \frac{2}{\frac{2\pi}{L_x}\times\frac{2\pi}{L_y}\times\frac{2\pi}{L_z}} = \frac{2V}{(2\pi)^3}$$



Properties of Bloch function

Bloch theorem

Bloch functions whose wave vectors differ by a reciprocal lattice vector, are the same!

$$\psi_{n,\vec{k}+\vec{G}}(\vec{r}) = \psi_{n,\vec{k}}(\vec{r}) \qquad \vec{G} = h\vec{g}_1 + k\vec{g}_2 + l\vec{g}_3$$

Proof:

$$\psi_{n,\vec{k}+\vec{G}}(\vec{r}) = u_{n,\vec{k}+\vec{G}}(\vec{r})\, e^{i(\vec{k}+\vec{G})\vec{r}} = \sum_{\vec{G}\prime} C\left(\vec{k}+\vec{G}-\vec{G}'\right) e^{-i\vec{G}'\vec{r}}\ e^{i(\vec{k}+\vec{G})\vec{r}} = \cdots$$

$$= \sum_{\vec{G}\prime\prime} C\left(\vec{k}-\vec{G}''\right) e^{-i\vec{G}''\vec{r}}\ e^{i(\vec{k})\vec{r}} = \psi_{n,\vec{k}}(\vec{r})$$

What about energies?

$$\left(\frac{\vec{p}^2}{2m_0} + V(\vec{r})\right)\psi_{n,\vec{k}}(\vec{r}) = E\left(n,\vec{k}\right)\ \psi_{n,\vec{k}}(\vec{r})$$

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$$\Rightarrow E(n,\vec{k}) = E(n,\vec{k}+\vec{G})$$

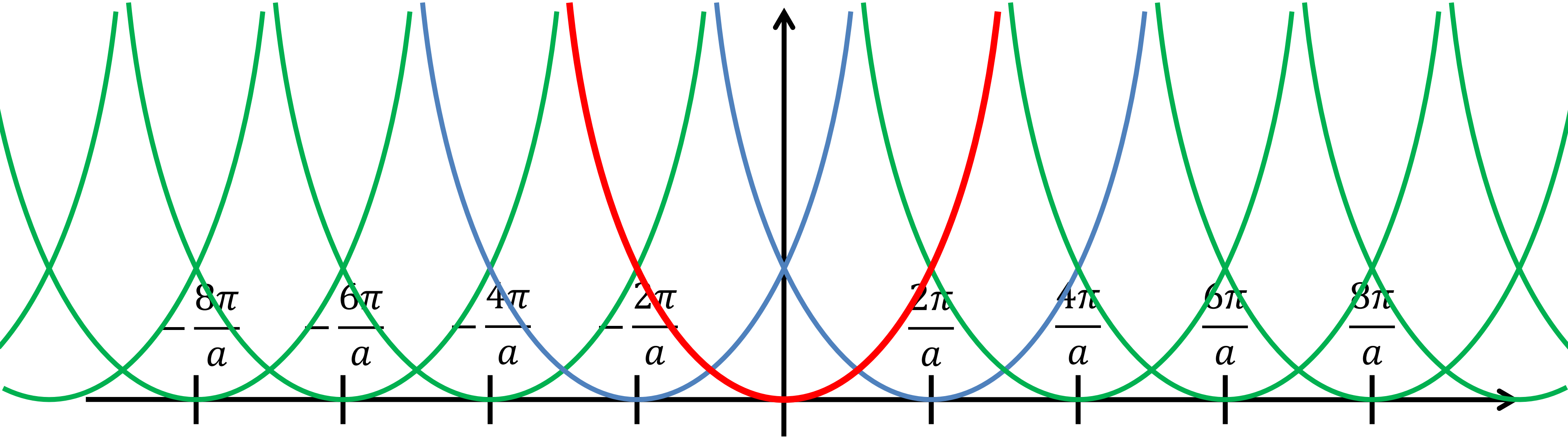
Energy eigenvalues are a periodic function of $\vec{k}$ (wave vectors of Bloch function).

Properties of Bloch function

The nearly free-electron approximation

Energy of the plane wave in empty space as the function of wave vector:

$$E\left(n,\vec{k}\right)=\frac{\hbar^2\vec{k}^2}{2m}=E\left(n,\vec{k}+\vec{G}\right)=\frac{\hbar^2\left(\vec{k}+\vec{G}\right)^2}{2m}$$



Periodic potential

The nearly free-electron approximation

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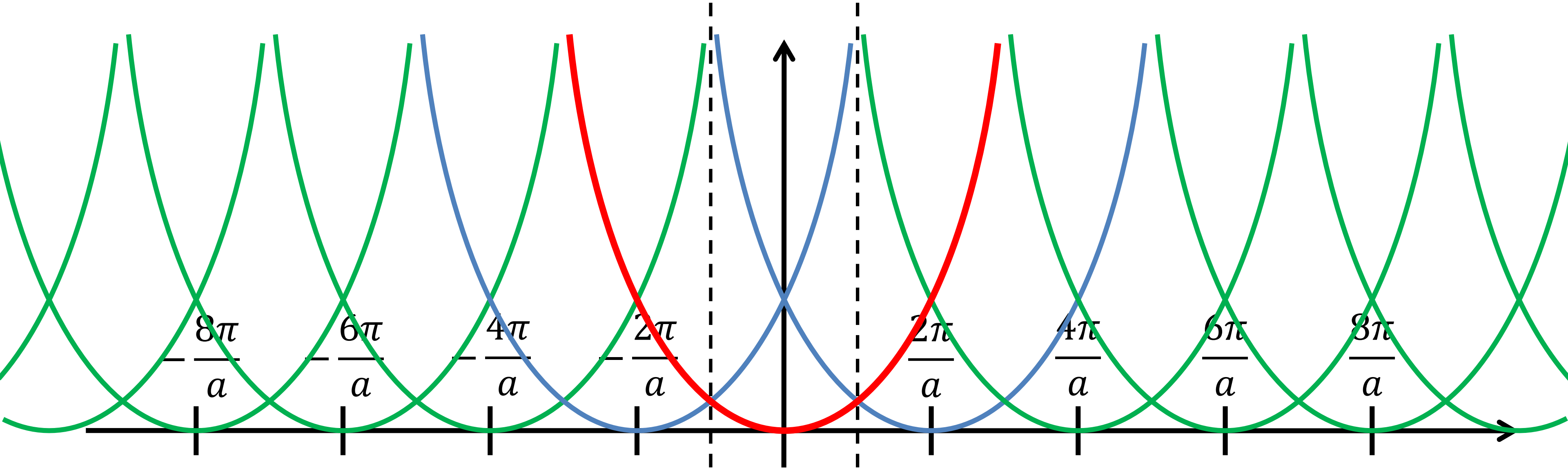

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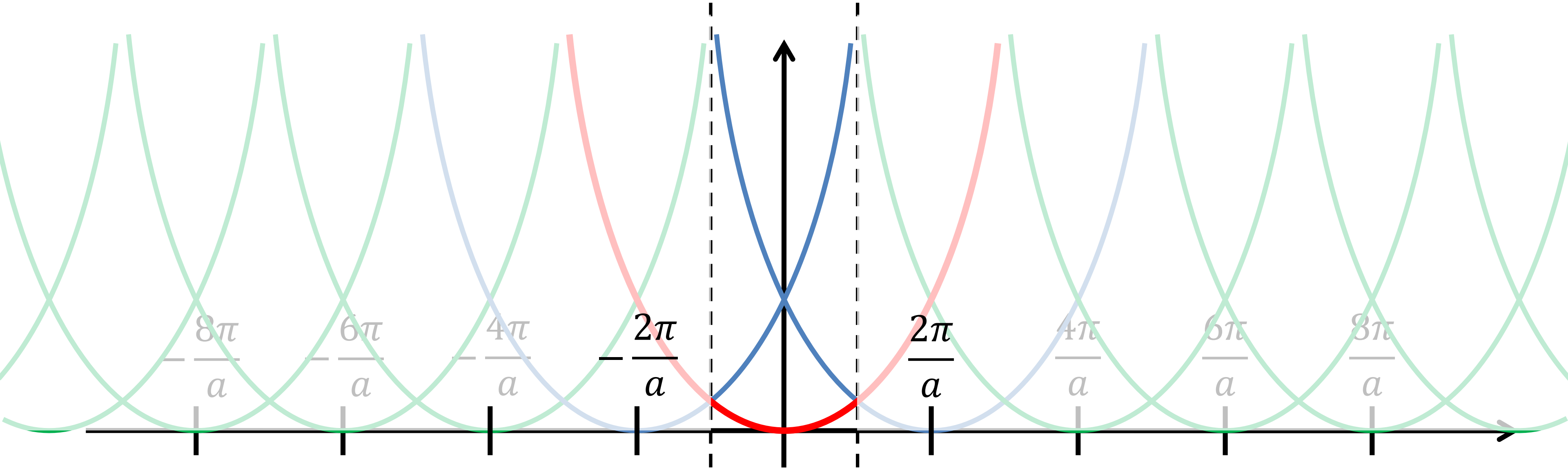

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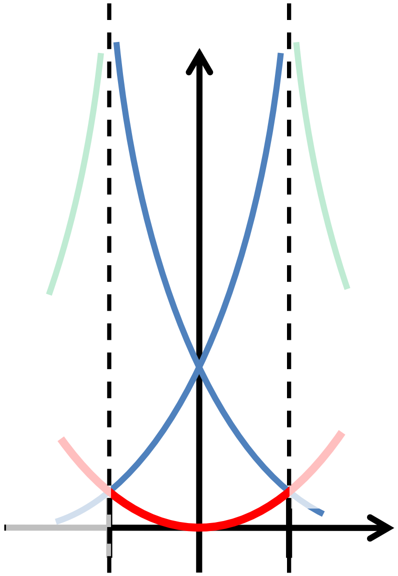
Reduced Brilloin zone.
On the border of the Brillouin zone energies are degenerated



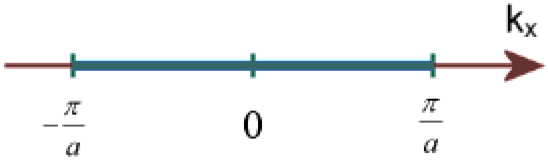
Periodic potential

Brillouin zones

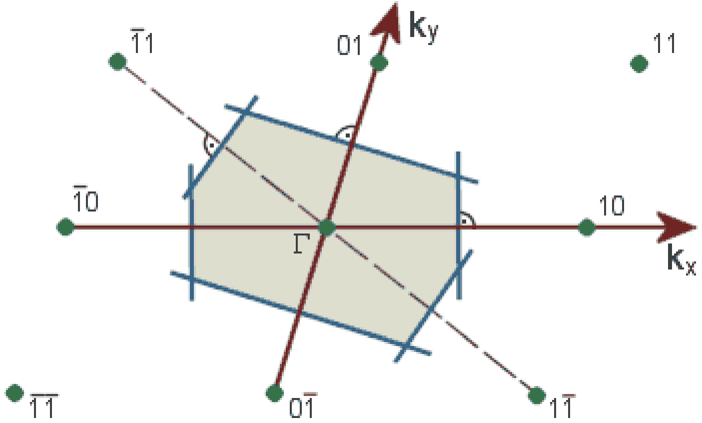
$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3, \qquad n_i \in \mathbb{Z}$$

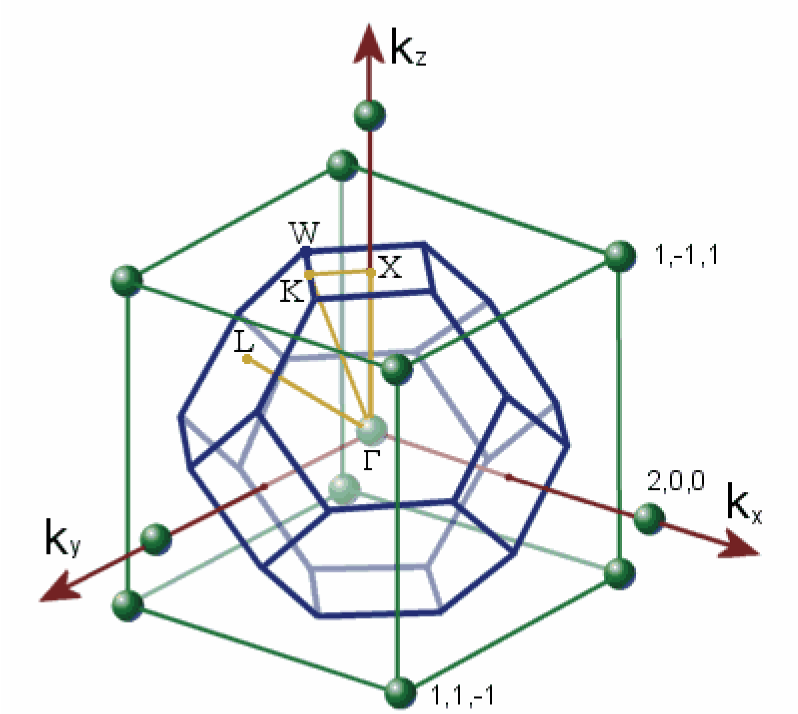
$$\vec{G} = m_1\vec{a}_1^* + m_2\vec{a}_2^* + m_3\vec{a}_3^*, \qquad m_i \in \mathbb{Z}$$

Brillouin zone in 1D



Brillouin zone in 2D, oblique lattice.





Brillouin zone for face centered cubic (fcc) lattice. The limiting zone walls comes from reciprocal lattice points (2,0,0) square and (1,1,1) hexagonal.

http://oen.dydaktyka.agh.edu.pl/dydaktyka/fizyka/c_teoria_pasmowa/2.php

Periodic potential

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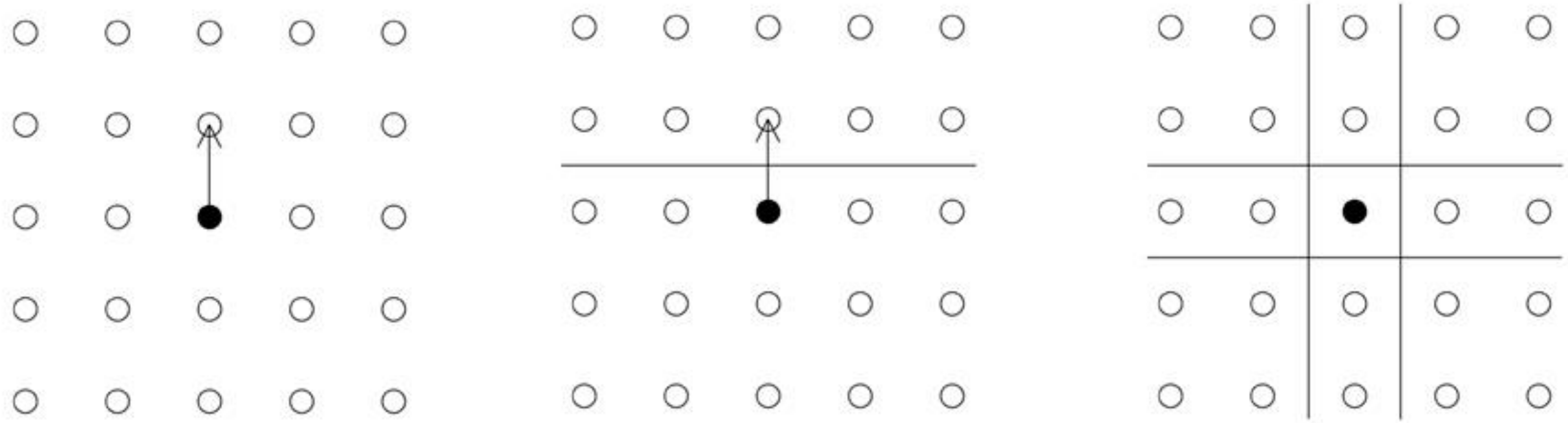
2-D square lattice

$$\vec{a}_i^*\vec{a}_j = 2\pi\delta_{ij}$$



http://www.doitpoms.ac.uk/tlplib/brillouin_zones/zone_construction.php

Periodic potential

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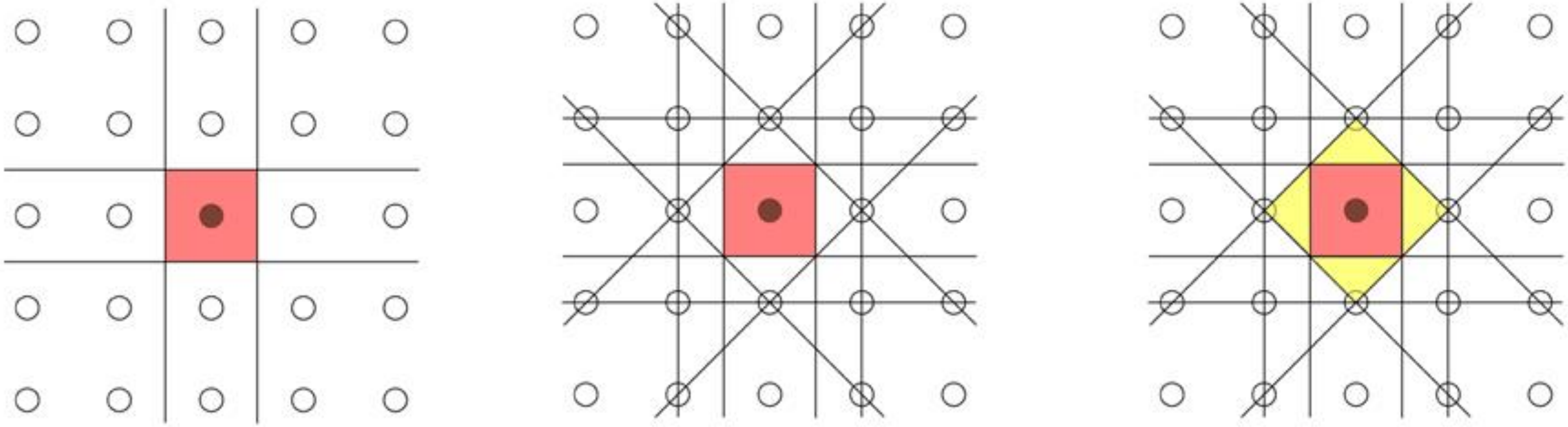

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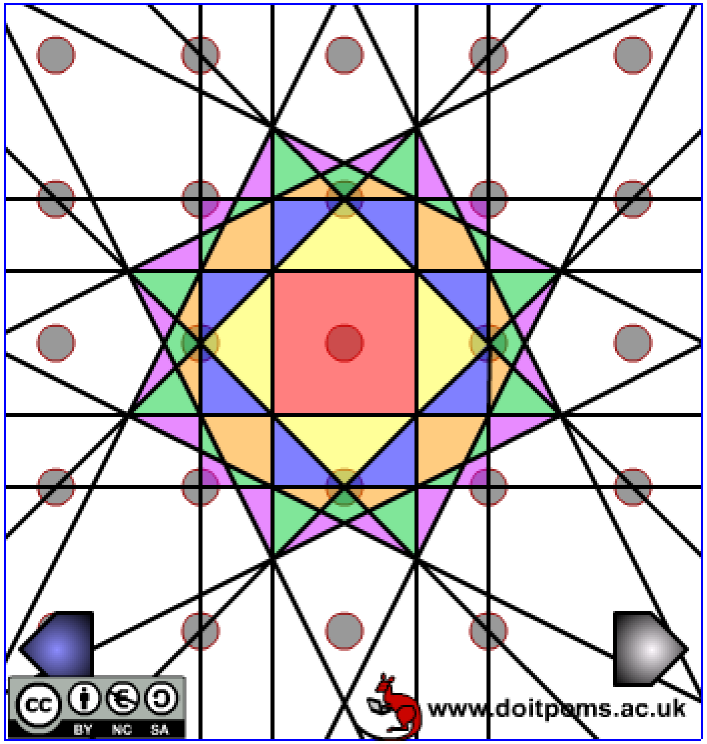

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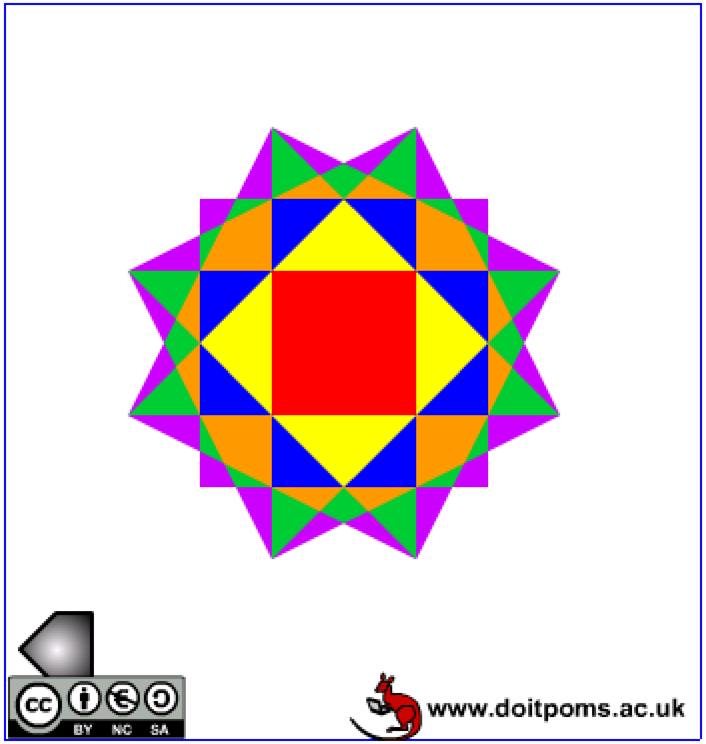

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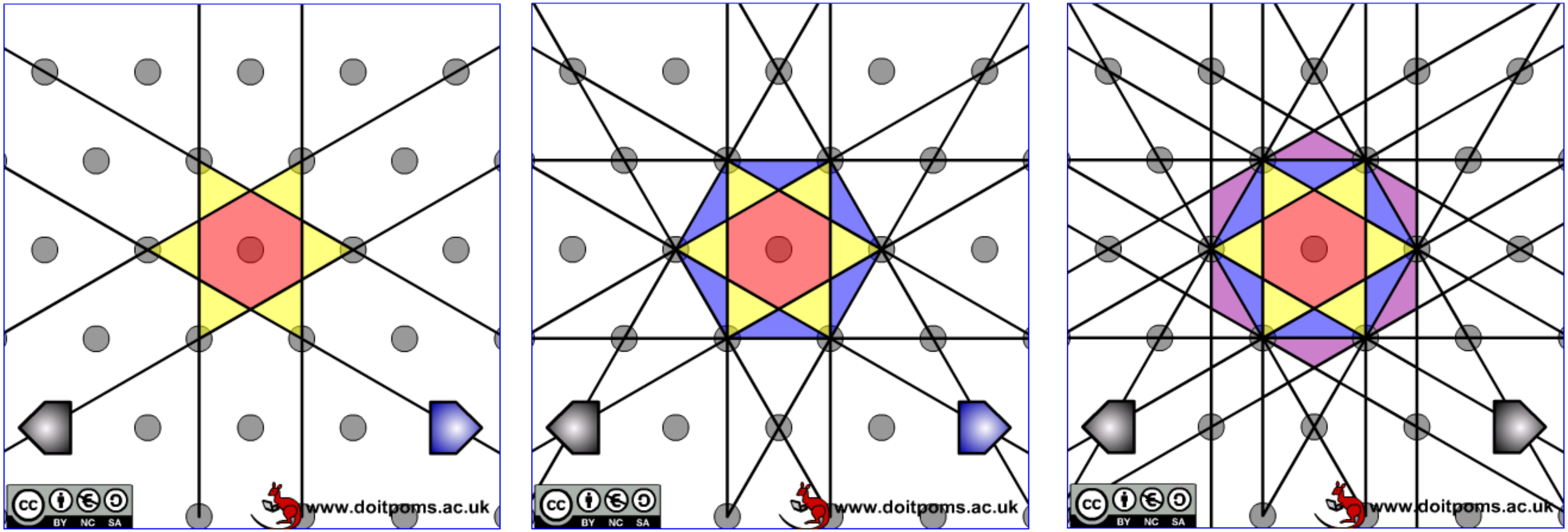
2-D hexagonal lattice

$$\vec{a}_i^*\vec{a}_j = 2\pi\delta_{ij}$$



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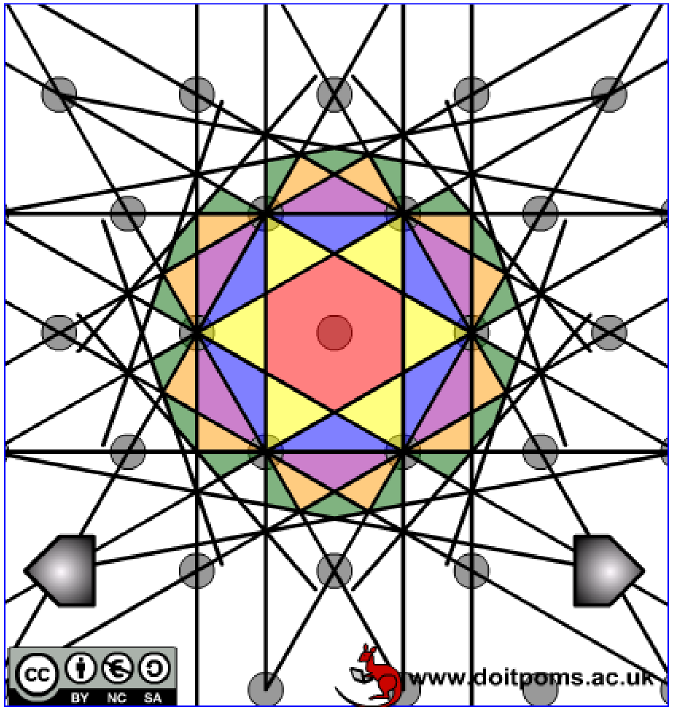

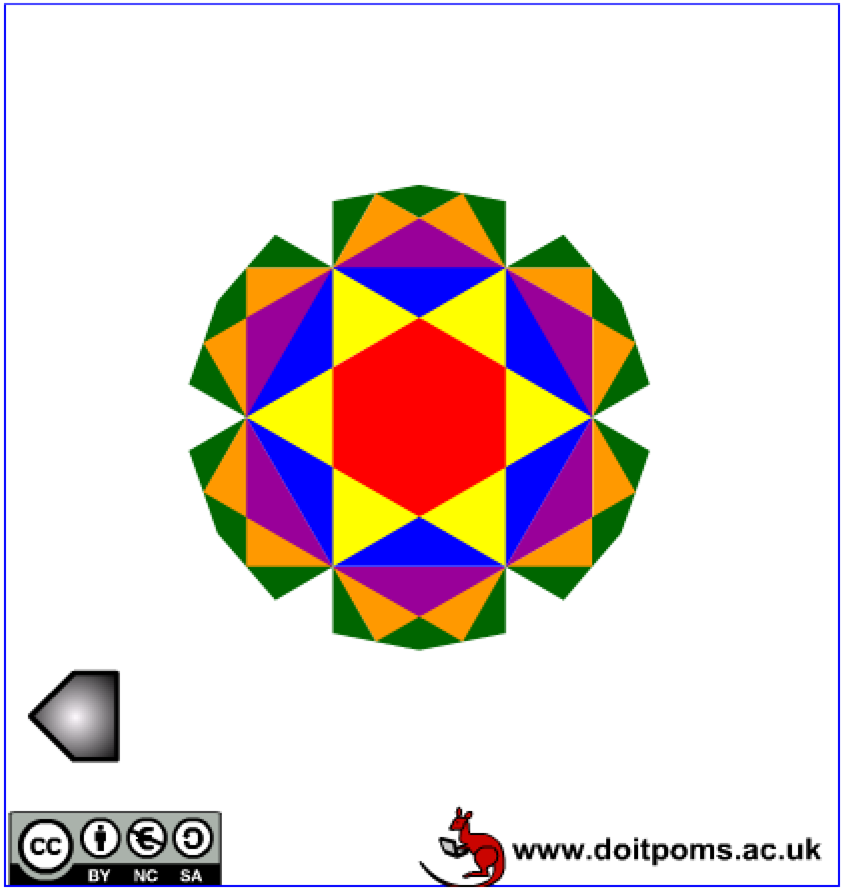

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Periodic potential

The nearly free-electron approximation

$$E(n,\vec{k}) = E(n,\vec{k}+\vec{G}) = \frac{\hbar^2(\vec{k}+\vec{G})^2}{2m}$$

$$\vec{G} = h\vec{g}_1 + k\vec{g}_2 + l\vec{g}_3$$

$$|g_i| = \frac{2\pi}{a_i}$$

The band structure of nearly free-electron cubic lattice

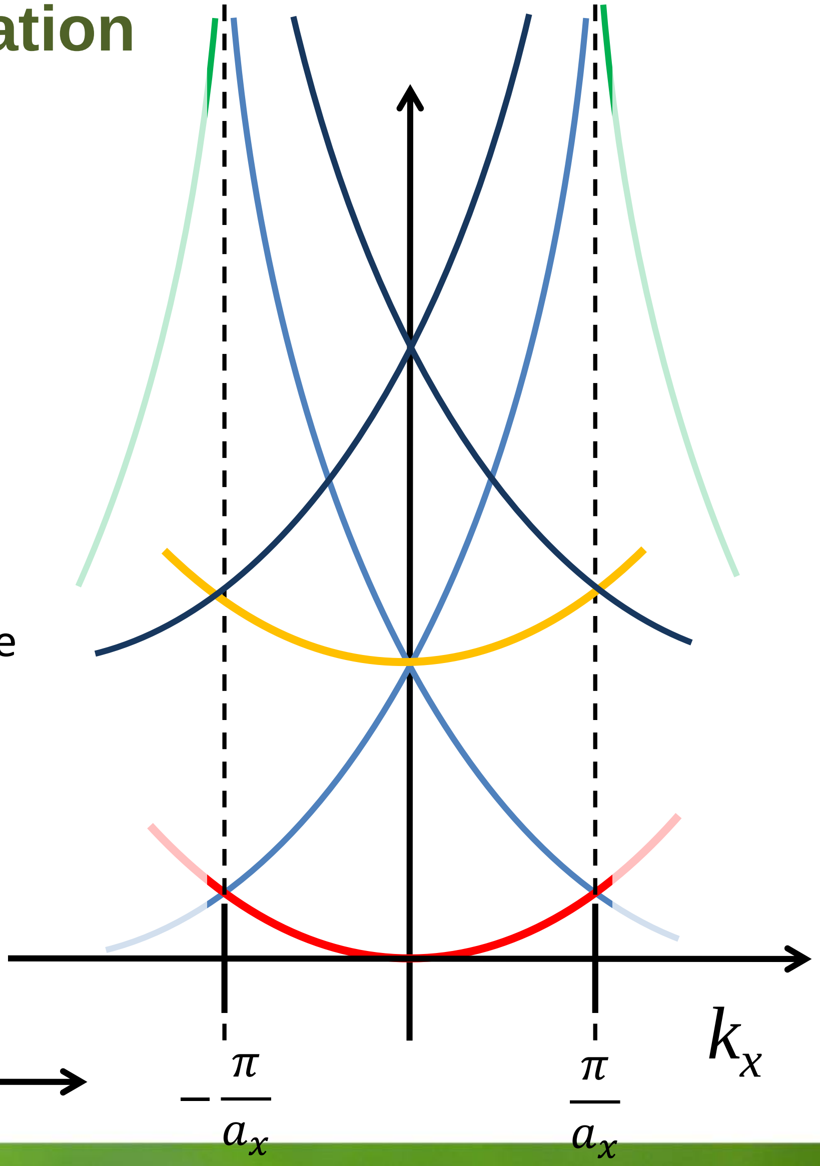
$[hkl]$=

000,

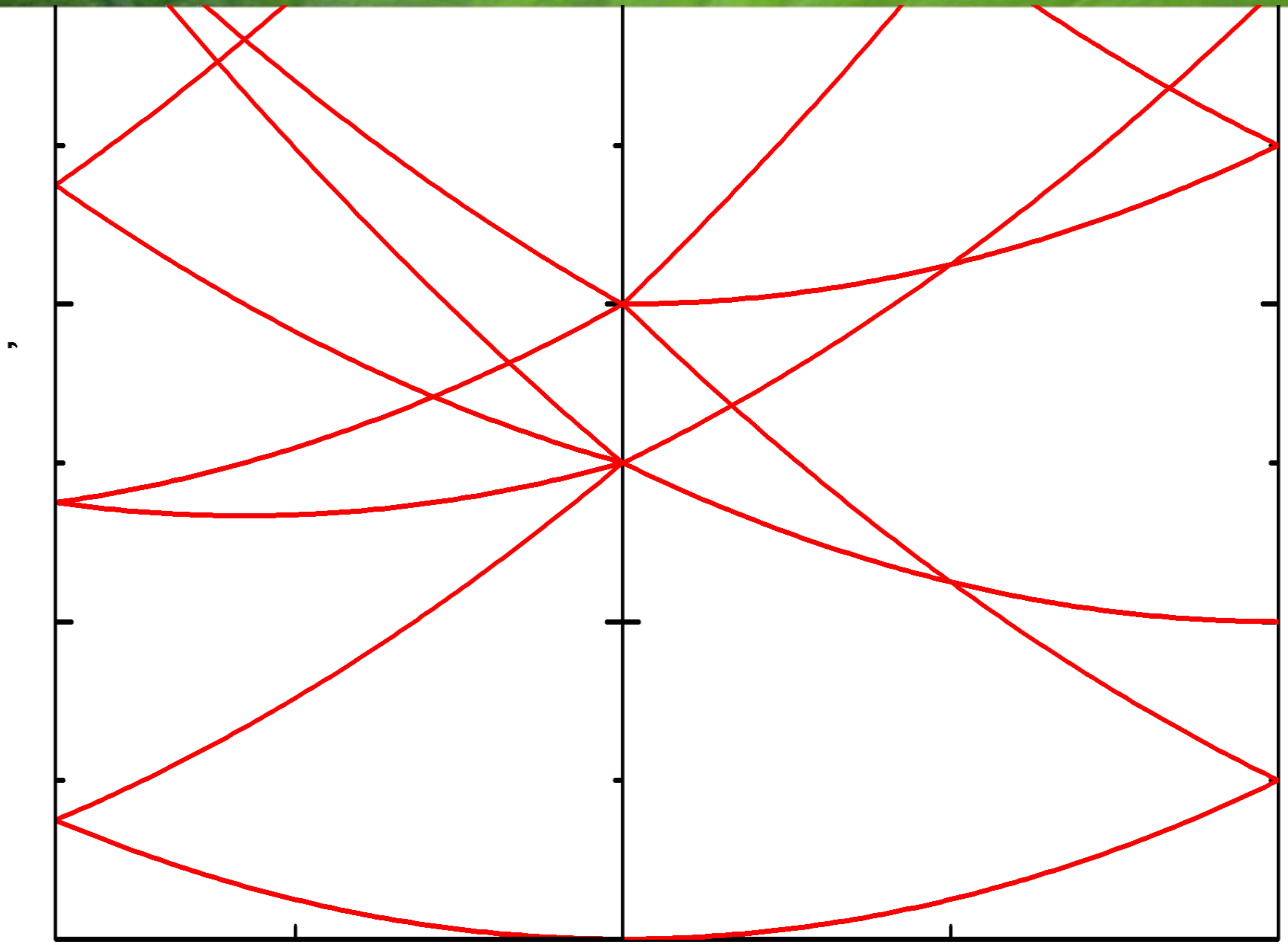
100, $\bar{1}00$, 200, $\bar{2}00$,

010, 010, 001, 001,

110, 101, $1\bar{1}0$, $10\bar{1}$, $\bar{1}01$, $\bar{1}\bar{1}0$, $\bar{1}0\bar{1}$, $\bar{1}10$ →

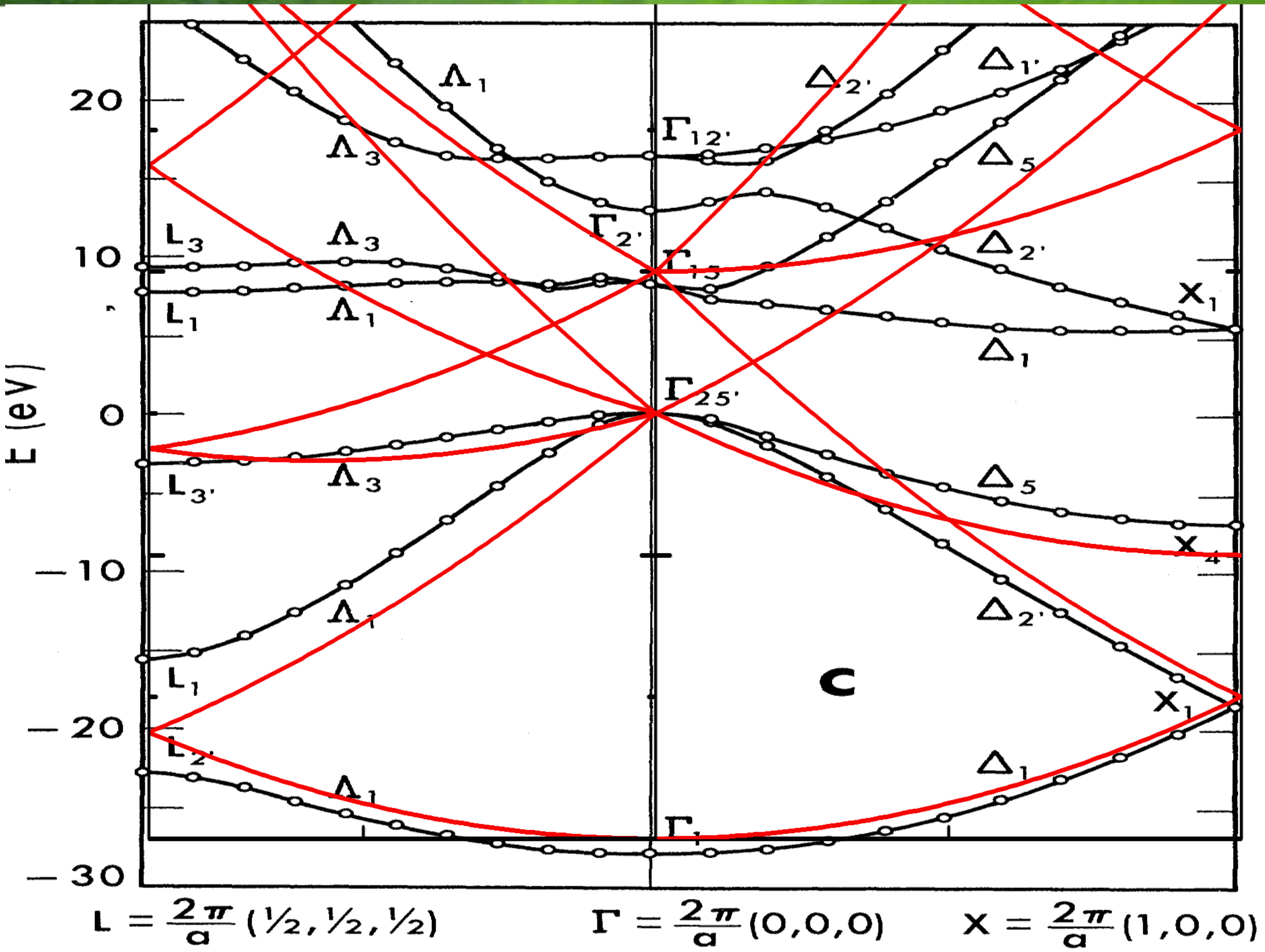


Periodic potential



$L = \frac{2\pi}{a}(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ $\Gamma = \frac{2\pi}{a}(0,0,0)$ $X = \frac{2\pi}{a}(1,0,0)$

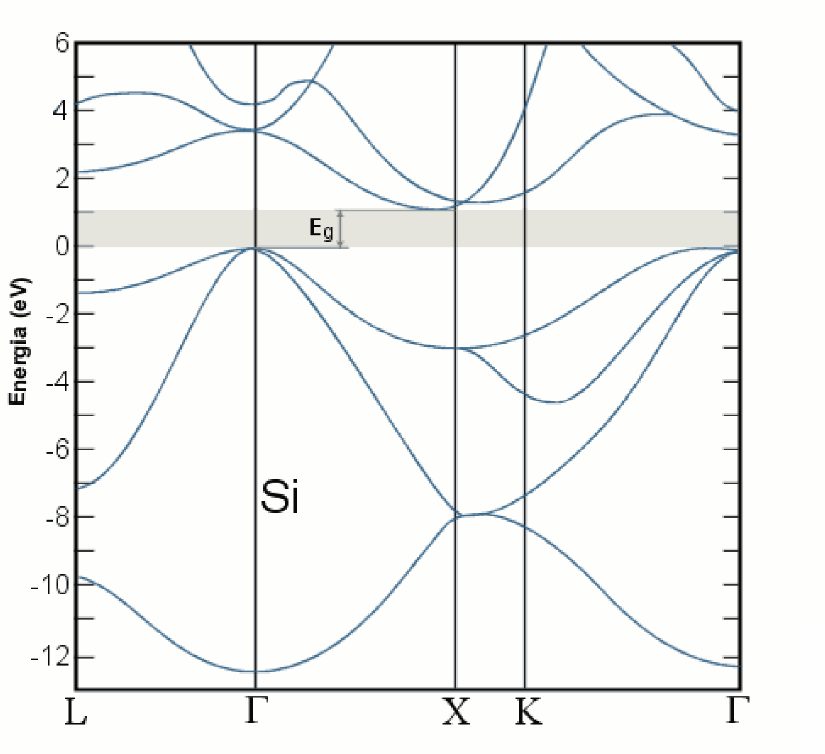
Periodic potential

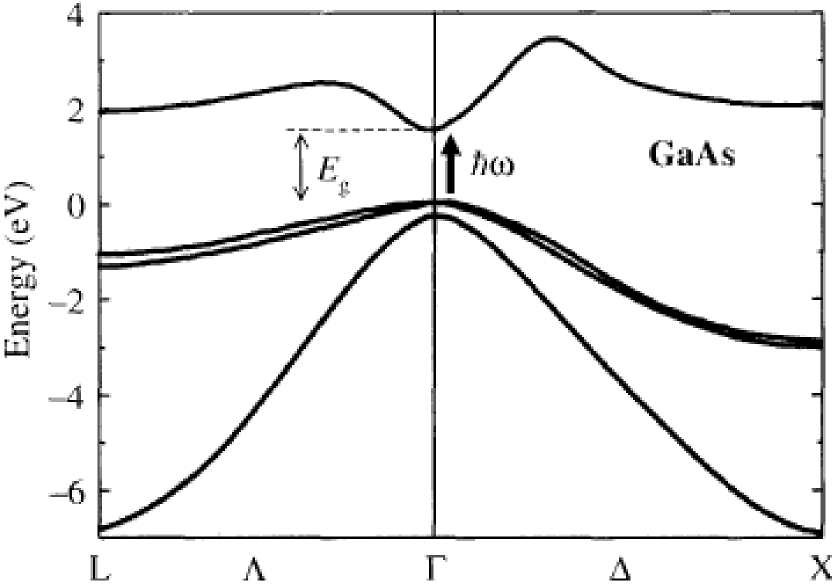


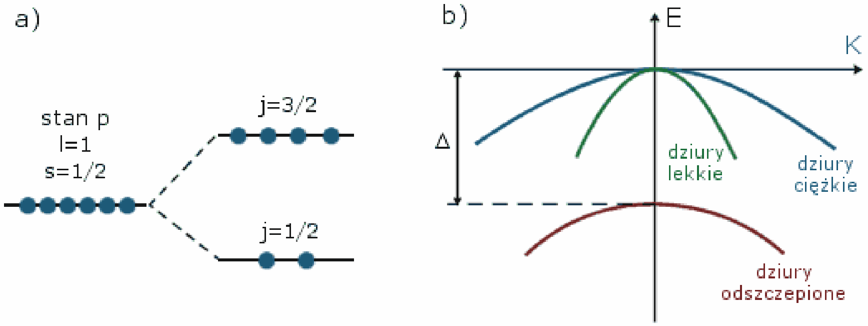
k·p perturbation theory – effective mass

The band theory of solids

Examples:



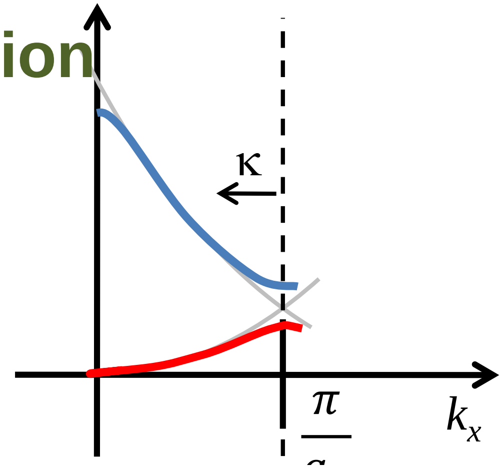


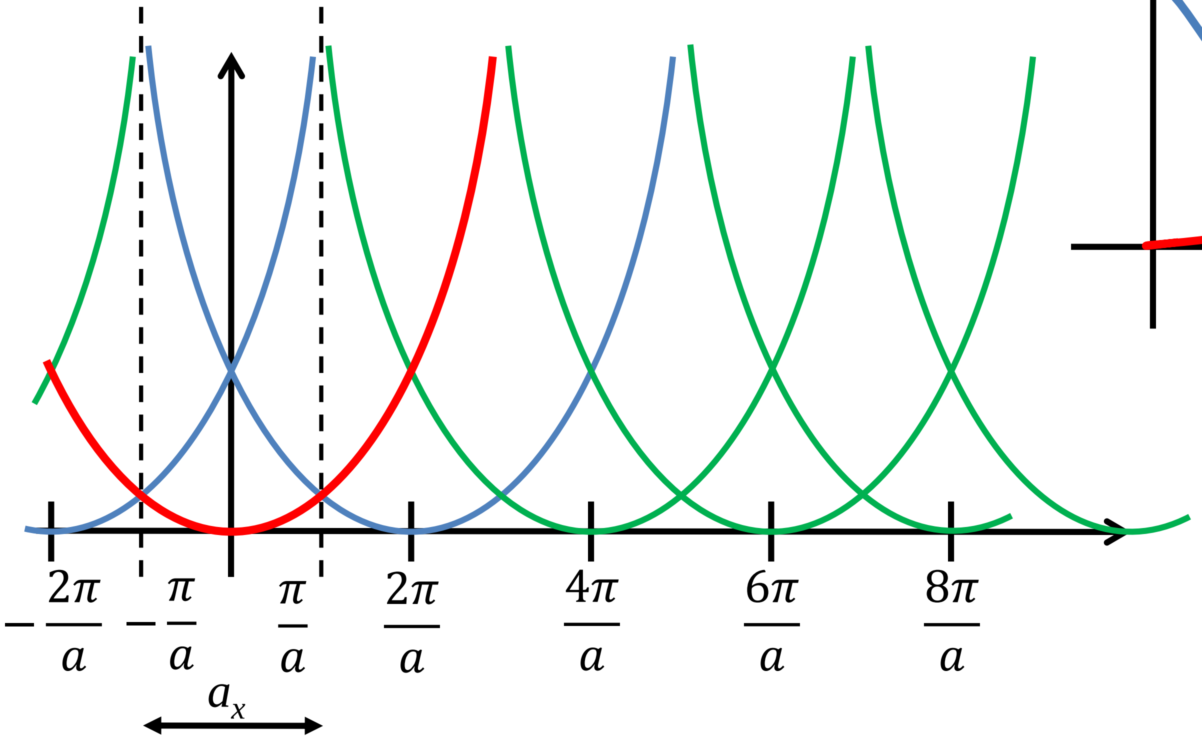


D. Wasik.

Periodic potential

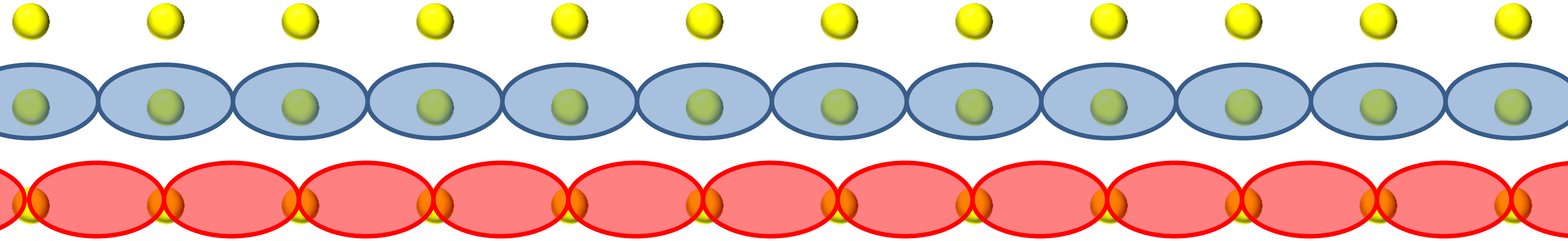
The nearly free-electron approximation





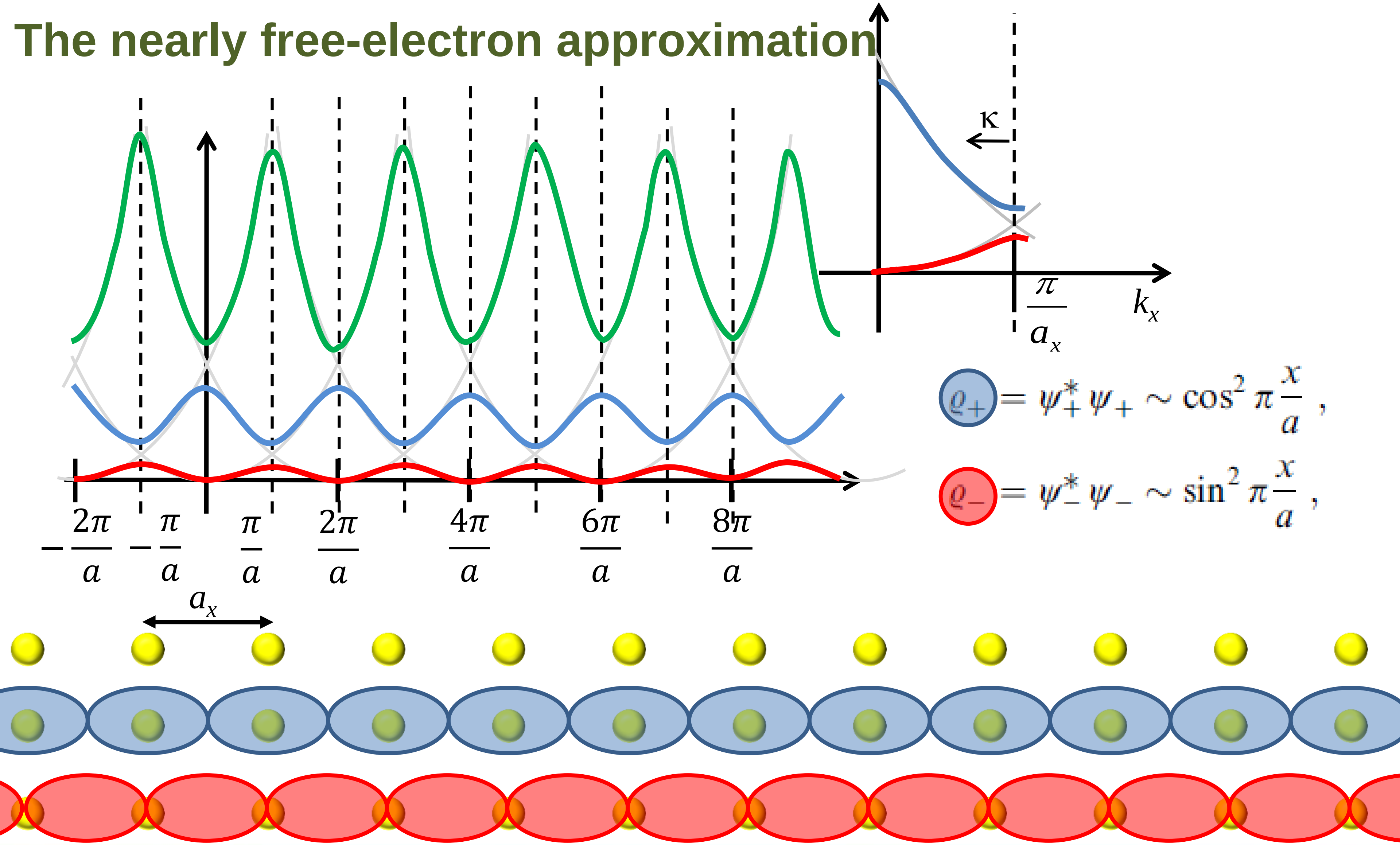
$$\varrho_+ = \psi_+^* \psi_+ \sim \cos^2 \pi \frac{x}{a} \ ,$$

$$\varrho_- = \psi_-^* \psi_- \sim \sin^2 \pi \frac{x}{a} \ ,$$



Periodic potential

The nearly free-electron approximation



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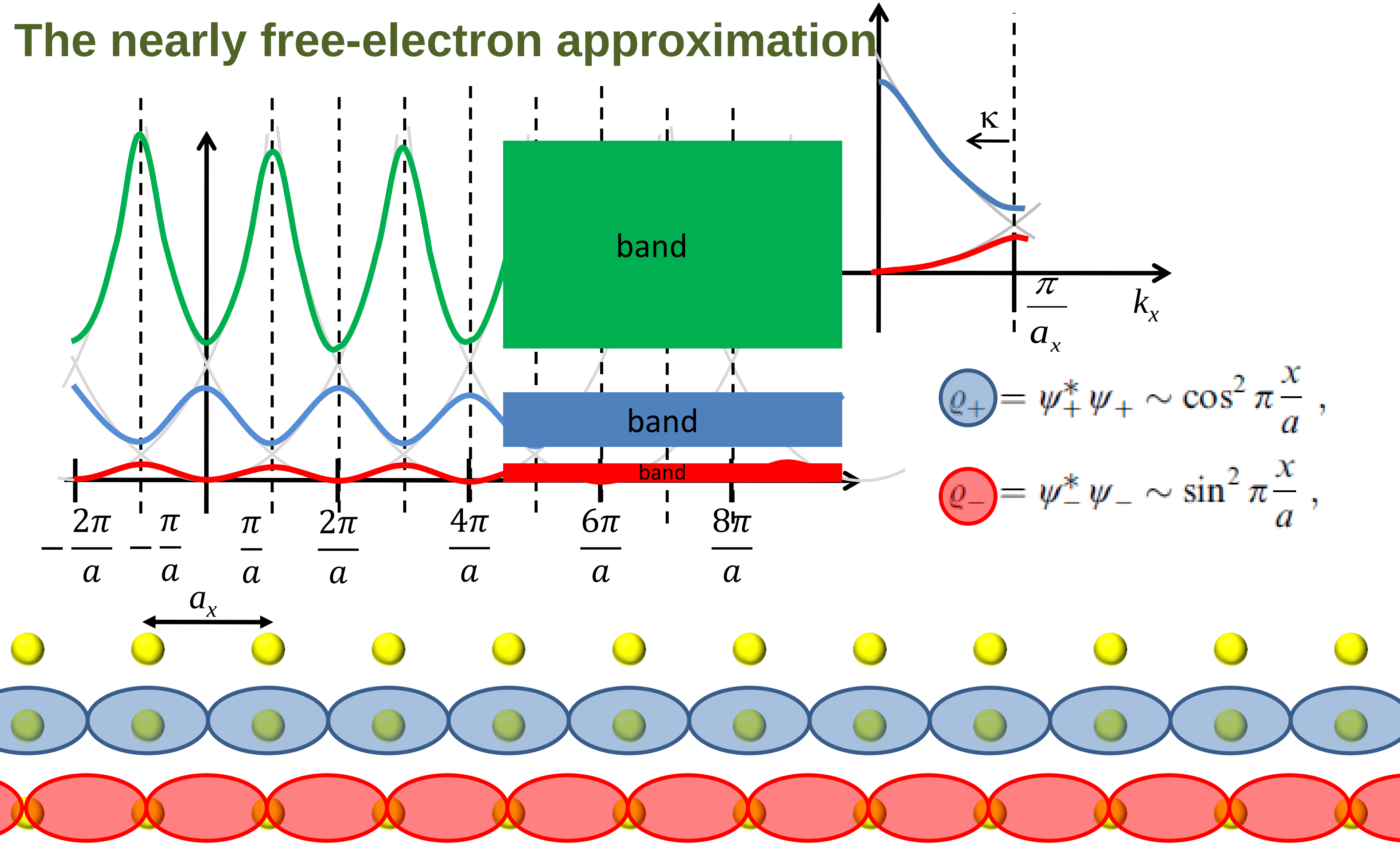

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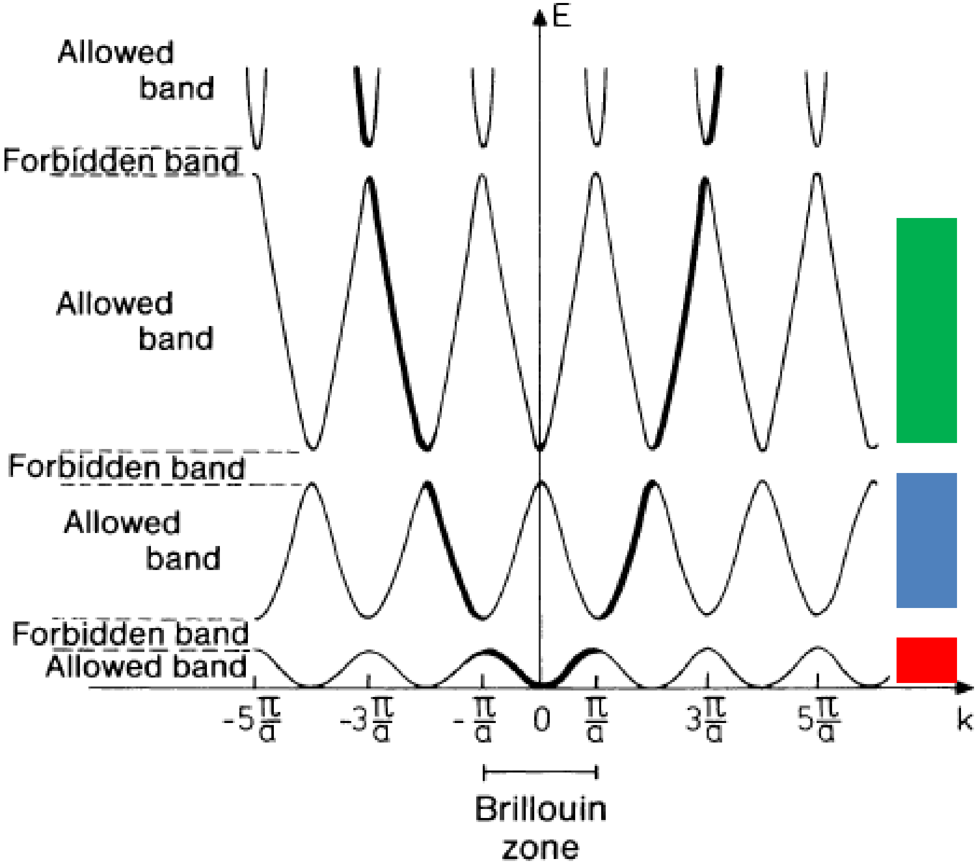
The electronic band structure

- It is convenient to present the energies only in the 1st Brillouin zone.
- The electron state in the solid state is given by the wave vector of the 1st Brillouin zone, band number and a spin.



Tight-Binding Approximation

The existence of the band structure arising from the discrete energy levels of isolated atoms due to the interaction between them. We can classify the electronic states as belonging to the electronic shells s, p, d etc.

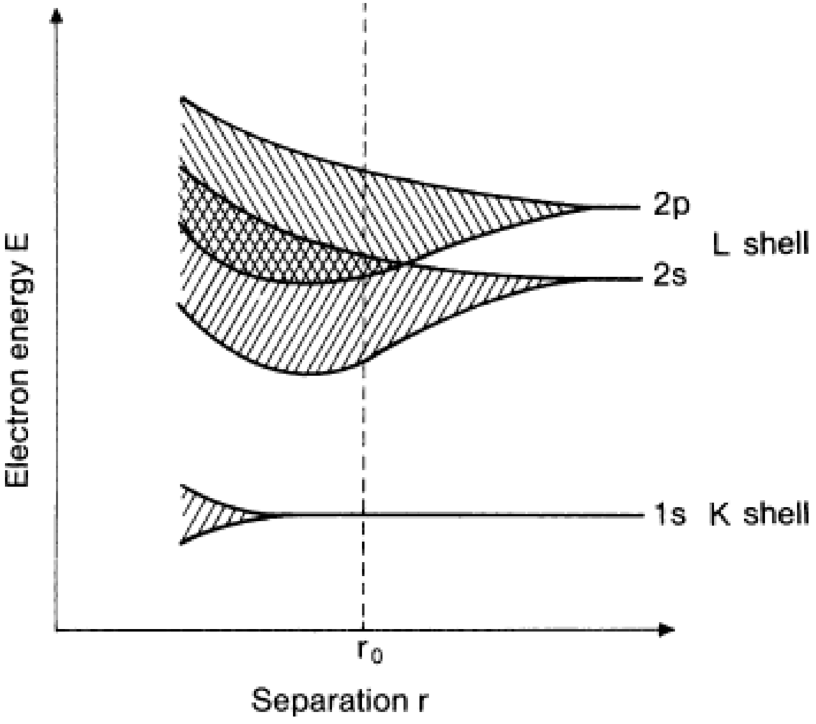


Fig. 1.1. Broadening of the energy levels as a large number of identical atoms from the first row of the periodic table approach one another (schematic). The separation r_0 corresponds to the approximate equilibrium separation of chemically bound atoms. Due to the overlap of the 2*s* and 2*p* bands, elements such as Be with two outer electrons also become metallic. Deep-lying atomic levels are only slightly broadened and thus, to a large extent, they retain their atomic character

H. Ibach, H. Lüth, Solid-State Physics

The existence of a forbidden gap is not tied to the periodicity of the lattice! Amorphous materials can also display a band gap.

If a crystal with a primitive cubic lattice contains N atoms and thus N primitive unit cells, then an **atomic energy level $\boldsymbol{E_i}$** of the free atom will split into N states (due to the interaction with the rest of $N - 1$ atoms).

Each band can be occupied by $2N$ electrons.

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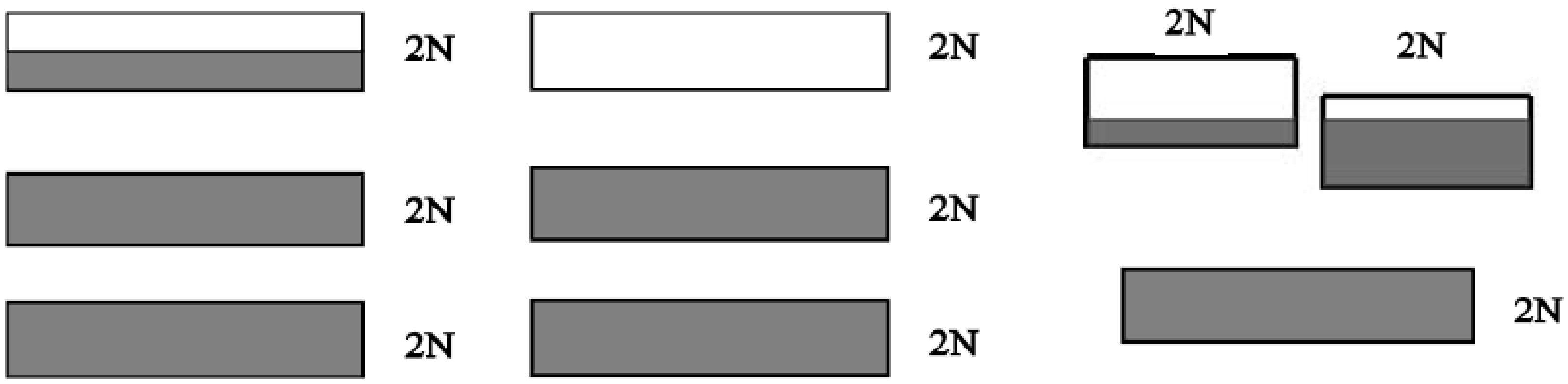


An odd number of electrons per cell (metal)

An even number of electrons per cell (non-metal)

An even number of electrons per cell but overlapping bands (metals of the II group, e.g. Be → next slide!)

H. Ibach, H. Lüth, Solid-State Physics

Tight-Binding Approximation

The states can mix: for instance sp^3 hybridization.

C, Si, Ge

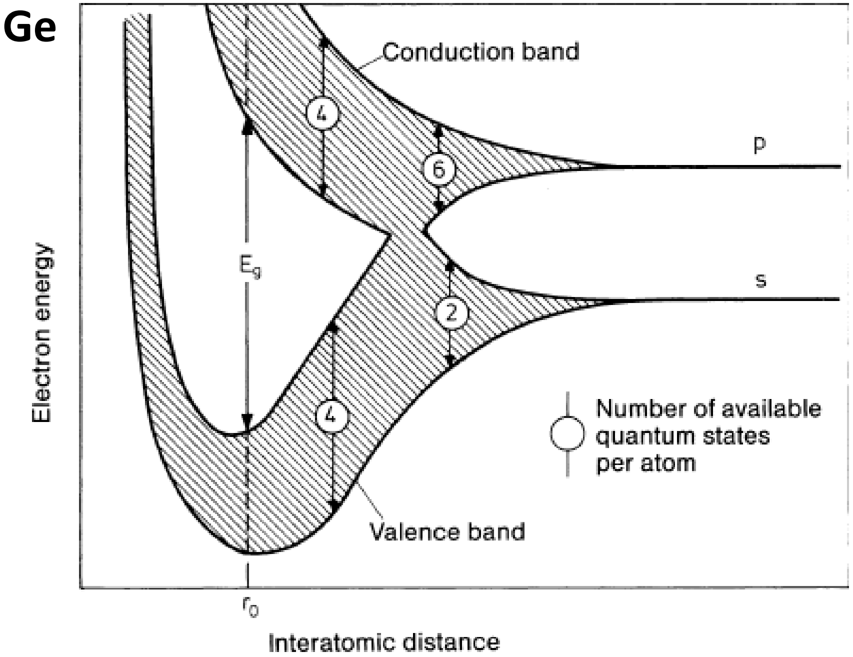


Fig. 7.9. Schematic behavior of the energy bands as a function of atomic separation for the tetrahedrally bound semiconductors diamond (C), Si, and Ge. At the equilibrium separation r_0 there is a forbidden energy gap of width E_g between the occupied and unoccupied bands that result from the sp^3 hybrid orbitals. For diamond, the sp^3 hybrid stems from the $2s$ and $2p^3$ atomic states, for Si from the $3s$ and $3p^3$, and for Ge from the $4s$ and $4p^3$. One sees from this figure that the existence of a forbidden energy region is not tied to the periodicity of the lattice. Thus amorphous materials can also display a band gap. (After [7.1])

Be

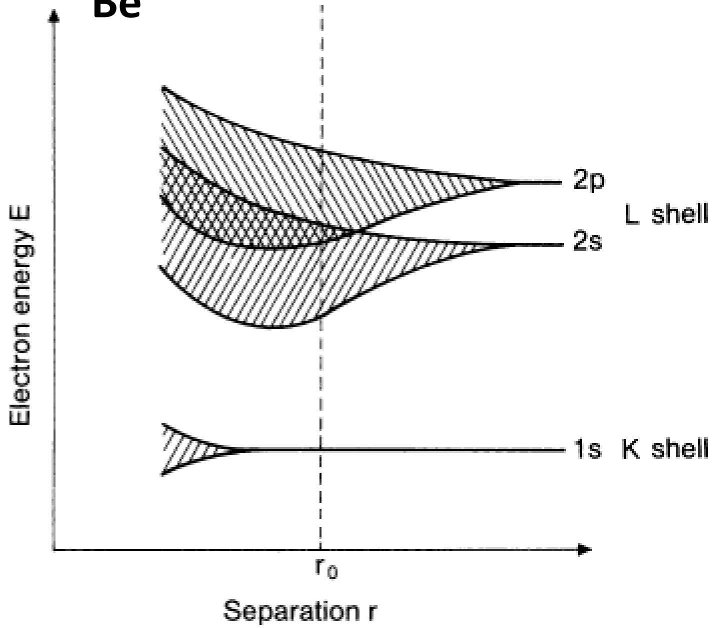


Fig. 1.1. Broadening of the energy levels as a large number of identical atoms from the first row of the periodic table approach one another (schematic). The separation r_0 corresponds to the approximate equilibrium separation of chemically bound atoms. Due to the overlap of the $2s$ and $2p$ bands, elements such as Be with two outer electrons also become metallic. Deep-lying atomic levels are only slightly broadened and thus, to a large extent, they retain their atomic character

H. Ibach, H. Lüth, Solid-State Physics

Tight-Binding Approximation

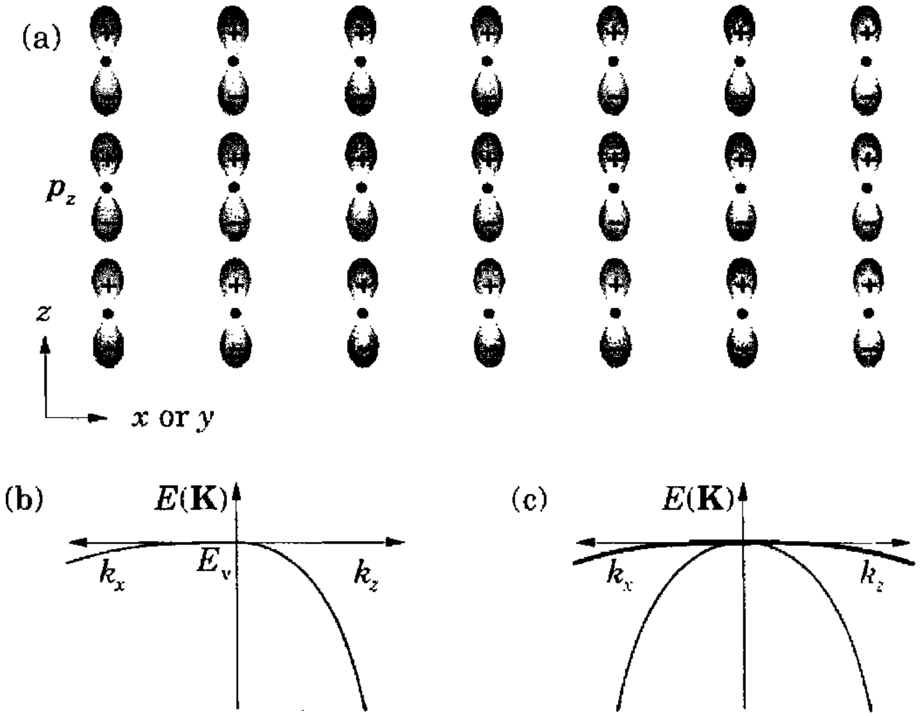


FIGURE 2.17. Valence bands constructed from p orbitals. (a) Lattice of p_z orbitals. (b) Band structure of the p_z orbitals only; the band is 'light' along k_z to the right and 'heavy' along k_x (or k_y) to the left. (c) Total bands from all three p orbitals, showing a doubly degenerate 'heavy' band and a single 'light' band.

Fermi surfaces of metals

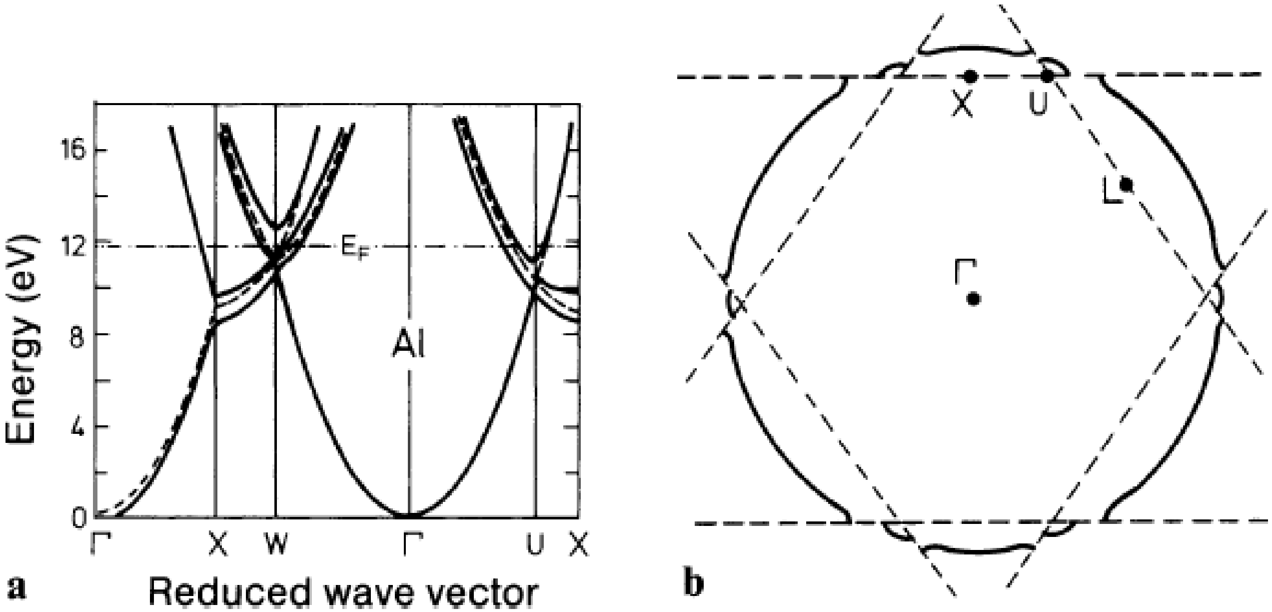


Fig. 7.11. **(a)** Theoretical bandstructure $E(\boldsymbol{k})$ for Al along directions of high symmetry (Γ is the center of the Brillouin zone). The dotted lines are the energy bands that one would obtain if the *s*- and *p*-electrons in Al were completely free ("empty" lattice). After [7.3]. **(b)** Cross section through the Brillouin zone of Al. The zone edges are indicated by the dashed lines. The Fermi "sphere" of Al (——) extends beyond the edges of the first Brillouin zone

Periodic potential

Bloch theorem

$\hat{p}\psi(\vec{r}) = -i\hbar\left(i\,\vec{k} + \nabla u_{n,\vec{k}}\right)e^{i\vec{k}\vec{r}} \neq \hbar\vec{k}\psi(\vec{r}).$

$\hbar\vec{k}$ is so-called *quasi-momentum* or *crystal momentum*.

If we consider interactions with other quasi-particles (electrons, phonons, magnons etc.) existing in the crystal and real particles penetrating through the crystal (e.g. photons, neutron) the momentum conservation law must be replaced by the **quasi-momentum conservation law** :

$$\sum_i \hbar\vec{k}_i + \sum_i \vec{p}_i = \sum_i \hbar\vec{k}_i{}' + \sum_i \vec{p}_i' + \hbar\vec{G}$$

The energy conservation is always the same:

$$\sum_i E_i = \sum_i E_i{}'$$

k·p perturbation theory – effective mass

$$\varphi_{n,\vec{k}}(\vec{r}) = e^{i\vec{k}\vec{r}} u_{n,\vec{k}}(\vec{r})$$

$\vec{k}$-vector is not the momentum (momentum operator $\hat{p} = -i\hbar\nabla$)

$$\hat{p}\varphi_{n,\vec{k}}(\vec{r}) = -i\hbar\left(i\vec{k} + \nabla u_{n,\vec{k}}(\vec{r})\right)e^{i\vec{k}\vec{r}} \neq \hbar\vec{k}\varphi_{n,\vec{k}}(\vec{r})$$

Bloch function in the Schrödinger equation:

$$\Delta\varphi_{n,\vec{k}}(\vec{r}) = \cdots = \left(\Delta u_{n,\vec{k}}(\vec{r}) + 2i\vec{k}\nabla u_{n,\vec{k}}(\vec{r}) - \vec{k}^2 u_{n,\vec{k}}(\vec{r})\right)e^{i\vec{k}\vec{r}}$$

By substitution of this expression and simplification by $e^{i\vec{k}\vec{r}}$ we got equation for $u_{n,\vec{k}}(\vec{r})$:

$$\left(-\frac{\hbar^2}{2m}\Delta - \frac{\hbar}{m}i\vec{k}\nabla + \frac{\hbar^2}{2m}\vec{k}^2\right)u_{n,\vec{k}}(\vec{r}) = \left(\frac{\hat{p}^2}{2m} + \frac{\hbar}{m}\vec{k}\hat{p} + \frac{\hbar^2\vec{k}^2}{2m}\right)u_{n,\vec{k}}(\vec{r})$$

The Schrodinger equation for the envelope $u_{n,\vec{k}}(\vec{r})$:

$$\left(\frac{\hat{p}^2}{2m} + \frac{\hbar}{m}\vec{k}\hat{p} + V(\vec{r})\right)u_{n,\vec{k}}(\vec{r}) = \left(E_n - \frac{\hbar^2\vec{k}^2}{2m}\right)u_{n,\vec{k}}(\vec{r})$$

k·p perturbation theory – effective mass

The Schrodinger equation for the envelope $u_{n,\vec{k}}(\vec{r})$:

$$\left(\frac{\hat{p}^2}{2m} + \frac{\hbar}{m}\,\vec{k}\hat{p} + V(\vec{r})\right)u_{n,\vec{k}}(\vec{r}) = \left(E - \frac{\hbar^2\vec{k}^2}{2m}\right)u_{n,\vec{k}}(\vec{r})$$

This is so-called ***kp* perturbation theory (*przybliżenie kp*)** used for the calculations of the energies and wavefunctions at some $\vec{k} = \vec{k}_0$.

The full Hamiltonian

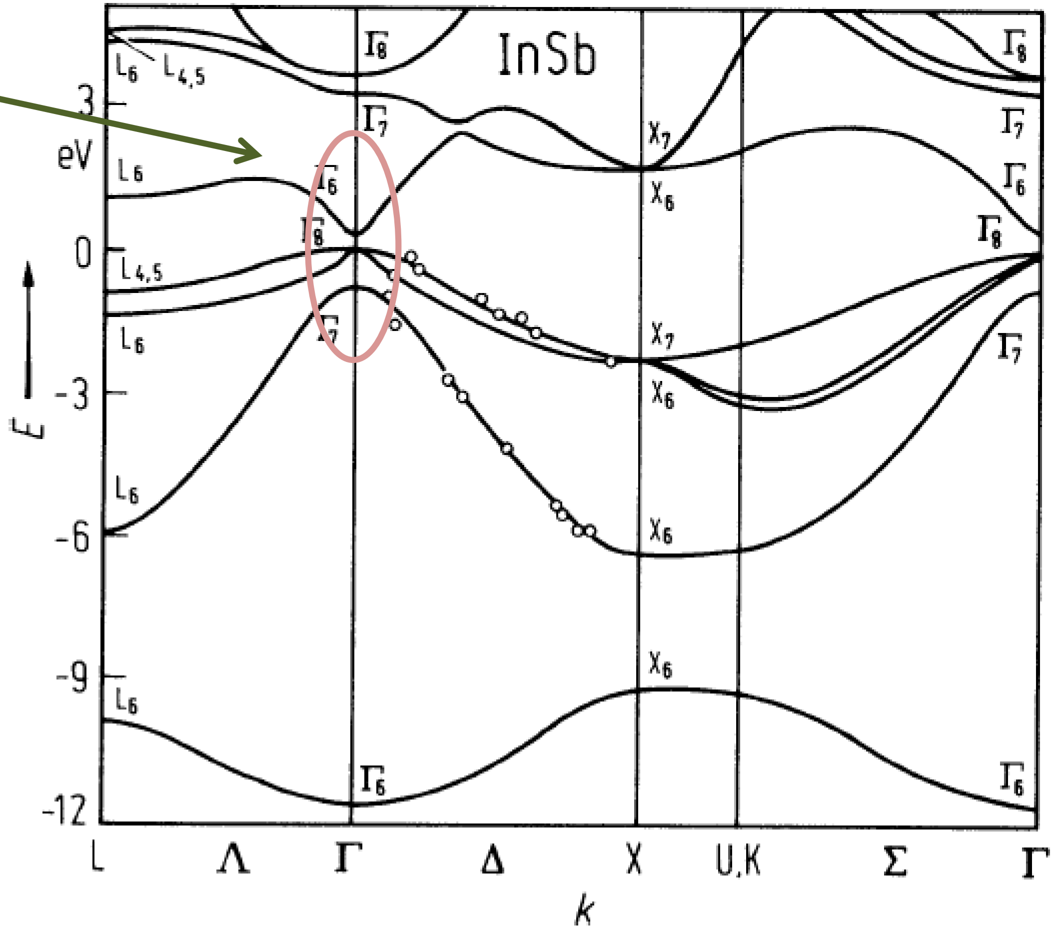
$$\hat{H}_{\vec{k}}u_{n,\vec{k}}(\vec{r}) = \left(\hat{H}_{\vec{k}_0} + \hat{H}'\right)u_{n,\vec{k}}(\vec{r}) = E_n\left(\vec{k}\right)u_{n,\vec{k}}(\vec{r})$$

Perturbation:

$$\hat{H}' = \frac{\hbar}{m}\,(\vec{k} - \vec{k}_0)\hat{p}$$

By the perturbation theory we find the function $u_{n,\vec{k}}(\vec{r})$ and the energy $E_n\left(\vec{k}\right)$.

k·p perturbation theory – effective mass



close bands

Expanding $E_n(\vec{k}) = \left(E_n - \frac{\hbar^2\vec{k}^2}{2m}\right)$ around an extreme point, e.g. $k = 0$:

Landolt-Boernstein

k·p perturbation theory – effective mass

We expand $E_n(\vec{k}) = \left(E_n - \frac{\hbar^2\vec{k}^2}{2m}\right)$ around an extreme point, e.g. $k = 0$:

$$E_n(\vec{k}) = E_n(0) + H'_{nn} + \sum_{l\neq n} \frac{|H'_{nl}|^2}{E_n(0) - E_l(0)} + \cdots$$

For

$$H'_{nl} = \int u_{n,0}(\vec{r})\hat{H}'\, u_{l,0}(\vec{r})\, d^3r = -\frac{i\hbar}{m}\,\vec{k}\int u_{n,0}(\vec{r})\nabla u_{l,0}(\vec{r})\, d^3r = \sum_{i=1}^{3} a_i k_i$$

Linear in $\vec{k}$

$$E_n(\vec{k}) = E_n(0) + \sum_{i=1}^{3} a_i k_i + \sum_{i=1}^{3}\sum_{j=1}^{3}\left(\frac{\hbar^2}{2m}\,\delta_{ij} + b_{ij}\right) k_i k_j + \cdots$$

the linear terms in extremum vanish

$$E_n(\vec{k}) = E_n(0) + \sum_{i=1}^{3}\sum_{j=1}^{3}\left(\frac{1}{m^*}\right)\frac{\hbar^2 k_i k_j}{2} + \cdots$$

k·p perturbation theory – effective mass

$$E_n(\vec{k}) = E_n(0) + \sum_{i=1}^{3}\sum_{j=1}^{3}\left(\frac{1}{m_{ij}^*}\right)\frac{\hbar^2 k_i k_j}{2} + \cdots$$

The inverse effective-mass tensor:

$$\frac{1}{m_{ij}^*} = \frac{\delta_{ij}}{m} + \frac{2\hbar^2}{m^2}\sum_{l\neq n}\frac{\int u_{n,0}\frac{\partial}{\partial x_i}u_{l,0}\,d^3r \;\cdot\; \int u_{n,0}\frac{\partial}{\partial x_j}u_{l,0}\,d^3r}{E_n(0) - E_l(0)}$$

This tensor is symmetric ($m_{ij} = m_{ji}$). If the energy extremum is in Γ(***k***=0) we obtain constant energy ellipsoid in $\vec{k}$-space, with principal axis $\frac{1}{m_i}$:

$$E_n(\vec{k}) \approx E_n(0) + \frac{\hbar^2}{2}\left(\frac{k_1^2}{m_1^*} + \frac{k_2^2}{m_2^*} + \frac{k_3^2}{m_3^*}\right)$$

where m_i^* are the inertial effective masses along these different axes.

k·p perturbation theory – effective mass

The energy $E_n(\boldsymbol{k})$ around extremum for the uniaxial crystal (np. GaN):

$$E_n(\vec{k}) = E_n(0) \pm \frac{\hbar^2}{2}\left(\frac{k_1^2 + k_2^2}{m_\perp^*} + \frac{k_3^2}{m_\parallel^*}\right)$$

For a cubic crystal:

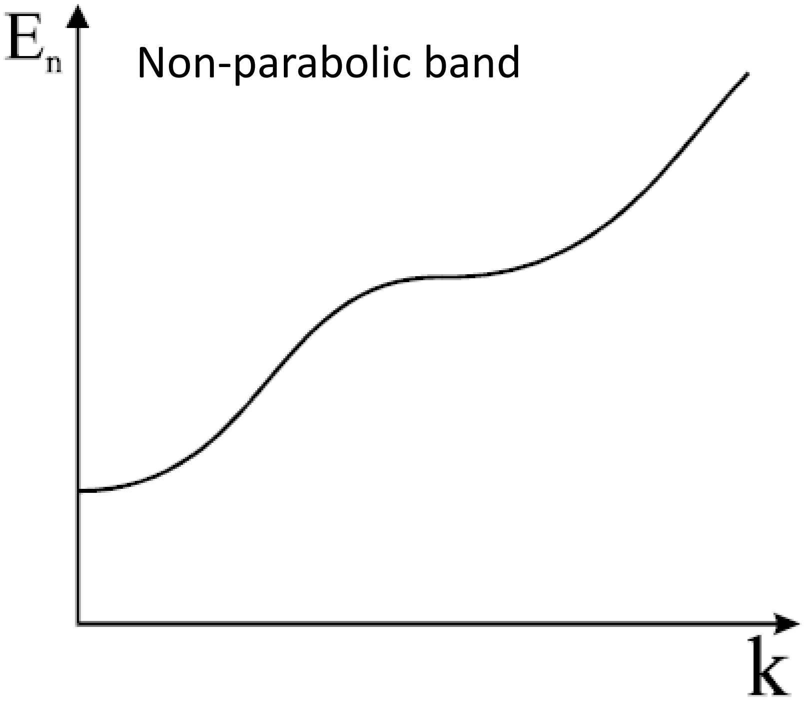
$$E_n(\vec{k}) = E_n(0) \pm \frac{\hbar^2 k^2}{2m^*}$$ so-called **spherical band**

Around the extremum (e.g. point $\Gamma(\boldsymbol{k}=0)$) we can restrict the solution to approximate **parabolic band**

In general, depending on the wave vector, also higher order perturbation terms exist.
The energy of the electron generally depends on $\boldsymbol{k}=(\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3)$. The energy isosurface can be very complex, and its shape depends on all bands.

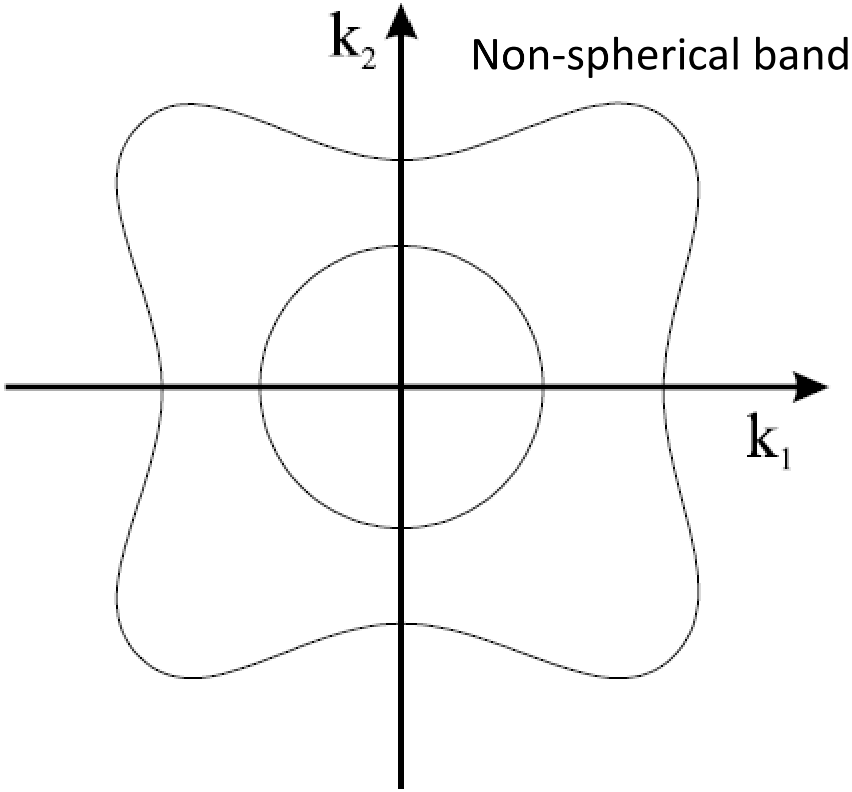
k·p perturbation theory – effective mass

The energy $E_n(\boldsymbol{k})$ around extremum



Non-parabolic band

Przykładowa zależność energii stanów pasma n od wektora falowego k.



Non-spherical band

Przykładowe powierzchnie stałej energii w dwuwymiarowej przestrzeni k.

R. Stępniewski

k·p perturbation theory – effective mass

The energy $E_n(\boldsymbol{k})$ around extremum for the uniaxial crystal (np. GaN):

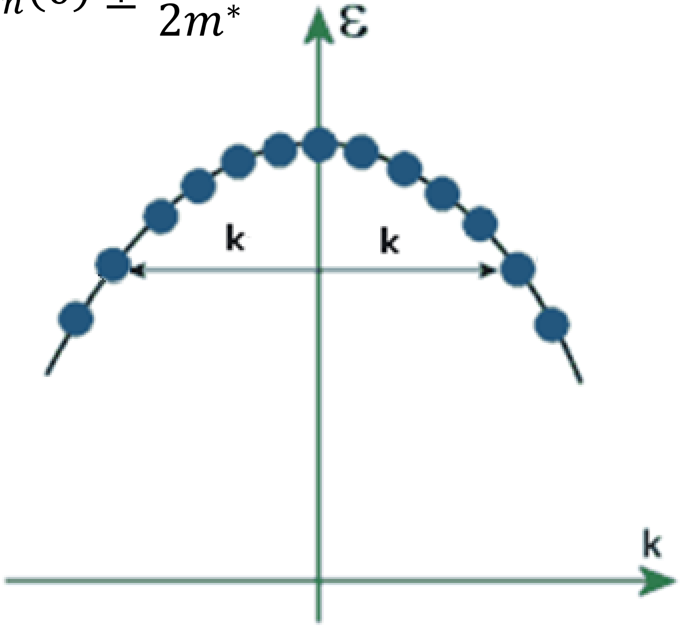
$$E_n(\vec{k}) = E_n(0) + \frac{\hbar^2}{2}\left(\frac{k_1^2 + k_2^2}{m_\perp^*} + \frac{k_3^2}{m_\parallel^*}\right)$$

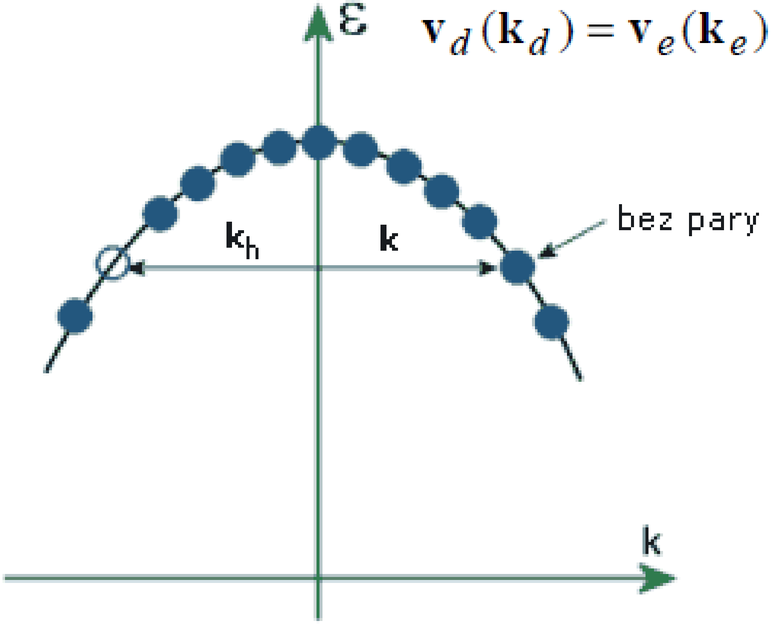
For a cubic crystal:

$$E_n(\vec{k}) = E_n(0) \pm \frac{\hbar^2 k^2}{2m^*}$$

$$\mathbf{v}_d(\mathbf{k}_e) = -\mathbf{v}_e(\mathbf{k}_e)$$

$$\mathbf{v}_d(\mathbf{k}_d) = \mathbf{v}_e(\mathbf{k}_e)$$





k·p perturbation theory – effective mass

Electrones and holes

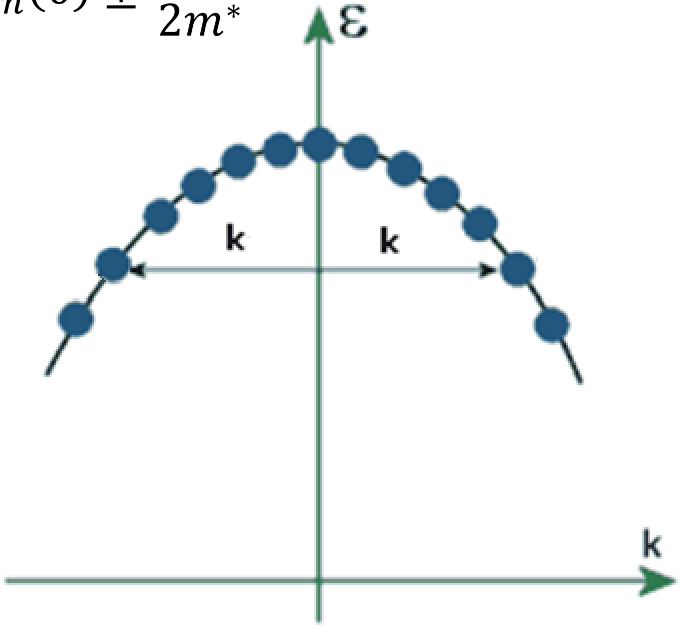
$$f_d = \sum_{\substack{i=1 \\ i \neq j}}^{2N} f(\mathbf{k}_i)$$

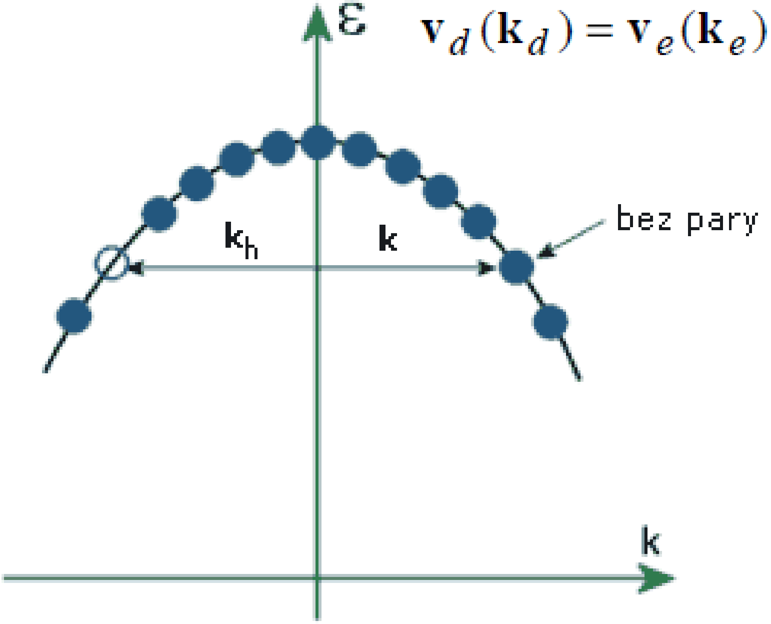
$$\mathbf{k}_d = \sum_{\substack{i=1 \\ i \neq j}}^{2N} \mathbf{k}_i = \sum_{i=1}^{2N} \mathbf{k}_i - \mathbf{k}_e = -\mathbf{k}_e$$

$$E_n(\vec{k}) = E_n(0) \pm \frac{\hbar^2 k^2}{2m^*}$$

$$\mathbf{v}_d(\mathbf{k}_e) = -\mathbf{v}_e(\mathbf{k}_e)$$

$$\mathbf{v}_d(\mathbf{k}_d) = \mathbf{v}_e(\mathbf{k}_e)$$





k·p perturbation theory – effective mass

Electrones and holes

$$f_d = \sum_{\substack{i=1 \\ i \neq j}}^{2N} f(\mathbf{k}_i) \qquad \mathbf{k}_d = \sum_{\substack{i=1 \\ i \neq j}}^{2N} \mathbf{k}_i = \sum_{i=1}^{2N} \mathbf{k}_i - \mathbf{k}_e = -\mathbf{k}_e$$

$$E_n(\vec{k}) = E_n(0) \pm \frac{\hbar^2 k^2}{2m^*}$$

$$\mathbf{v}_d(\mathbf{k}_e) = -\mathbf{v}_e(\mathbf{k}_e)$$
$$\mathbf{v}_d(\mathbf{k}_d) = \mathbf{v}_e(\mathbf{k}_e)$$

For any periodic function $f(\vec{r}) = f(\vec{r} + \vec{R})$ $\quad I(\mathbf{r}') := \int_\Omega d_3\mathbf{r}\, f(\mathbf{r} + \mathbf{r}') = const$

$$0 = \nabla' I(\mathbf{r}') := \int_\Omega d_3\mathbf{r}\, \nabla' f(\mathbf{r} + \mathbf{r}') = \int_\Omega d_3\mathbf{r}\, \nabla f(\mathbf{r} + \mathbf{r}')$$
$$0 = \nabla'^2 I(\mathbf{r}') := \int_\Omega d_3\mathbf{r}\, \nabla'^2 f(\mathbf{r} + \mathbf{r}') = \int_\Omega d_3\mathbf{r}\, \nabla^2 f(\mathbf{r} + \mathbf{r}')$$

k·p perturbation theory – effective mass

Electrones and holes

$$f_d = \sum_{\substack{i=1\\ i\neq j}}^{2N} f(\mathbf{k}_i)$$

$$\mathbf{k}_d = \sum_{\substack{i=1\\ i\neq j}}^{2N} \mathbf{k}_i = \sum_{i=1}^{2N} \mathbf{k}_i - \mathbf{k}_e = -\mathbf{k}_e$$

$$E_n(\vec{k}) = E_n(0) \pm \frac{\hbar^2 k^2}{2m^*}$$

For any periodic function $f(\vec{r}) = f(\vec{r} + \vec{R})$

$$0 = \nabla' I(\mathbf{r}') := \int_{\Omega} d_3\mathbf{r}\, \nabla' f(\mathbf{r} + \mathbf{r}') = \int_{\Omega} d_3\mathbf{r}\, \nabla f(\mathbf{r} + \mathbf{r}')$$

$$0 = \nabla'^2 I(\mathbf{r}') := \int_{\Omega} d_3\mathbf{r}\, \nabla'^2 f(\mathbf{r} + \mathbf{r}') = \int_{\Omega} d_3\mathbf{r}\, \nabla^2 f(\mathbf{r} + \mathbf{r}')$$

$$\langle \mathbf{v} \rangle = \frac{1}{4\pi^3 \hbar} \int_{SB} \nabla_k E(\mathbf{k})\, d_3\mathbf{k} = 0$$

$$\left\langle \overline{\overline{\mathbf{m}}}^{-1} \right\rangle = \frac{1}{4\pi^3 \hbar^2} \int_{SB} \nabla_k \nabla_k E(\mathbf{k})\, d_3\mathbf{k} = 0$$

$$\langle j \rangle = -e \sum_{i=1}^{2N} \mathbf{v}_i = -e \langle \mathbf{v} \rangle = 0$$

$$\langle \dot{\mathbf{v}} \rangle = \left\langle \overline{\overline{\mathbf{m}}}^{-1} \mathbf{F} \right\rangle = \left\langle \overline{\overline{\mathbf{m}}}^{-1} \right\rangle \mathbf{F} = 0$$

k·p perturbation theory – effective mass

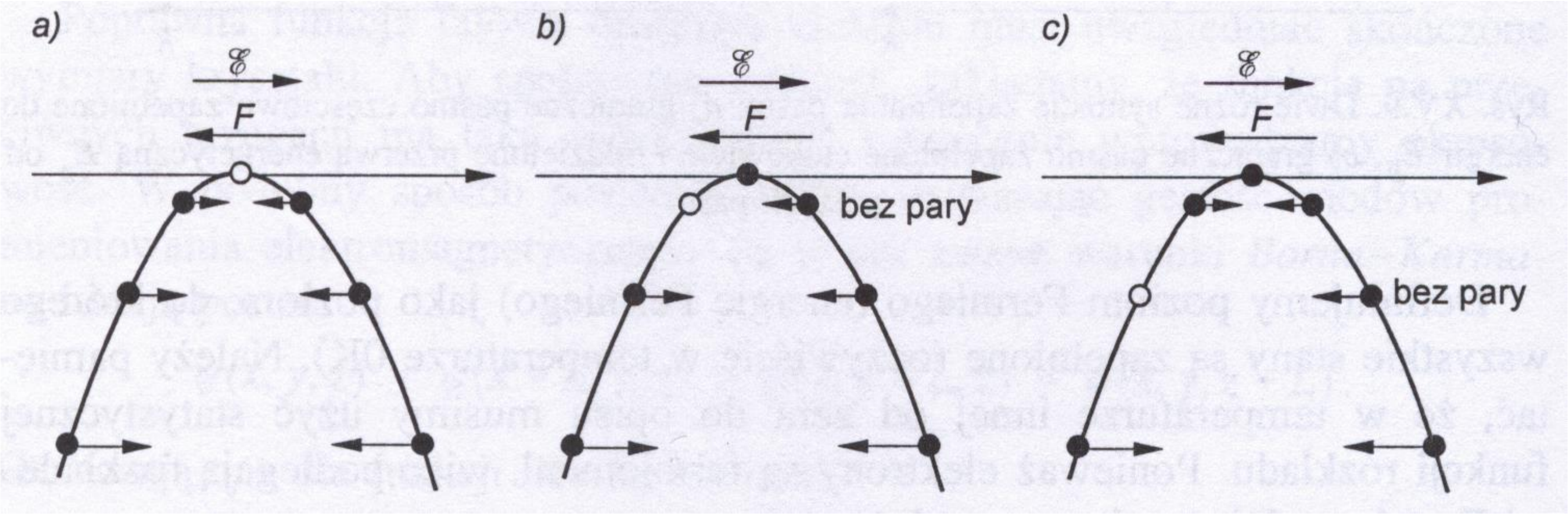
Electrones and holes

$$f_d = \sum_{\substack{i=1 \\ i \neq j}}^{2N} f(\mathbf{k}_i)$$

$$\mathbf{k}_d = \sum_{\substack{i=1 \\ i \neq j}}^{2N} \mathbf{k}_i = \sum_{i=1}^{2N} \mathbf{k}_i - \mathbf{k}_e = -\mathbf{k}_e$$

$$E_n(\vec{k}) = E_n(0) \pm \frac{\hbar^2 k^2}{2m^*}$$

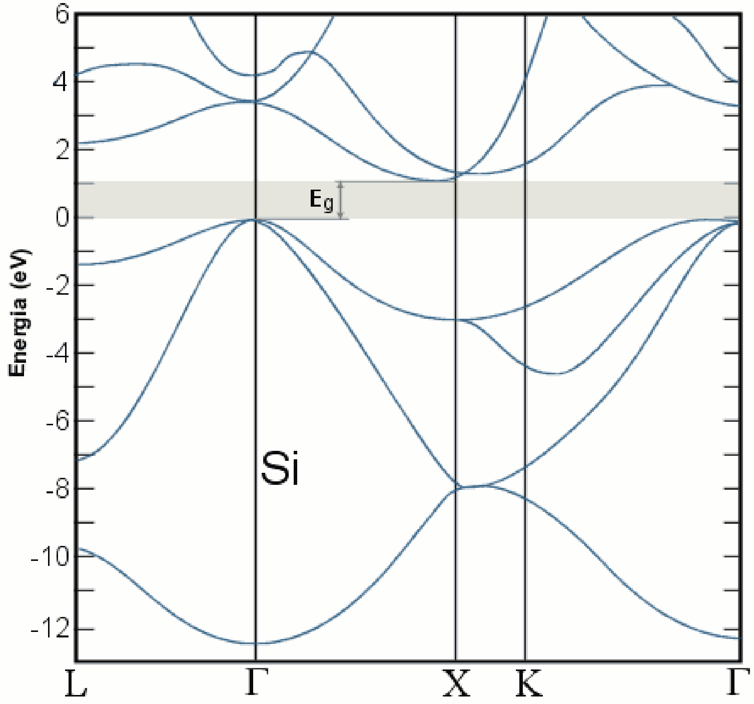
$$\mathbf{v}_d(\mathbf{k}_e) = -\mathbf{v}_e(\mathbf{k}_e)$$
$$\mathbf{v}_d(\mathbf{k}_d) = \mathbf{v}_e(\mathbf{k}_e)$$

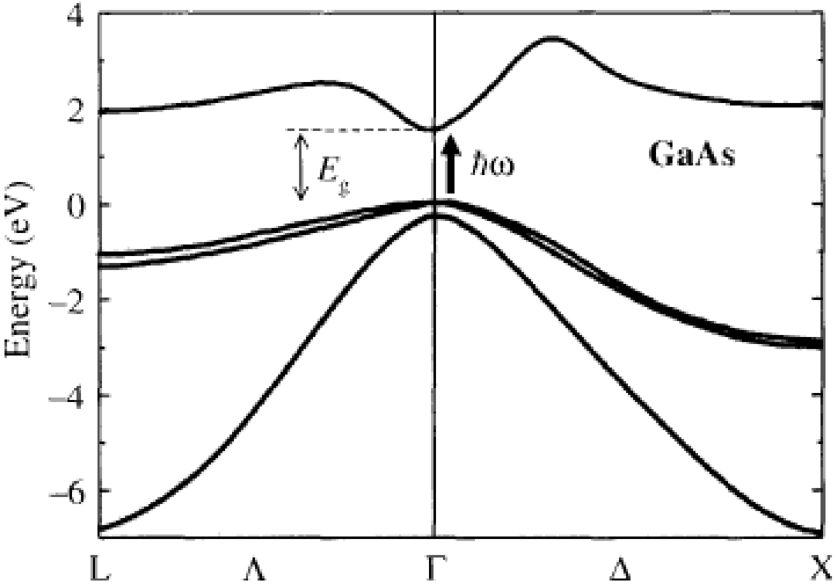


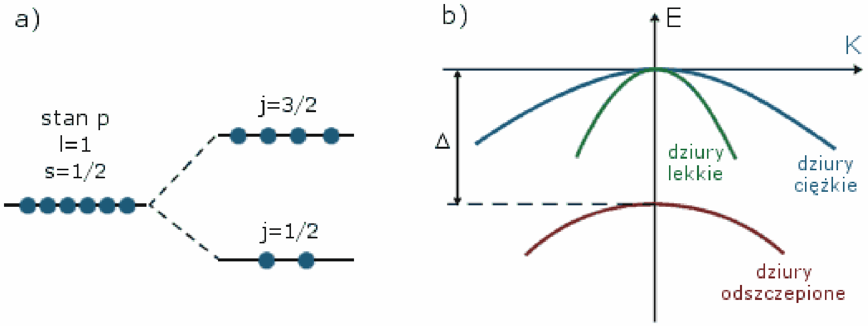
k·p perturbation theory – effective mass

The band theory of solids

Examples:







D. Wasik.

The band theory of solids.

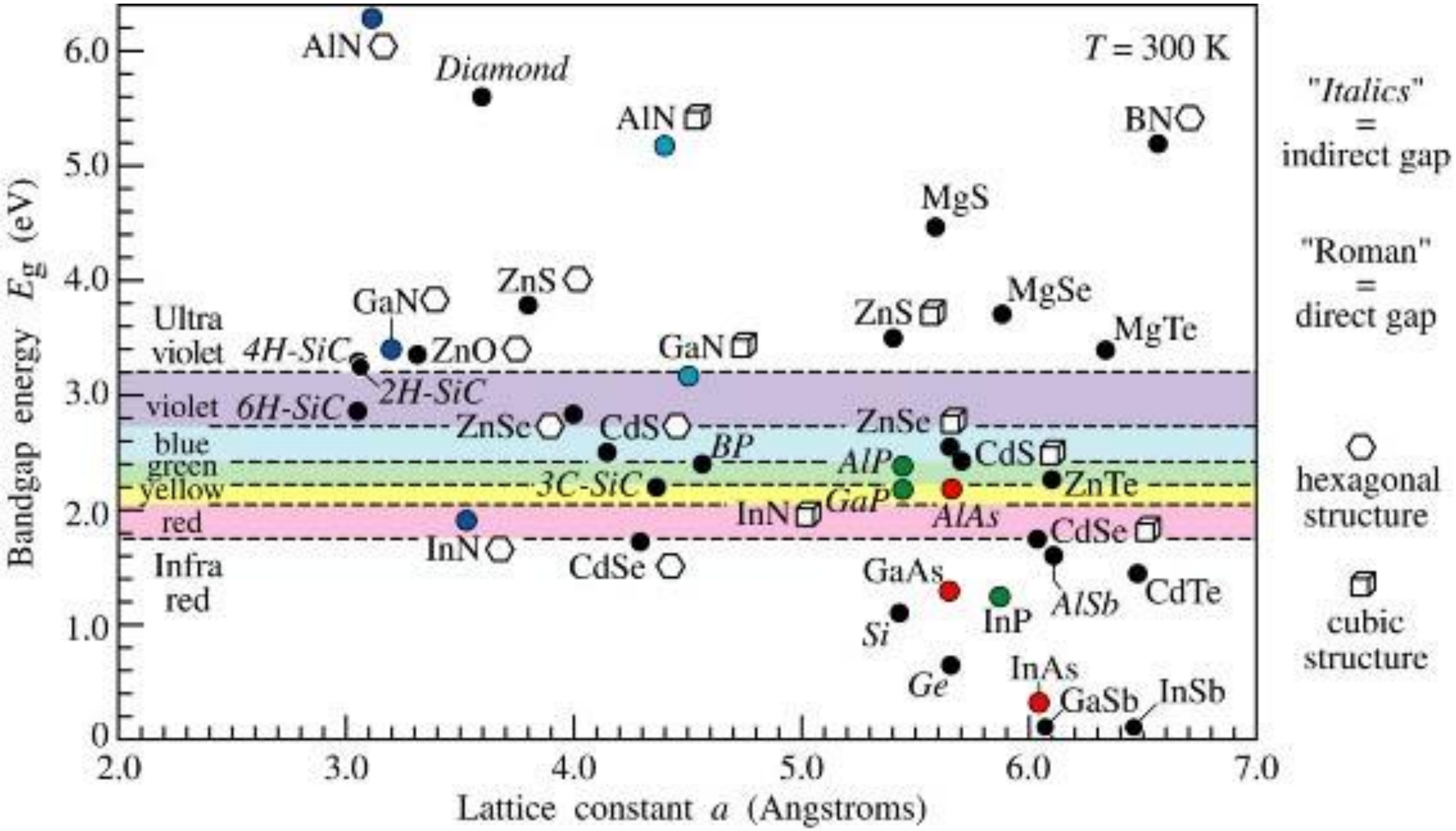


Fig. 11.4. Room-temperature bandgap energy versus lattice constant of common elemental and binary compound semiconductors.

The Fermi-Dirac distribution

The probability that a state of the energy E will be occupied

E_F – chemical potential

Fermions:

$$f_0 = \frac{1}{e^{\frac{E-E_F}{k_B T}} + 1}$$

Electrons

Holes

Trions (charged excitons)

Bosons:

$$f_0 = \frac{1}{e^{\frac{E-E_F}{k_B T}} - 1}$$

Polaritons

Phonons

Magnons

Excitons, biexcitons

Plasmons

Boltzman distribution:

$$f_0 = \frac{1}{e^{\frac{E-E_F}{k_B T}} \pm 1} \approx e^{-\frac{E-E_F}{k_B T}}$$

$$E_F = \frac{\partial F}{\partial n}$$

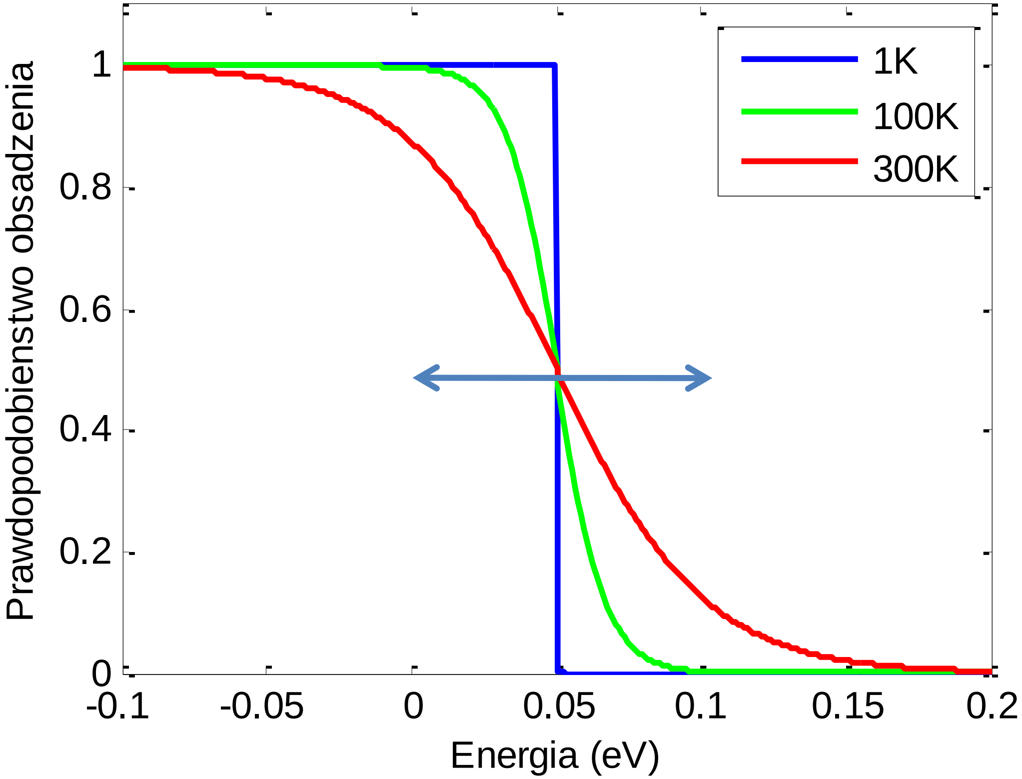
$$F = U - TS$$

Anyons – eg. composite fermions $|\Psi_1\Psi_2\rangle = e^{i\theta}|\Psi_2\Psi_1\rangle$

Slave fermions (chargon, holon, spinon) = fermion+bozon with the charge-spin separation

The Fermi-Dirac distribution

$$f_0 = \frac{1}{e^{\frac{E-E_F}{k_B T}} + 1}$$

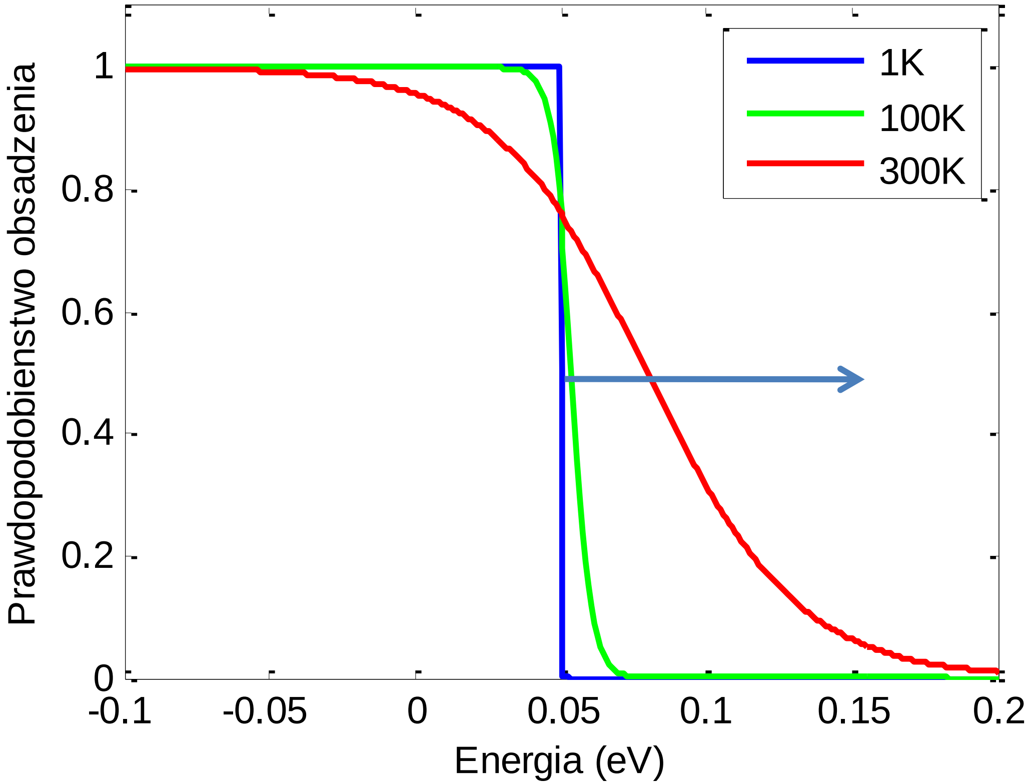


Enrico Fermi
1901 – 1954

Paul Adrian
Maurice Dirac
1902 – 1984

The Fermi-Dirac distribution

$$f_0 = \frac{1}{e^{\frac{E-E_F}{k_B T}} + 1}$$



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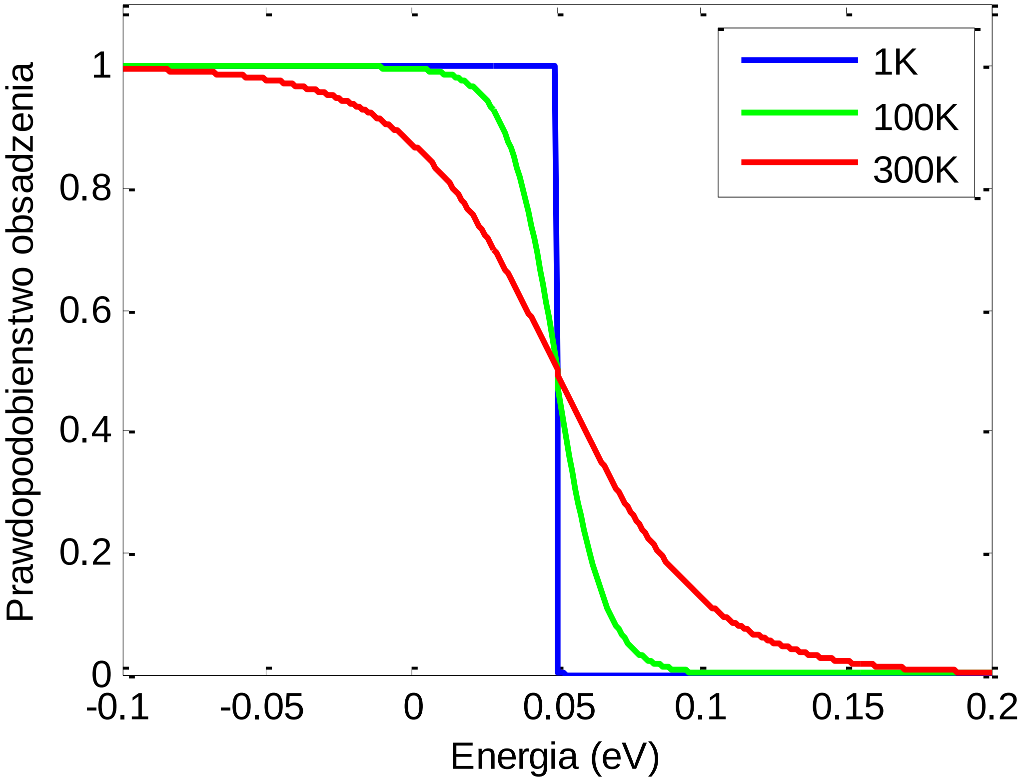

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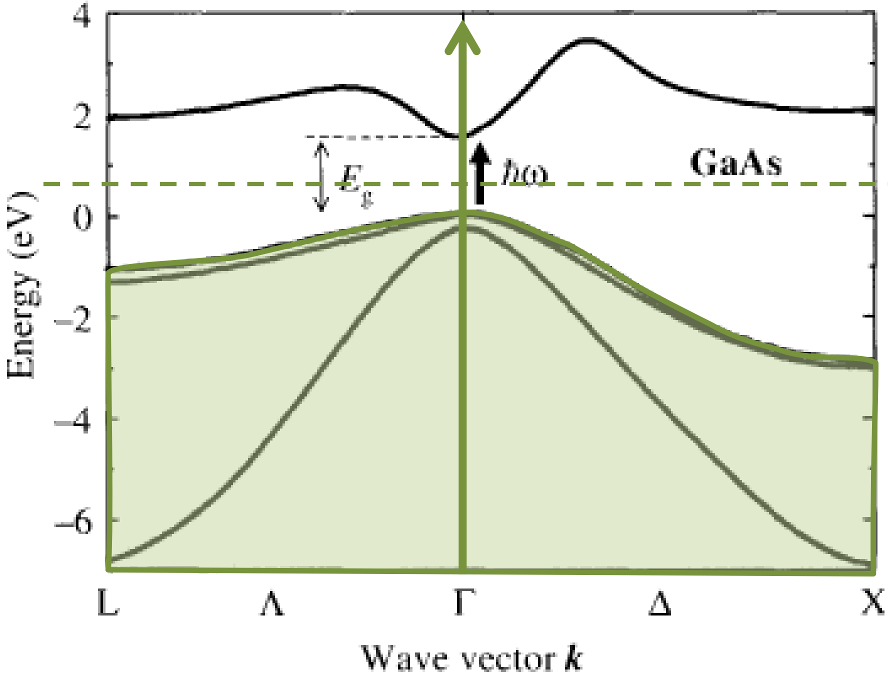

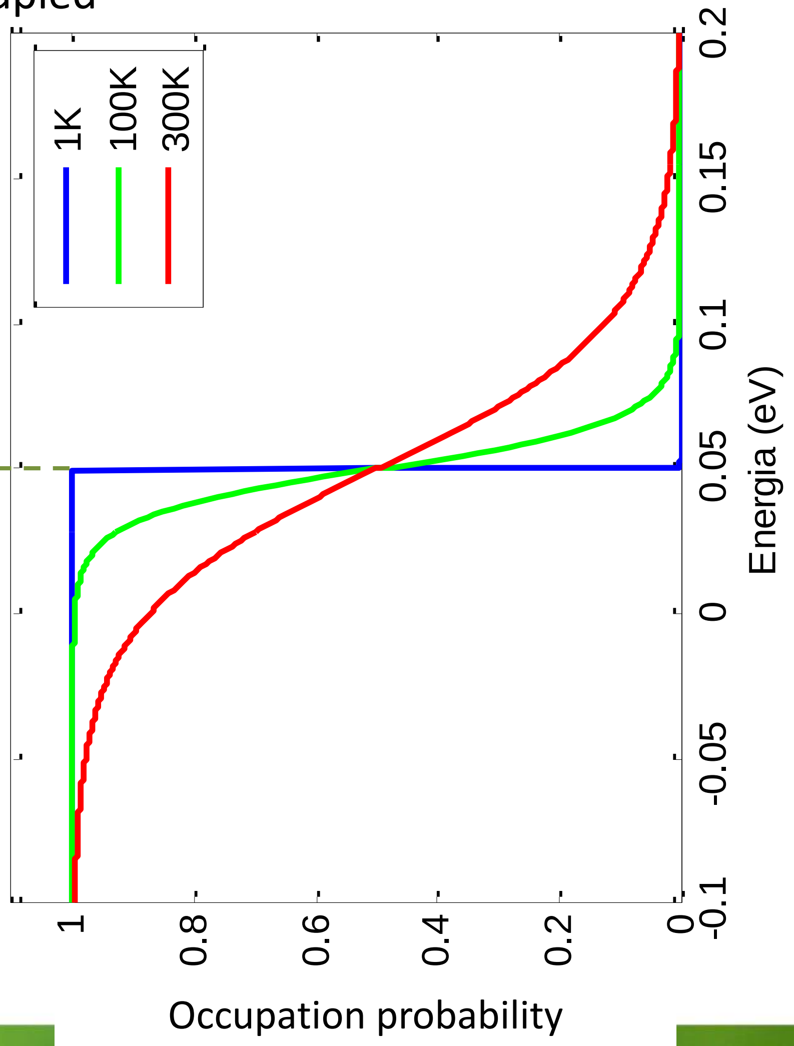

The Fermi-Dirac distribution

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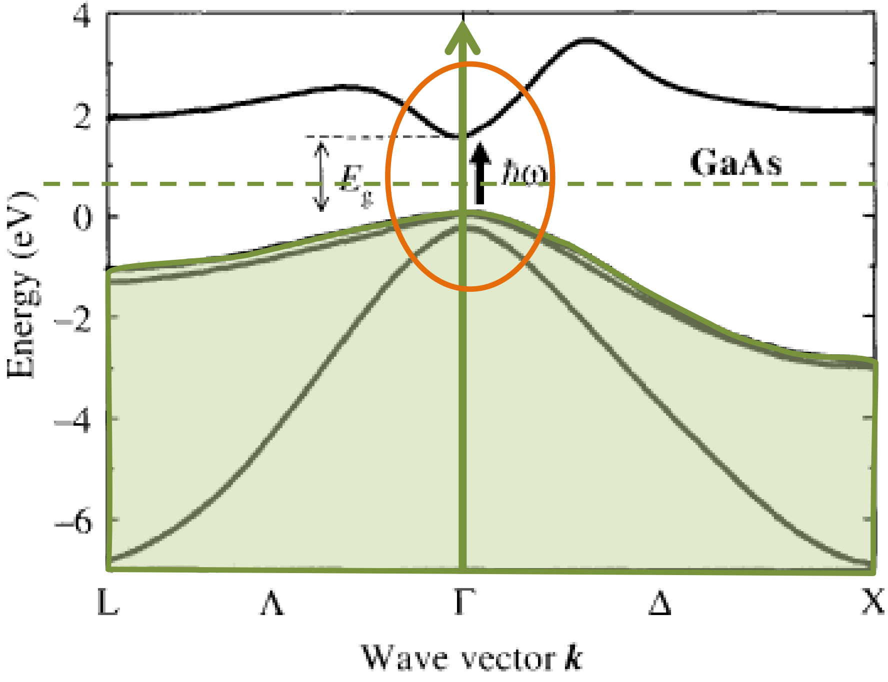
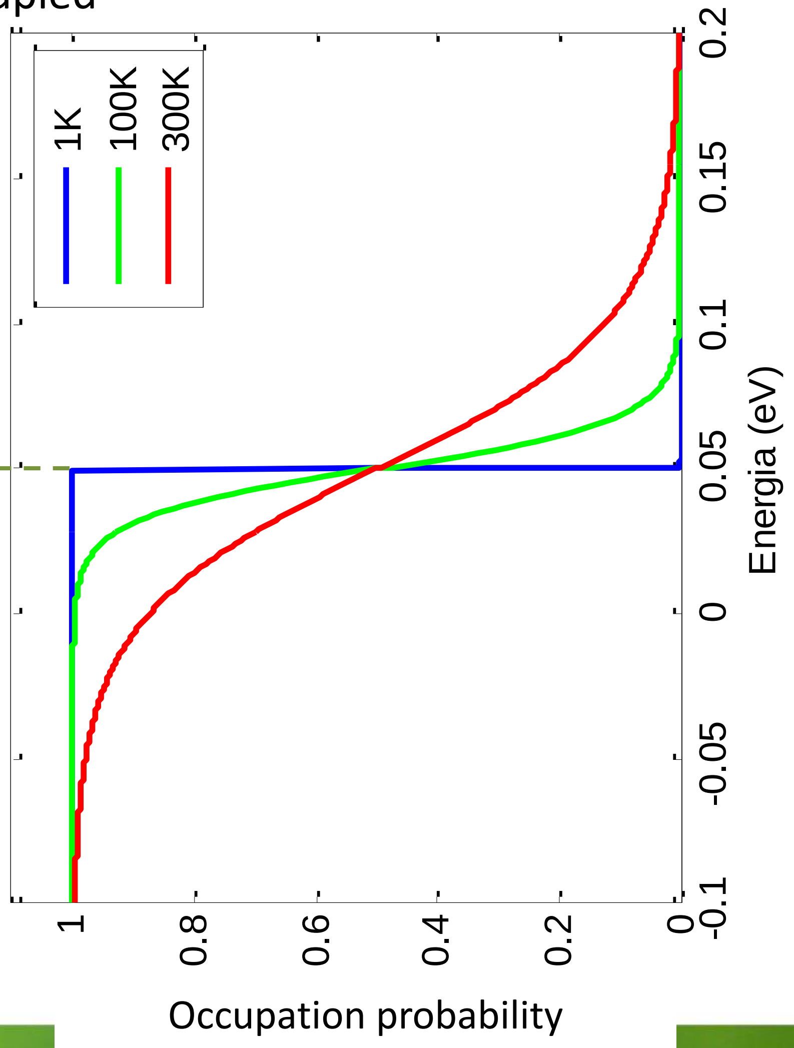
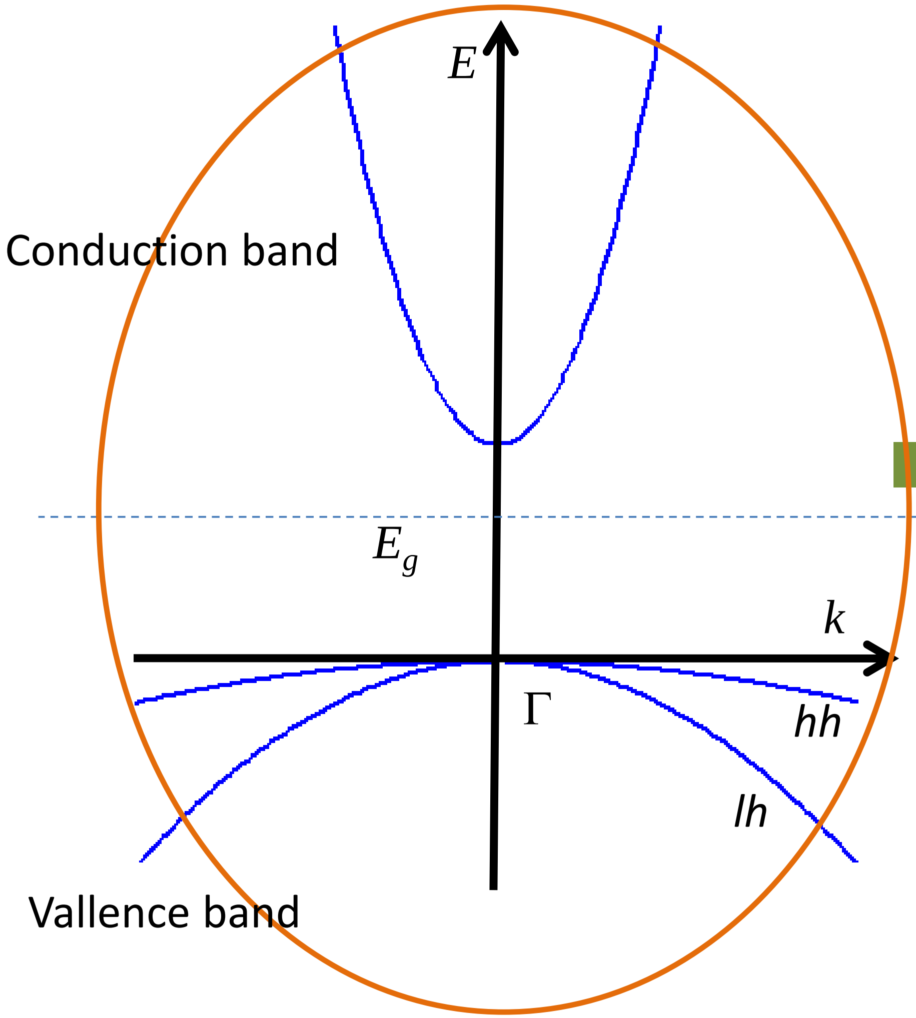
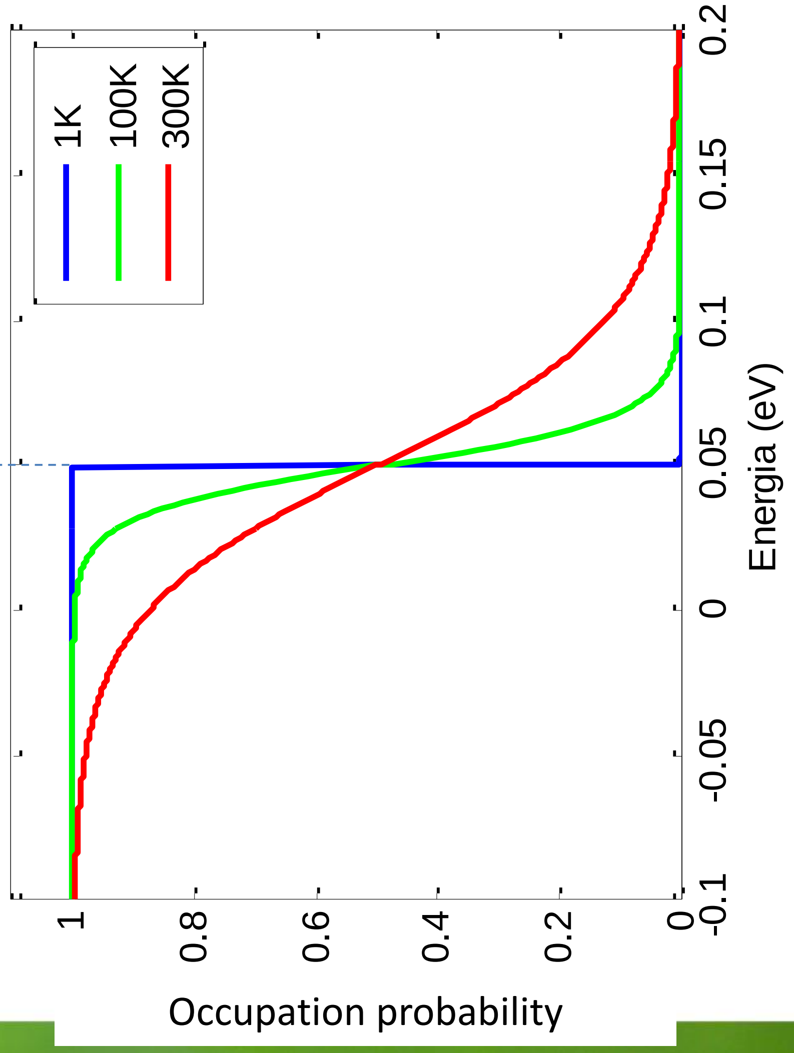




The Fermi-Dirac distribution





Density of states

Density of states Number of states per unit energy $\rho^{nD}(E)$ depends on the dimension

If our crystal has a finite size the set of k –vectors is finite (though enormous!).
For example: we can assume periodic boundary conditions and then:

Born- von Karman boundary conditions

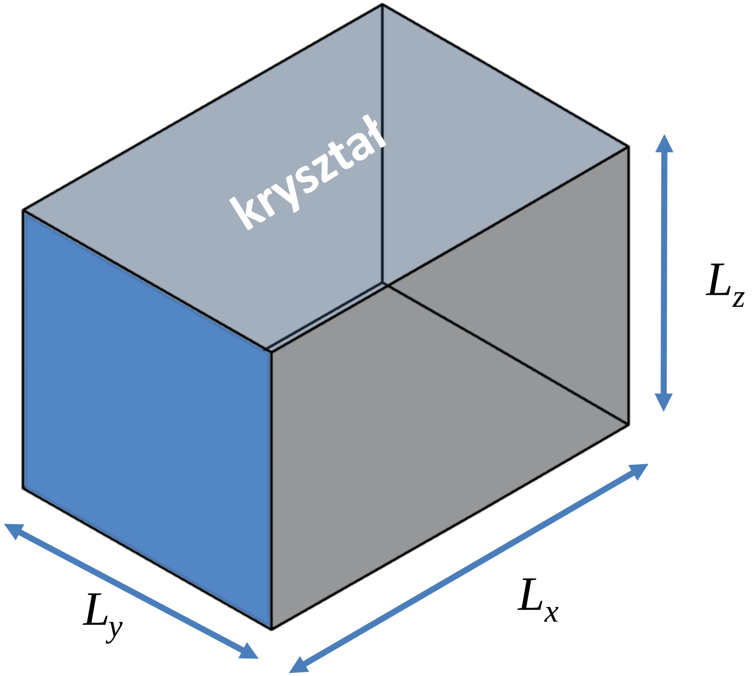
Finite size of the crystal L_x, L_y, L_z

Ψ – the Bloch function

$$\Psi(x + L_x, y, z) = \Psi(x, y + L_y, z) = \Psi(x, y, z + L_z)$$

$$\boxed{\begin{aligned} e^{ik_xL_x} &= 1 \\ e^{ik_yL_y} &= 1 \\ e^{ik_zL_z} &= 1 \end{aligned}}$$

$$\vec{k}_i = 0, \pm\frac{2\pi}{L_i}, \pm\frac{4\pi}{L_i}, \dots, \pm\frac{2\pi n_i}{L_i}$$



Number of states in the volume V $= \dfrac{2}{\dfrac{2\pi}{L_x} \times \dfrac{2\pi}{L_y} \times \dfrac{2\pi}{L_z}} = \dfrac{2V}{(2\pi)^3}$

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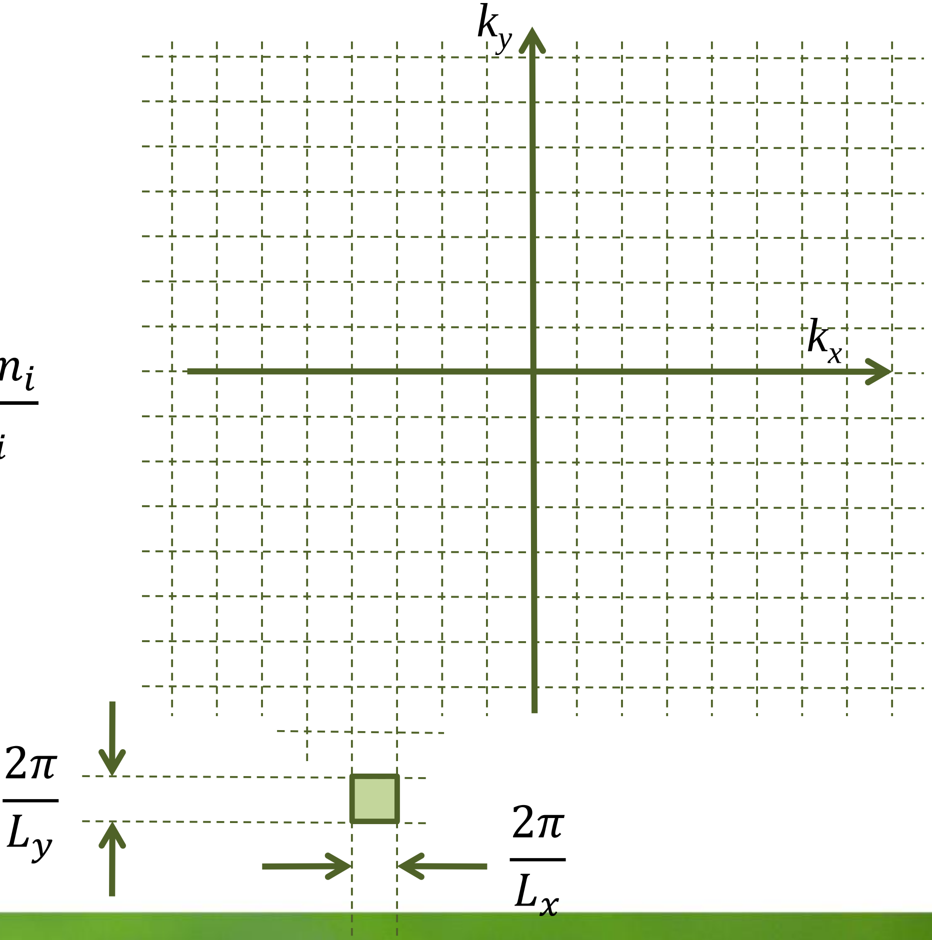
$$\boxed{\begin{array}{l} e^{ik_xL_x} = 1 \\ e^{ik_yL_y} = 1 \\ e^{ik_zL_z} = 1 \end{array}}$$

$$\vec{k}_i = 0, \pm\frac{2\pi}{L_i}, \pm\frac{4\pi}{L_i}, \dots, \pm\frac{2\pi n_i}{L_i}$$

$$\text{Number of states in the volume } V = \frac{2}{\frac{2\pi}{L_x}\times\frac{2\pi}{L_y}\times\frac{2\pi}{L_z}} = \frac{2V}{(2\pi)^3}$$



Density of states

Density of states Number of states per unit energy $\rho^{nD}(E)$ depends on the dimension

The density of states in k-space of n dimension (and the unite volume) $\rho_k^{nD} = 2\left(\frac{1}{2\pi}\right)^{n}$

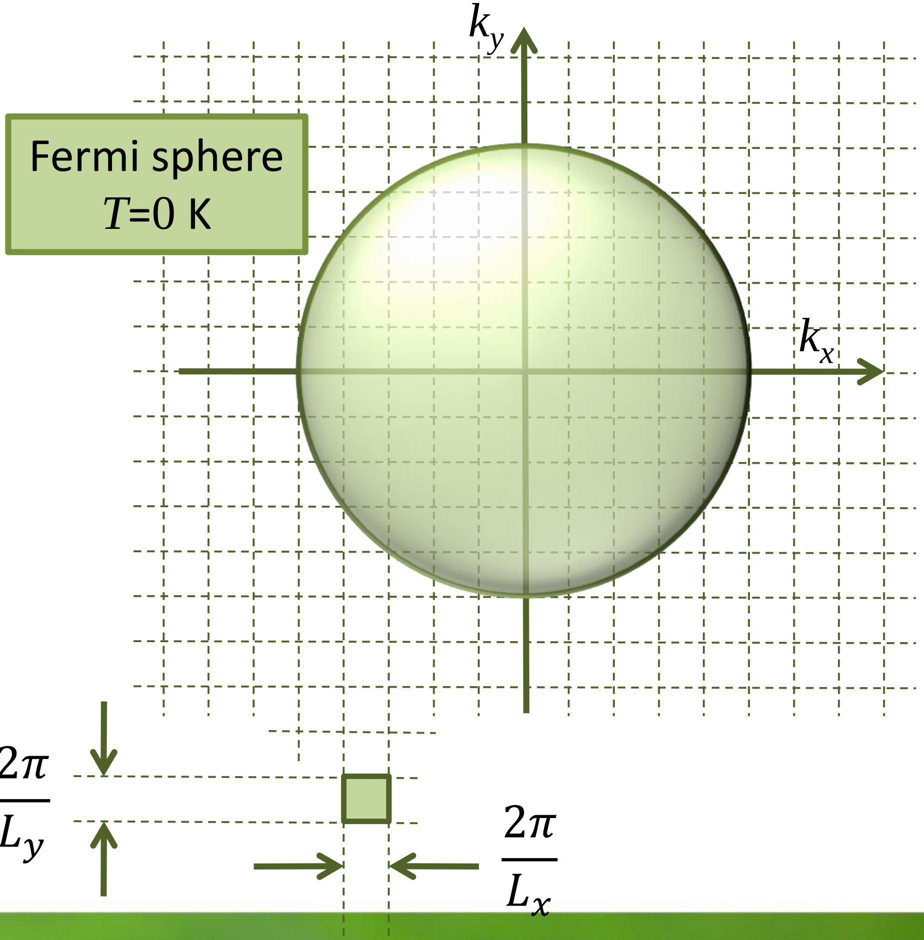
3D case

$$\rho^{3D}(E)dE = \rho_k^{3D}d\vec{k} = 2\left(\frac{1}{2\pi}\right)^3 4\pi k^2 dk$$

For a spherical and parabolic band:

$$\rho_c^{3D}(E) = \frac{1}{2\pi^2}\left(\frac{2m_0 m_c^*}{\hbar^2}\right)^{3/2}\sqrt{E-E_c}$$

$$\rho_v^{3D}(E) = \frac{1}{2\pi^2}\left(\frac{2m_0 m_h^*}{\hbar^2}\right)^{3/2}\sqrt{E_v-E}$$



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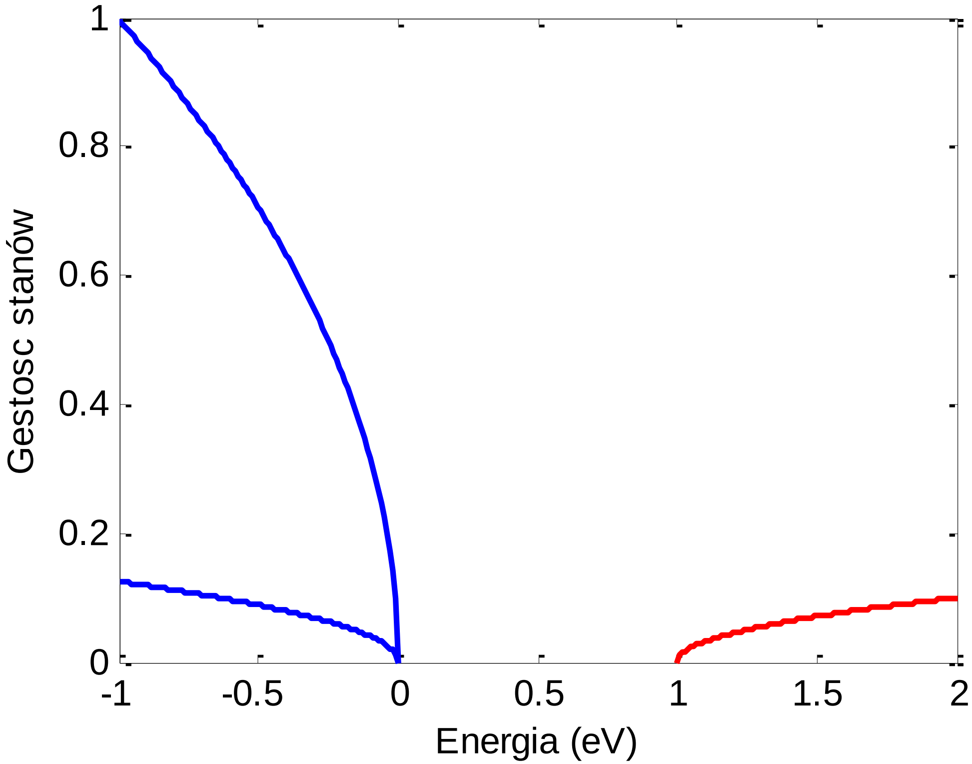

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3D case

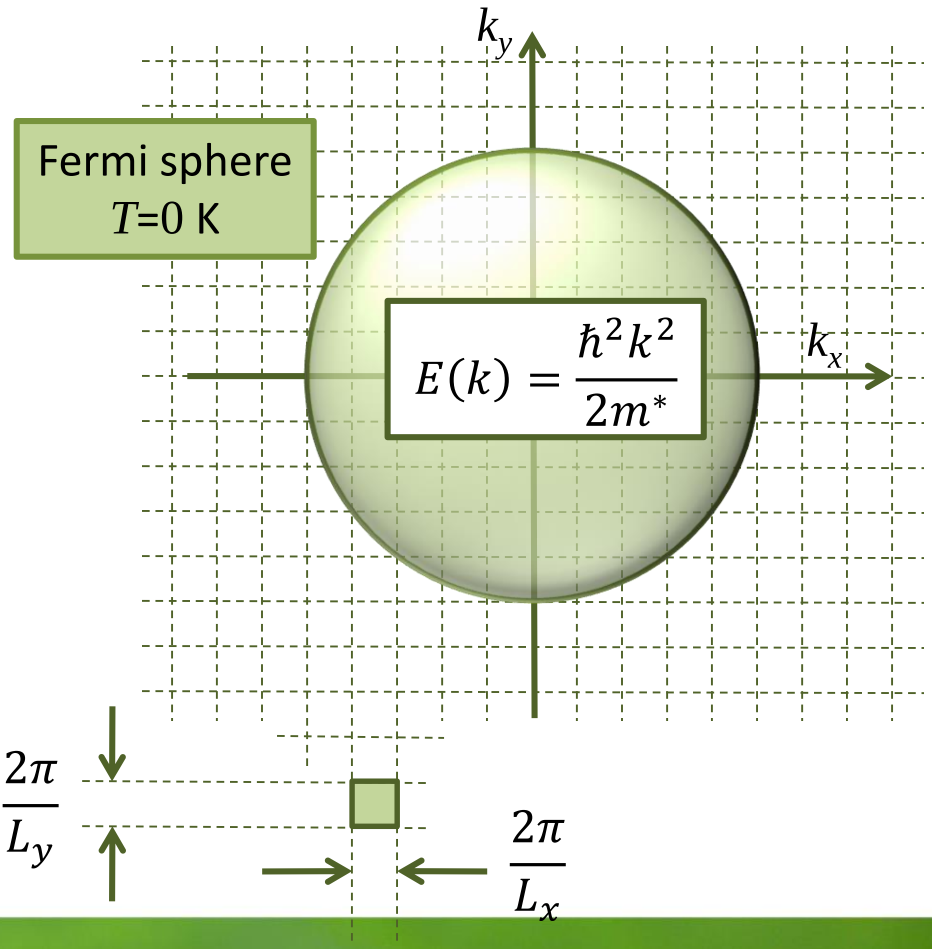
$$\rho^{3D}(E)dE = \rho_k^{3D}d\vec{k} = 2\left(\frac{1}{2\pi}\right)^3 4\pi k^2 dk$$

2D case

$$\rho^{2D}(E)dE = \rho_k^{2D}d\vec{k} = 2\left(\frac{1}{2\pi}\right)^2 2\pi k\, dk$$

1D case

$$\rho^{1D}(E)dE = \rho_k^{1D}d\vec{k} = 2\left(\frac{1}{2\pi}\right)^1 2\, dk$$



Fermi sphere
T=0 K

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

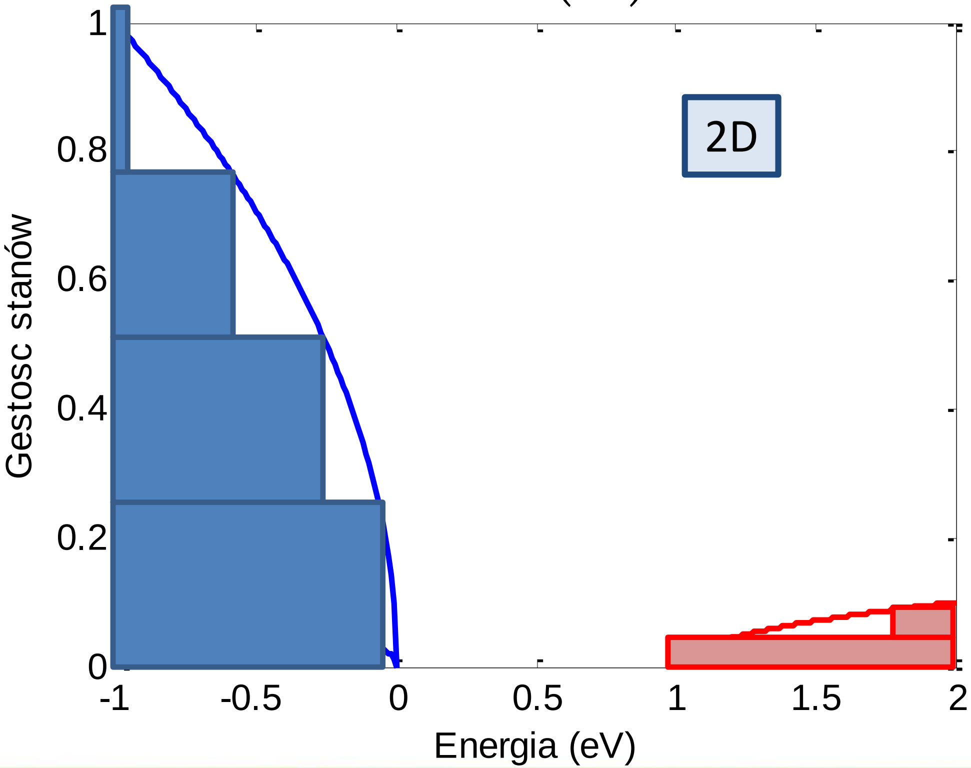
Density of states

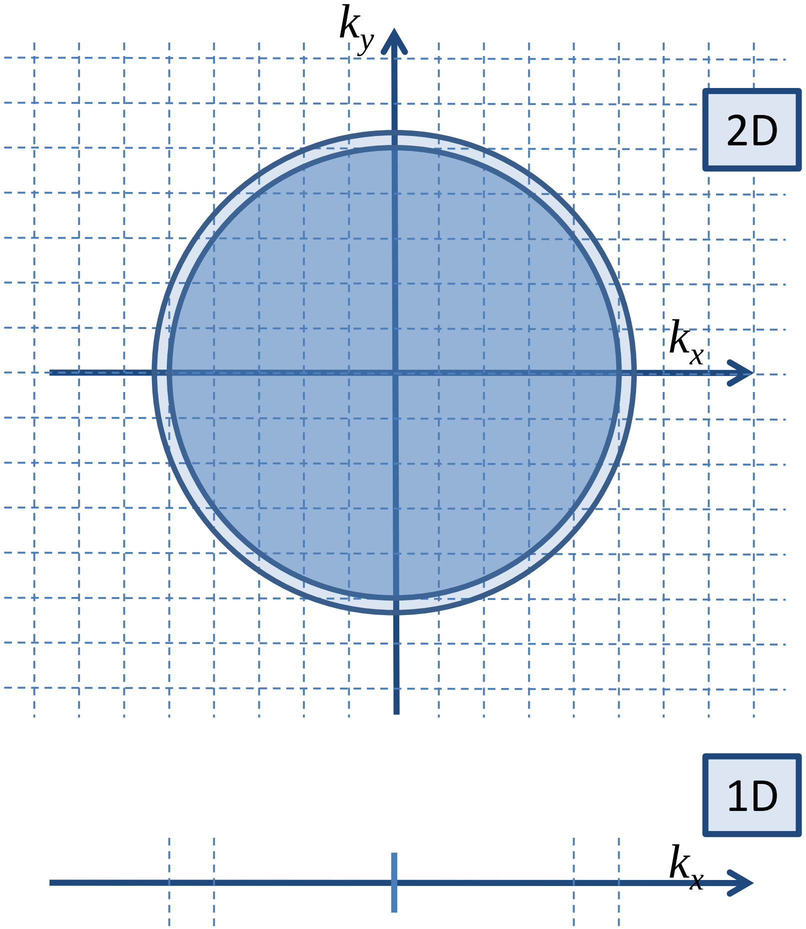
Density of states Number of states per unit energy $\rho^{nD}(E)$ depends on the dimension

The density of states in k-space of n dimension (and the unite volume)
$$\rho_k^{nD} = 2\left(\frac{1}{2\pi}\right)^n$$

2D case

$$\rho^{2D}(E)dE = \rho_k^{2D} d\vec{k} = 2\left(\frac{1}{2\pi}\right)^2 2\pi k\, dk$$



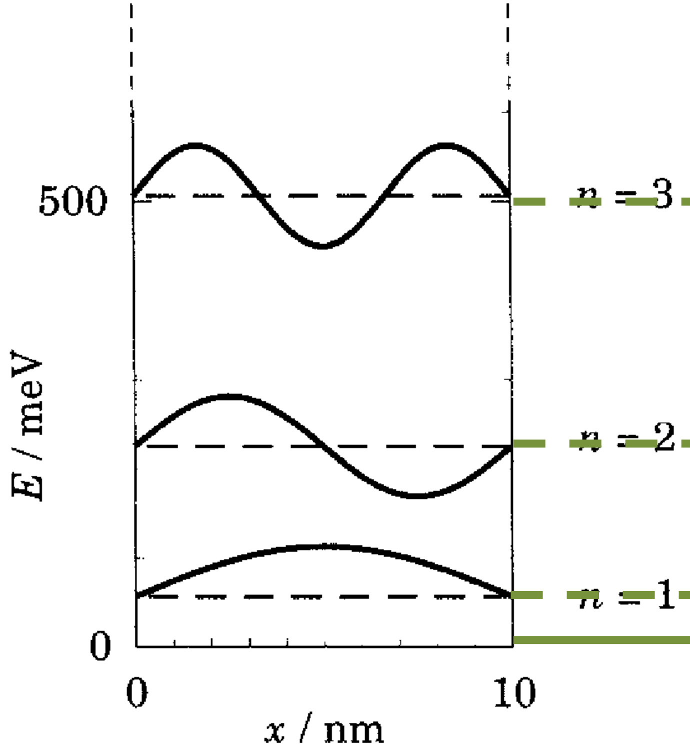


Density of states

Inside the well:

$$\psi(x,t) = \sqrt{\frac{2}{L}}\sin(k_n x\ )\, e^{-i\omega t} \qquad k_n = \frac{n\pi}{L}$$

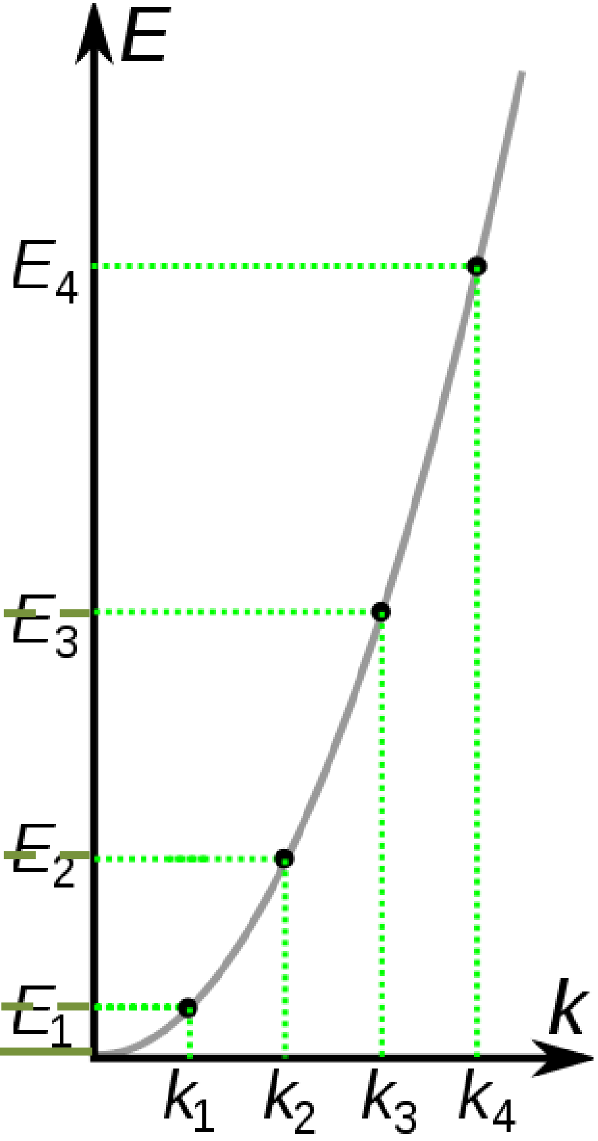
$$\varepsilon_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$



$$\varepsilon_3 = E_c + \frac{9\hbar^2\pi^2}{2m_0 m^* L^2}$$

$$\varepsilon_2 = E_c + \frac{2\hbar^2\pi^2}{m_0 m^* L^2}$$

$$\varepsilon_1 = E_g + \frac{\hbar^2\pi^2}{2m_0 m^* L^2}$$



Density of states

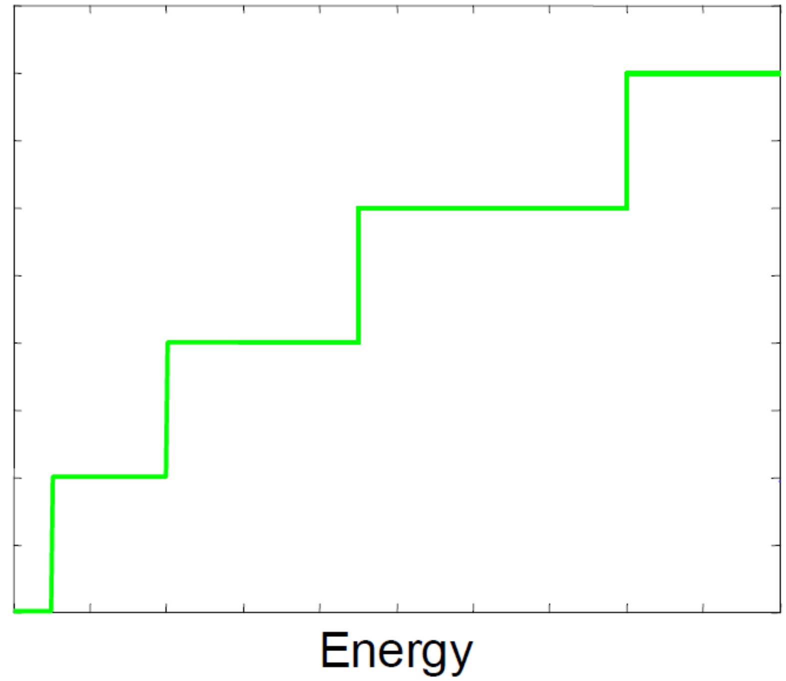
2D density of states for a spherical and parabolic band:

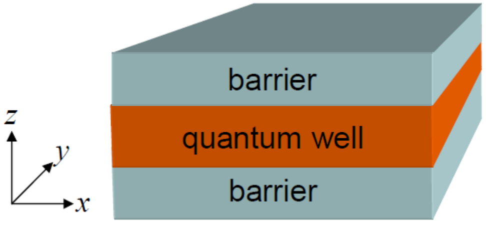
$$\rho^{2D}(E)dE = \rho_k^{2D} d\vec{k} = 2\left(\frac{1}{2\pi}\right)^2 2\pi k\, dk$$

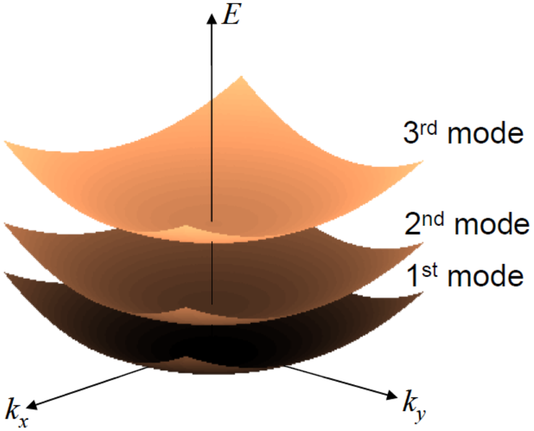
$$\rho_a^{2D}(E)dE = \frac{m_0 m^*}{\pi\hbar^2}\theta(E - E_a)\, dE$$

Step-like θ Heaviside function

$$\rho^{2D}(E)dE = \frac{m_0 m^*}{\pi\hbar^2}\sum_a \theta(E - E_a)\, dE$$







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Density of states – 2D

$$\psi_{k_x,k_y,n}(x,y,z) = \exp(ik_x x)\exp(ik_y y)\,u_n(z) = \psi_{\boldsymbol{k},n}(\boldsymbol{r},z) = \exp(i\boldsymbol{k}\cdot\boldsymbol{r})\,u_n(z)$$

$$E_n(k_x,k_y) = \varepsilon_n + \frac{\hbar^2 k_x^2}{2m} + \frac{\hbar^2 k_y^2}{2m} \qquad E_n(\boldsymbol{k}) = \varepsilon_n + \frac{\hbar^2 \boldsymbol{k}^2}{2m}$$

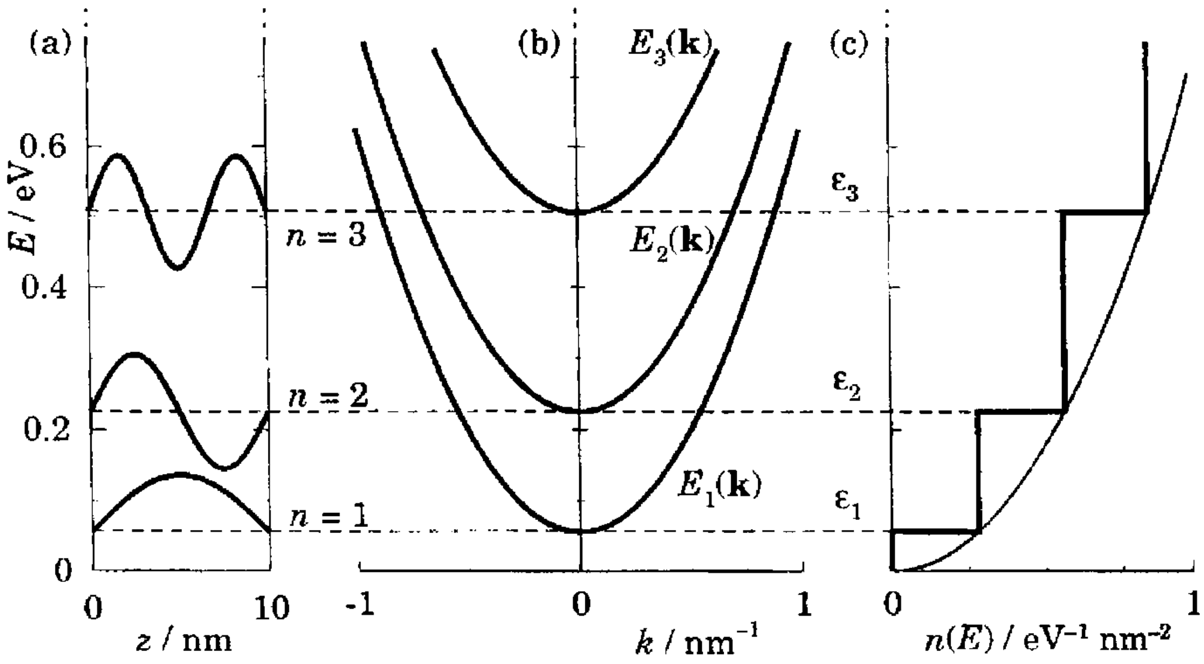


FIGURE 4.7. (a) Potential well with energy levels, (b) total energy including the transverse kinetic energy for each subband, and (c) steplike density of states of a quasi-two-dimensional system. The example is an infinitely deep square well in GaAs of width 10 nm. The thin curve in (c) is the parabolic density of states for unconfined three-dimensional electrons.

Density of states – 2D

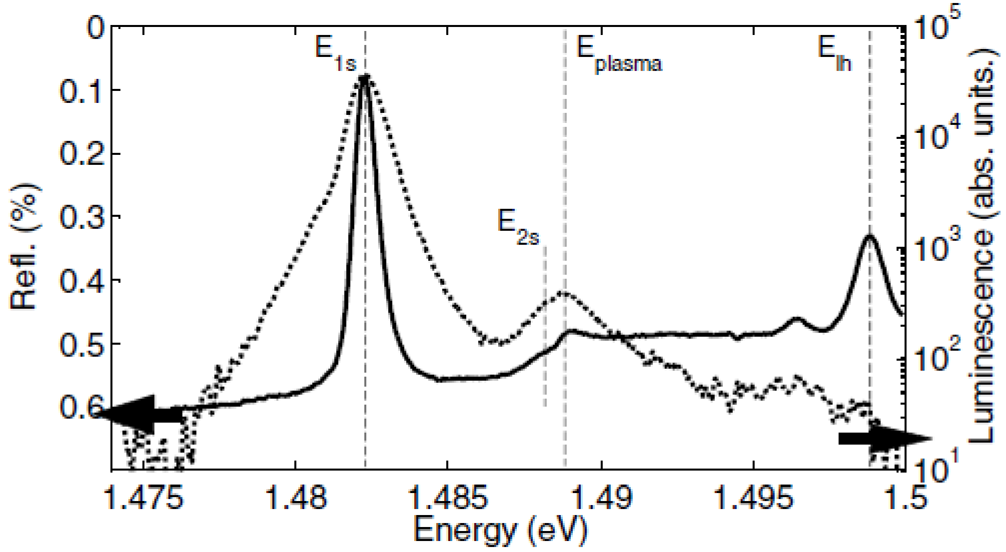


FIG. 1. cw absorption (i.e., 1 − reflectivity; bold line, left axis) and the TR-PL integrated over 1300 ps (logarithmic scale, right) results. $E_{1s} = 1.4823$ eV ($E_{2s} = 1.4882$ eV) is the 1s (2s) heavy-hole exciton, $E_{\mathrm{plasma}} = 1.4888$ eV, light-hole exciton $E_{\mathrm{lh}} = 1.4988$ eV (vertical lines). The low energy exponential tail of the excitonic transition originates from the trion at 1.4807 eV (discussed in [18]).

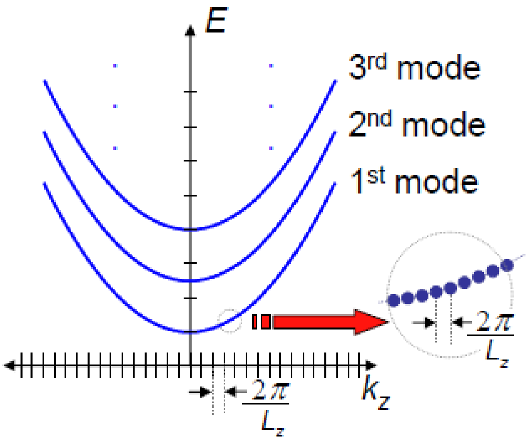
J. Szczytko, et al. Phys. Rev. Lett. 93, 137401 (2004)

Density of states – 1D

1D density of states for a spherical and parabolic band:

$$\rho^{1D}(E)dE = \rho_k^{1D} d\vec{k} = 2\left(\frac{1}{2\pi}\right)^1 2\,dk$$

$$\rho^{1D}(E)dE = \frac{2}{\pi}\sqrt{\frac{m_0 m^*}{2\hbar^2}} \sum_{a_x,a_y} \frac{\theta\left(E - E_{a_x,a_y}\right)}{\sqrt{E - E_{a_x,a_y}}}\,dE$$



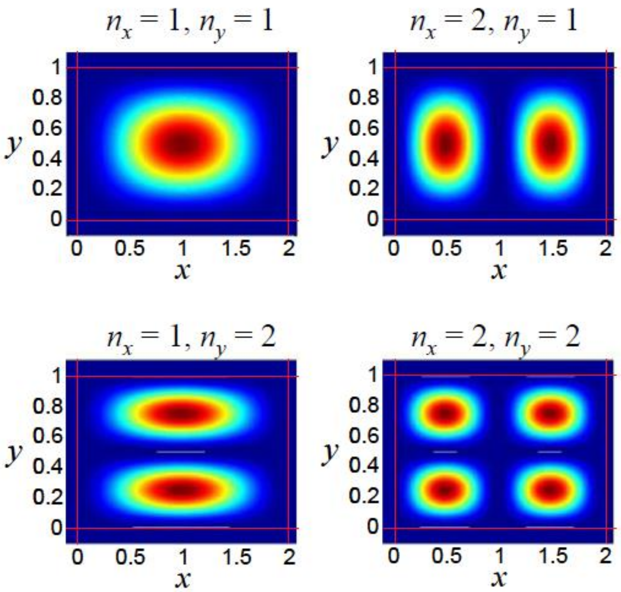
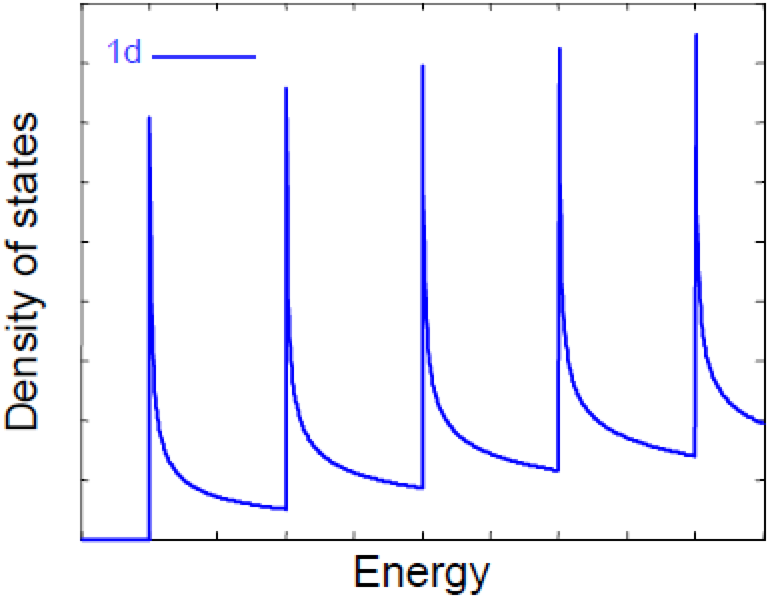


Fig. 2.13. The first four modes of the quantum wire. Since in this example, $L_x > L_y$ the $n_x = 2$, $n_y = 1$ mode has lower energy than the $n_x = 1$, $n_y = 2$ mode.



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Density of states – 1D

0D density of states

For the ISOLATED QD: $\Delta E \rightarrow 0, \Delta t \rightarrow \infty$ $\rho^{0D}(E)dE = g_n \delta(E - E_n)dE$

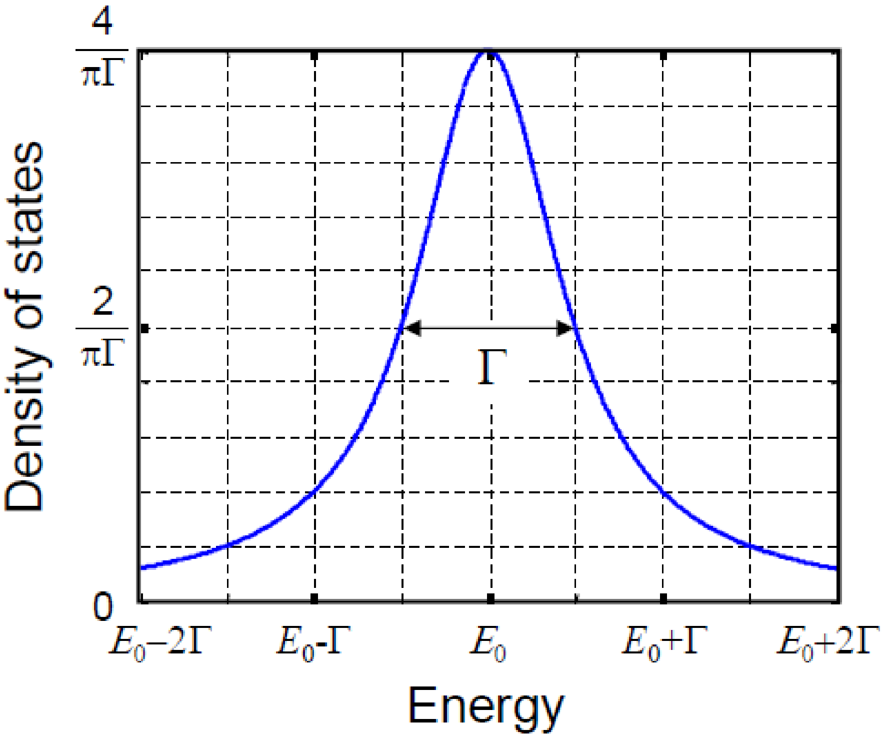
Suppose that the lifetime of the state energy E is equal to τ, we assume an exponential decay

$$|\psi(t)|^2 = |A|^2 \exp\left(-\frac{t}{\tau}\right), \qquad t > 0$$

$$\psi(t) = \mathrm{A} \exp\left(-i\frac{E_0 t}{\hbar} - \frac{t}{2\tau}\right), \qquad t > 0$$

Fourrier transform

$$\psi(\omega) = \frac{A}{\frac{1}{2\tau} + i\left(\frac{E_0}{\hbar} - \omega\right)}$$



Lorentz profile

$$\rho^{0D}(E)dE = \frac{1}{2\pi}|\psi(\omega)|^2 \frac{d\omega}{dE} = \frac{2}{\pi} \frac{\frac{\hbar}{2\tau}}{(E - E_0)^2 + \left(\frac{\hbar}{2\tau}\right)^2}$$

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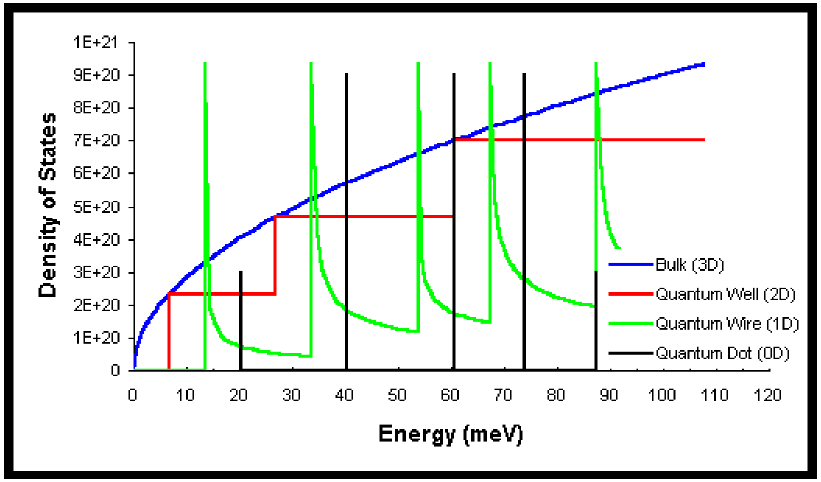
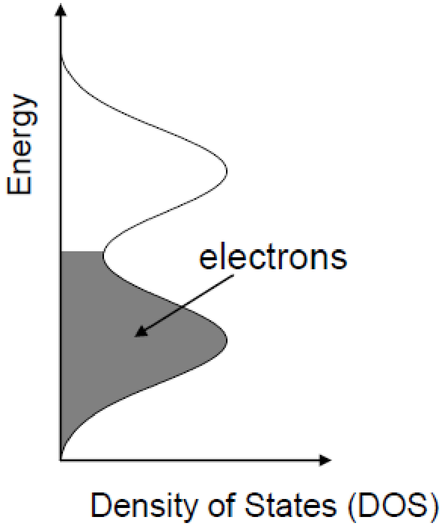
Density of states – the summary

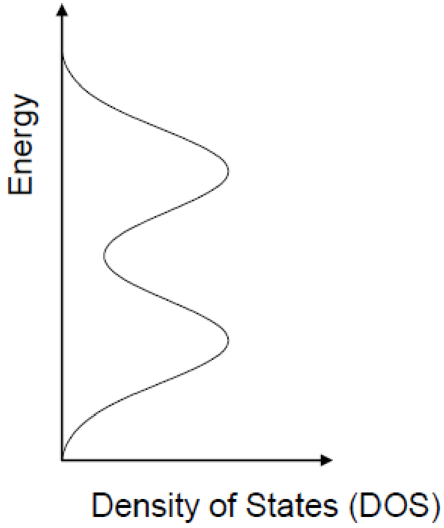
Density of states



(a) Partly filled = metal



(b) Completely filled or empty
= insulator or semiconductor



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Electrons statistics in crystals

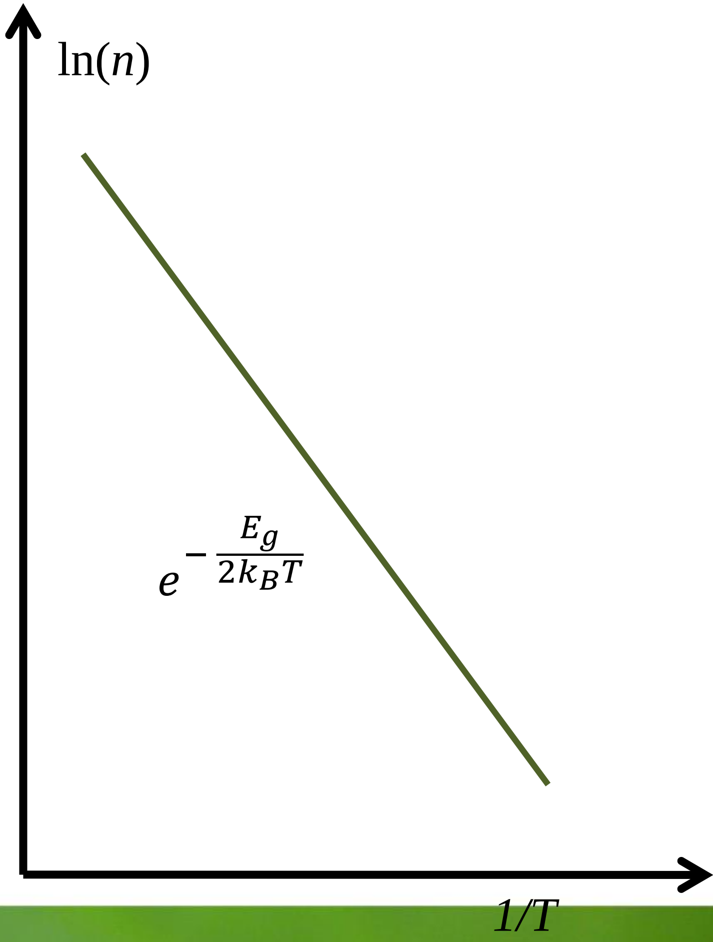
What is the concentration of carriers for T>0?

In the thermodynamic equilibrium for an intrinsic semiconductors (*półprzewodniki samoistne*), the concentration of electrons in the conduction band is equal to the concnetration of holes in the valence band (because they appear only as a result of excitation from the valence band).

$n = p = n_i$ (an intrinsic case)

$$n \cdot p = n_i^2 = 4\left(\frac{k_B T}{2\pi\hbar^2}\right)^3 (m_e^* m_h^*)^{\frac{3}{2}}\, e^{-\frac{E_g}{k_B T}} = N_c N_v e^{-\frac{E_g}{k_B T}}$$

$$n = p = n_i = 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}} (m_e^* m_h^*)^{\frac{3}{4}}\, e^{-\frac{E_g}{2k_B T}} = \sqrt{N_c N_v} e^{-\frac{E_g}{2k_B T}}$$



Intrinsic carrier concentration

What is the concentration of carriers for T>0?

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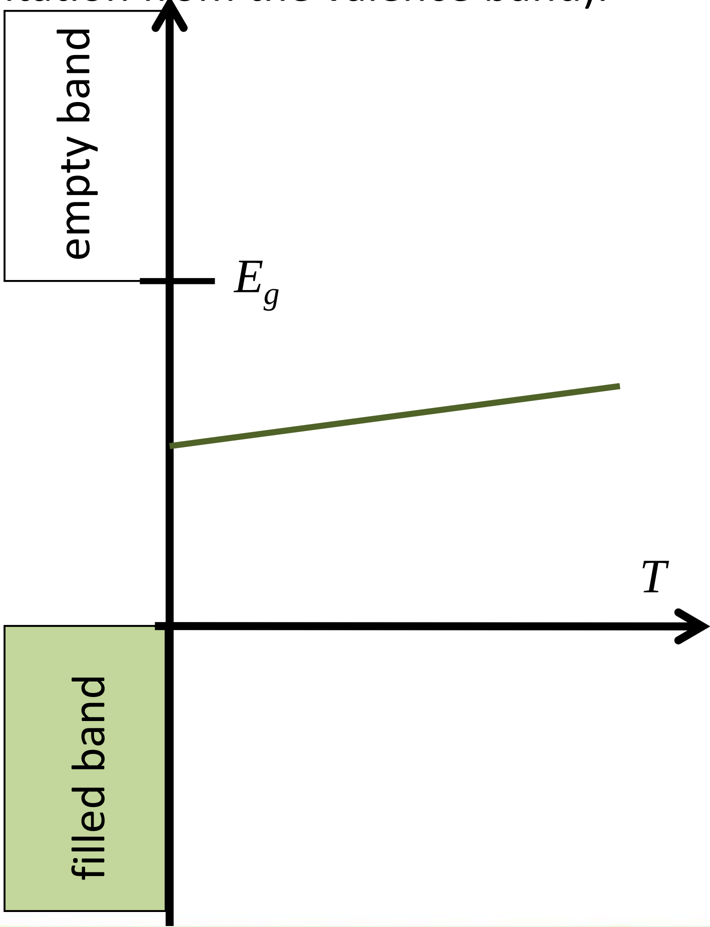
(general formula)

$n = p = n_i$ (an intrinsic case)

$$n = p = n_i = 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}} (m_e^* m_h^*)^{\frac{3}{4}}\, e^{-\frac{E_g}{2k_B T}} = \sqrt{N_c N_v}\, e^{-\frac{E_g}{2k_B T}}$$

$$\frac{N_c}{N_v} = e^{\frac{2\xi - E_g}{k_B T}} \Rightarrow \xi = \frac{1}{2}(E_c + E_v) + \frac{3}{4} k_B T \ln\left(\frac{m_h^*}{m_e^*}\right)$$

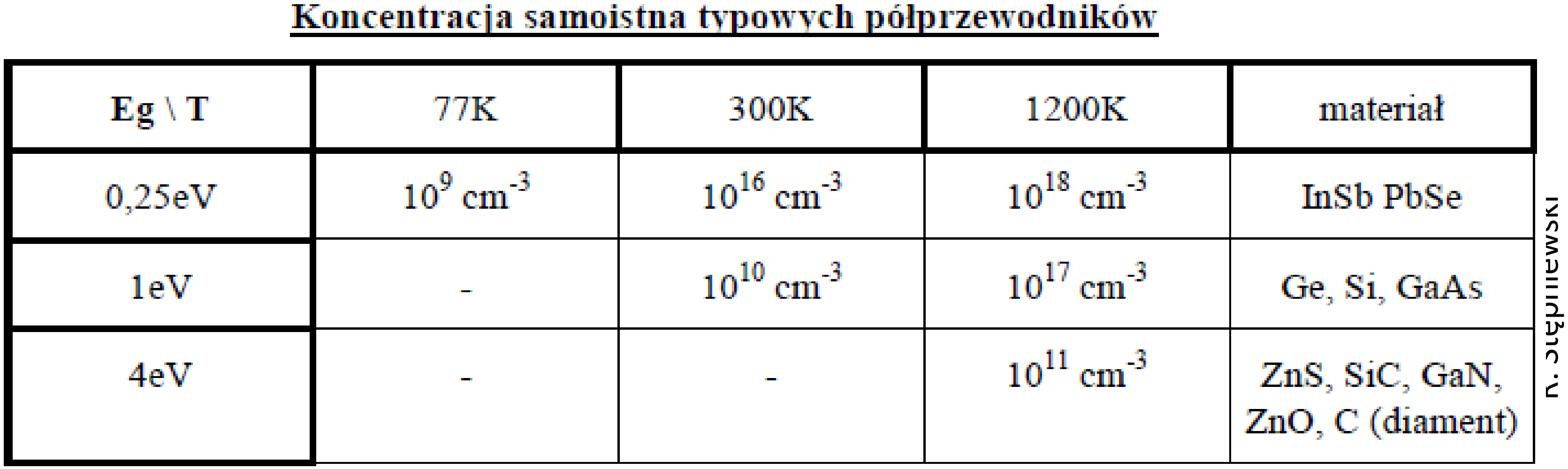
in our notation the middle of the band is 0



Intrinsic carrier concentration

What is the concentration of carriers for T>0?

The intrinsic semiconductors (*półprzewodniki samoistne*) in thermal equilibrium, the concentration of electrons in the conduction band is equal to the concnetration of holes in the valence band.



Koncentracja samoistna typowych półprzewodników

Eg \ T	77K	300K	1200K	materiał
0,25eV	10^9 cm^{-3}	10^{16} cm^{-3}	10^{18} cm^{-3}	InSb PbSe
1eV	-	10^{10} cm^{-3}	10^{17} cm^{-3}	Ge, Si, GaAs
4eV	-	-	10^{11} cm^{-3}	ZnS, SiC, GaN, ZnO, C (diament)

R. Stępniewski

The concentration values less than 10^{10} cm^{-3} do not make sense because the concentration of impurities, and thus the concentration resulting from unintentional doping, is greater

$$n = p = \sqrt{N_c N_v} e^{-\frac{Eg}{2k_B T}}$$

$$n = N_c \, e^{\frac{E_F - E_c}{k_B T}}$$

$$p = N_v \, e^{-\frac{E_F - E_v}{k_B T}}$$

Dopants, impurities and defects

Carriers:

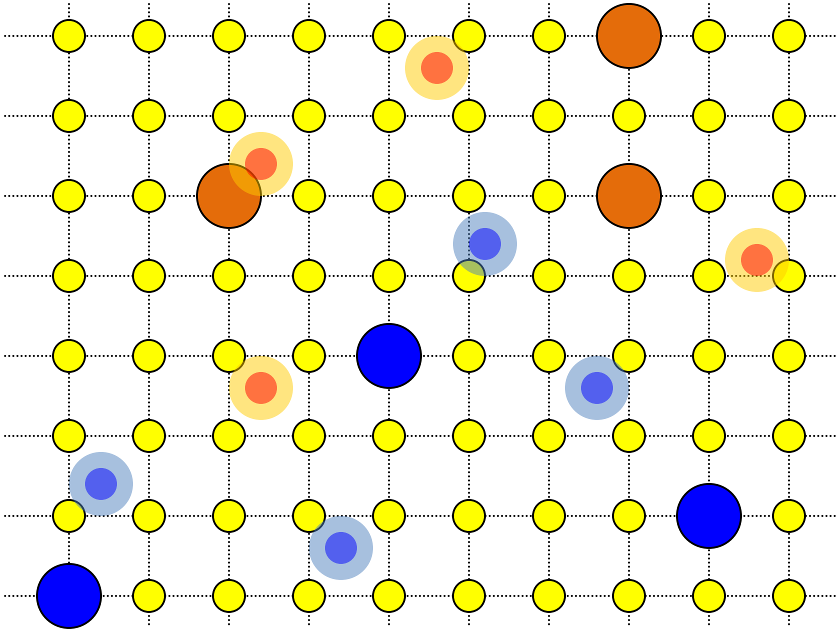
holes ● +

electrons ● -

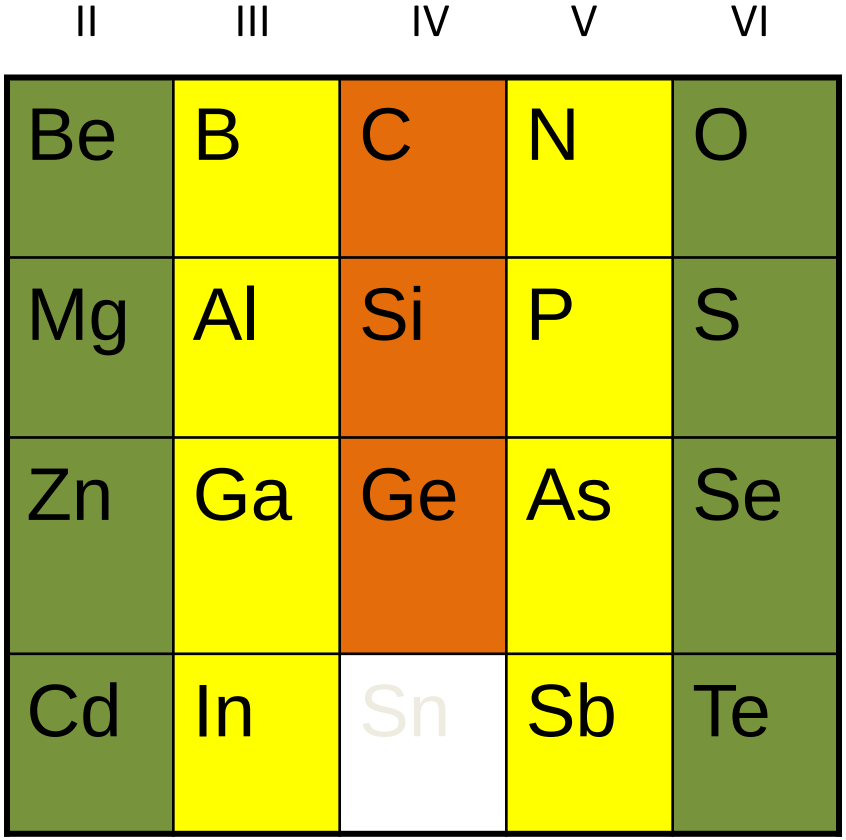
Dopants:

● Acceptors (p-type)

● Donors (n-type)



Semiconductors



II	III	IV	V	VI
Be	B	C	N	O
Mg	Al	Si	P	S
Zn	Ga	Ge	As	Se
Cd	In	Sn	Sb	Te

Group IV: diamond, Si, Ge

Group III-V: GaAs, AlAs, InSb, InAs...

Group II-VI: ZnSe, CdTe, ZnO, SdS...

Dopants, impurities and defects

How to control the concentration of carriers?

In semiconductors we can find several deviations from the ideal crystal structure:
· Defects of the crystal structure, vacancies, the atoms in interstitial positions, dislocations created eg. during the growth process.
· Foreign atoms (dopants) introduced intentionally or by adding impurities

As a result of their presence:
· allowed states in the forbidden gap due to deviations from the ideal crystalline potential
· space charges in insulators
· screening by free carriers

Dopant states can be classified into:
· Deep - the short-range potential located mainly in the area of one unit cell - eg. a vacancy, izoelectronics dopant (the same valency as atom of the base material e.g. N InP).
· Shallow - mainly long-range Coulomb potential

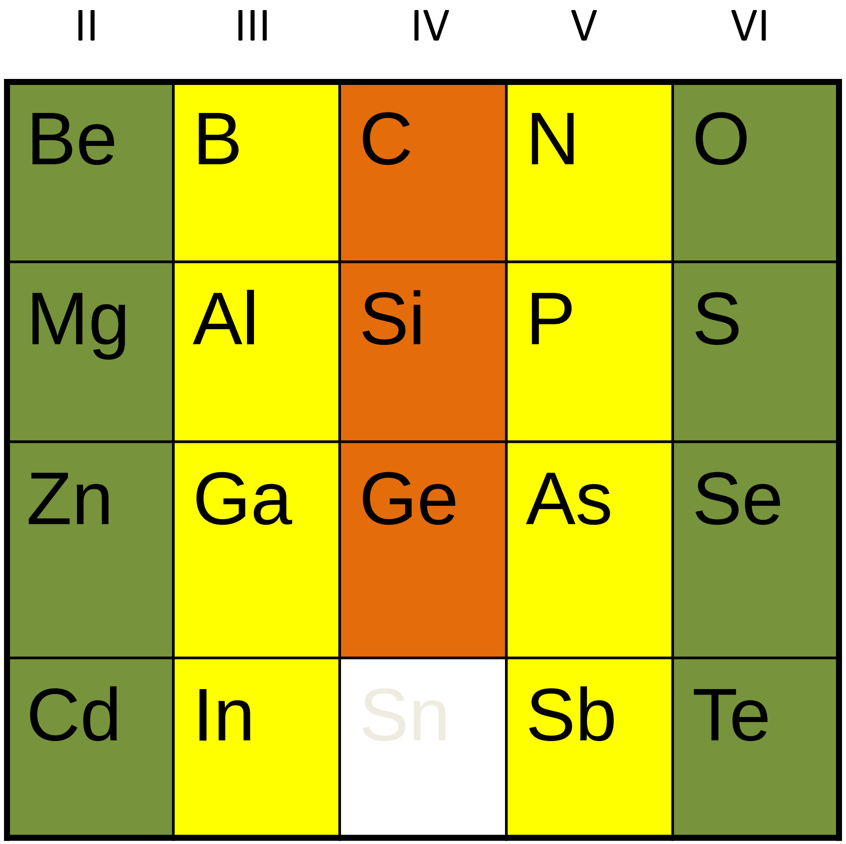
Dopants, impurities and defects

Hydrogen-like model

Atom of a valency higher than the base material atom becomes a source of Coulomb potential (modified by the dielectric constant of the crystal ε_r) caused by an extra proton in the nucleus. Extra electron in the conduction band feels this potential. The states are described by the effective mass equation:

$$T = -\frac{\hbar^2}{2m^*}\Delta \qquad U = -\frac{1}{4\pi\varepsilon_0}\frac{e^2}{\varepsilon_r r}$$

$$[T+U]\phi(\vec{r}) = E\phi(\vec{r})$$



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Dopants, impurities and defects

Hydrogen-like model

Finally, the problem reduces to the problem of hydrogen atpom with a free carrier of mass m^* in the medium of dielectric constant ε and with a small "perturbation" potential.

$$E_n = -\left(\frac{m^*}{m_0}\right)\frac{1}{\varepsilon_r^2}Ry\frac{1}{n^2}$$

For typical semiconductors $m_e^* \approx 0.1 m_e$ $\varepsilon_s \approx 10$

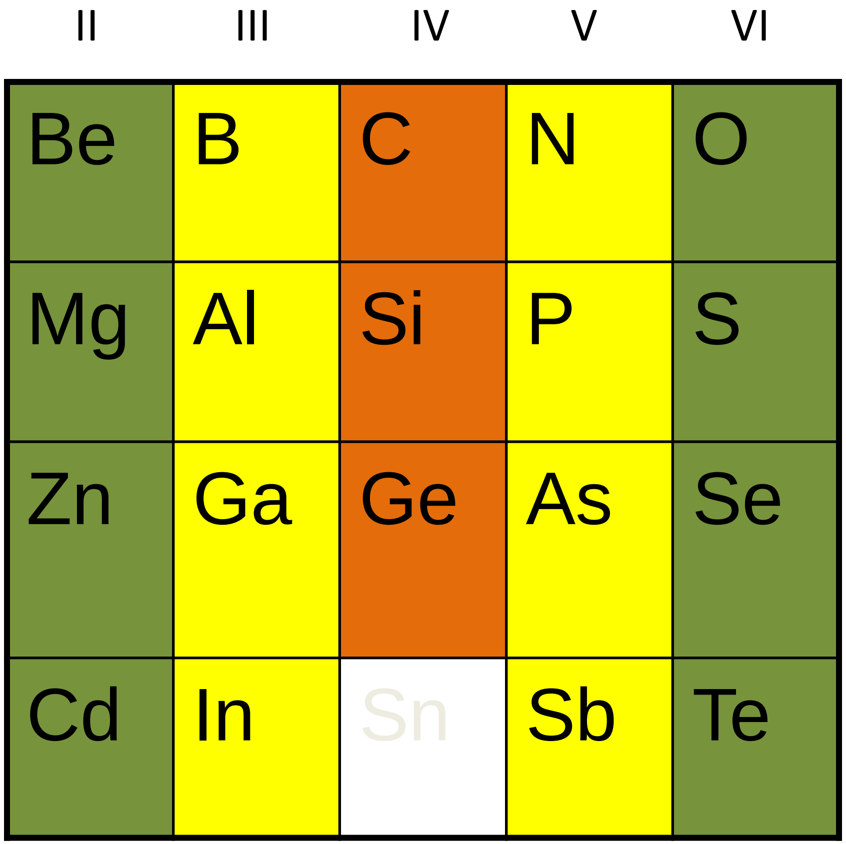
$$a_B^* = \frac{4\pi\varepsilon_r\varepsilon_0\hbar^2}{m_0 e^2}\left(\frac{m_0}{m^*}\right) = a_B\varepsilon_r\left(\frac{m_0}{m^*}\right)$$

For Hydrogen

$Ry = 13.6$ eV and $a_B = 0.053$ nm

For GaAs semiconductor

$Ry^* \approx 5$ meV and $a_B^* \approx 10$ nm



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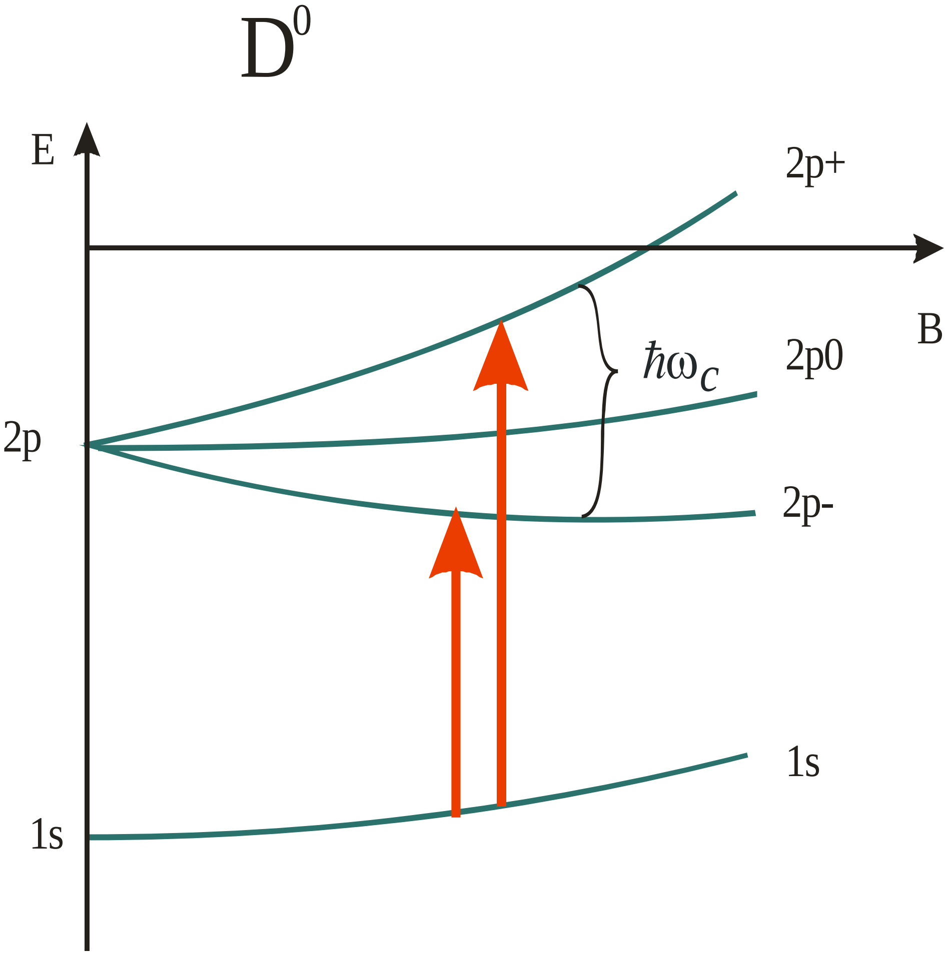
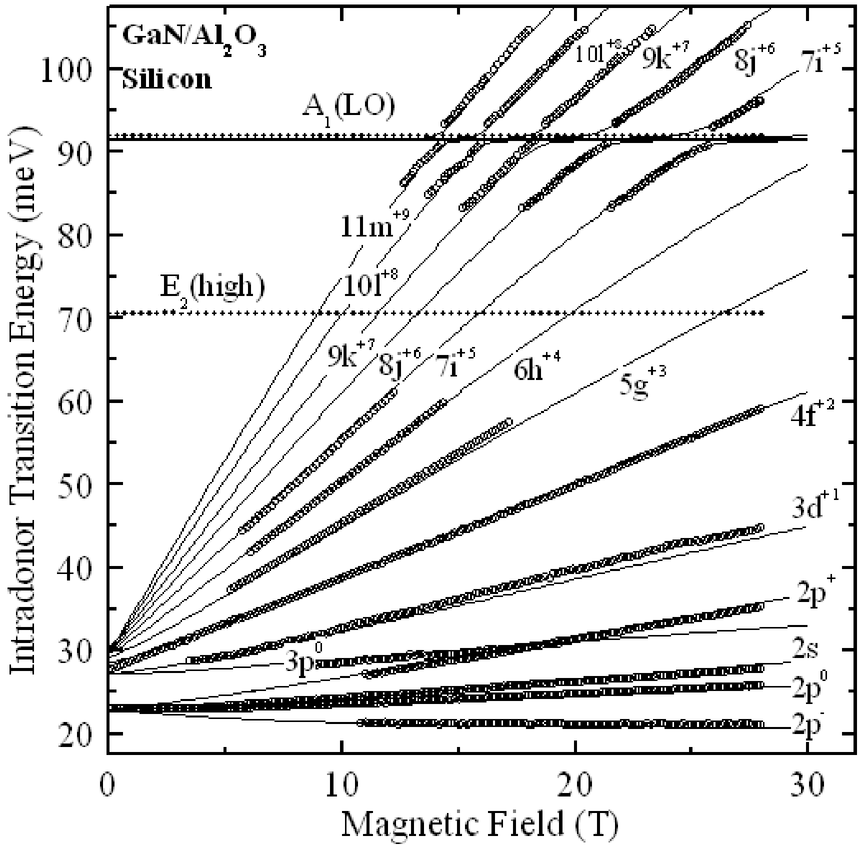
Far infrared spectroscopy

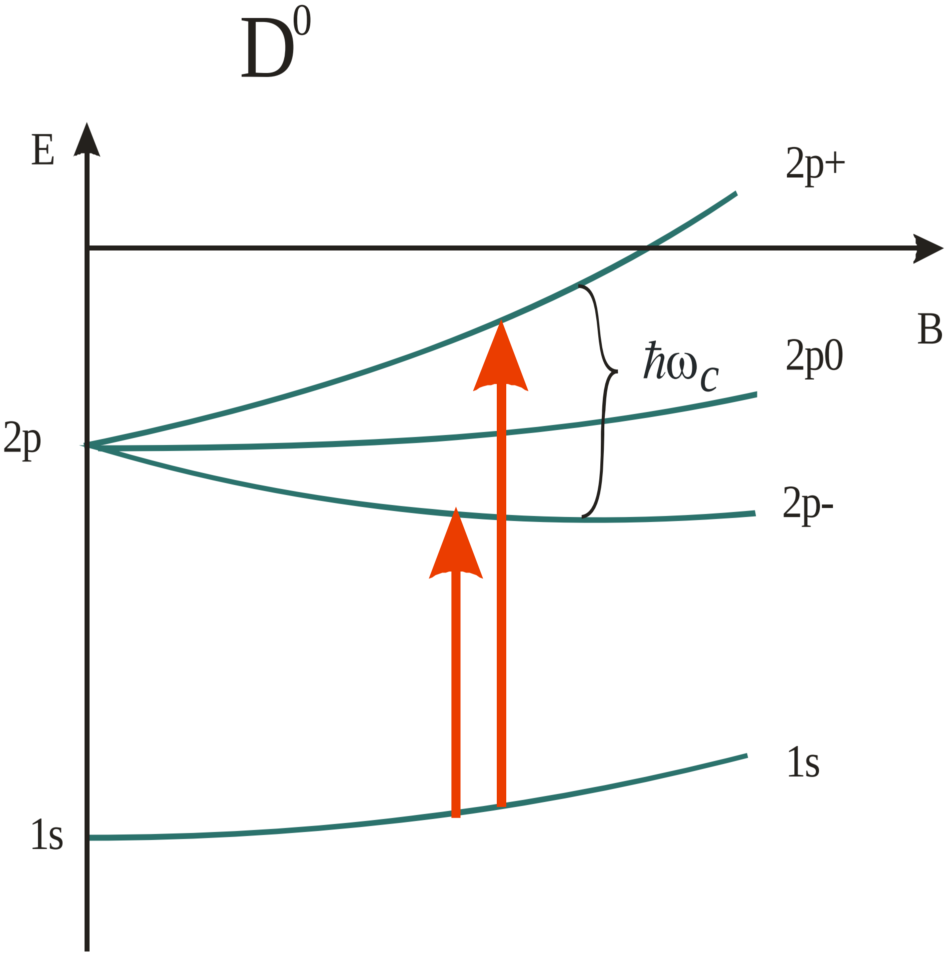


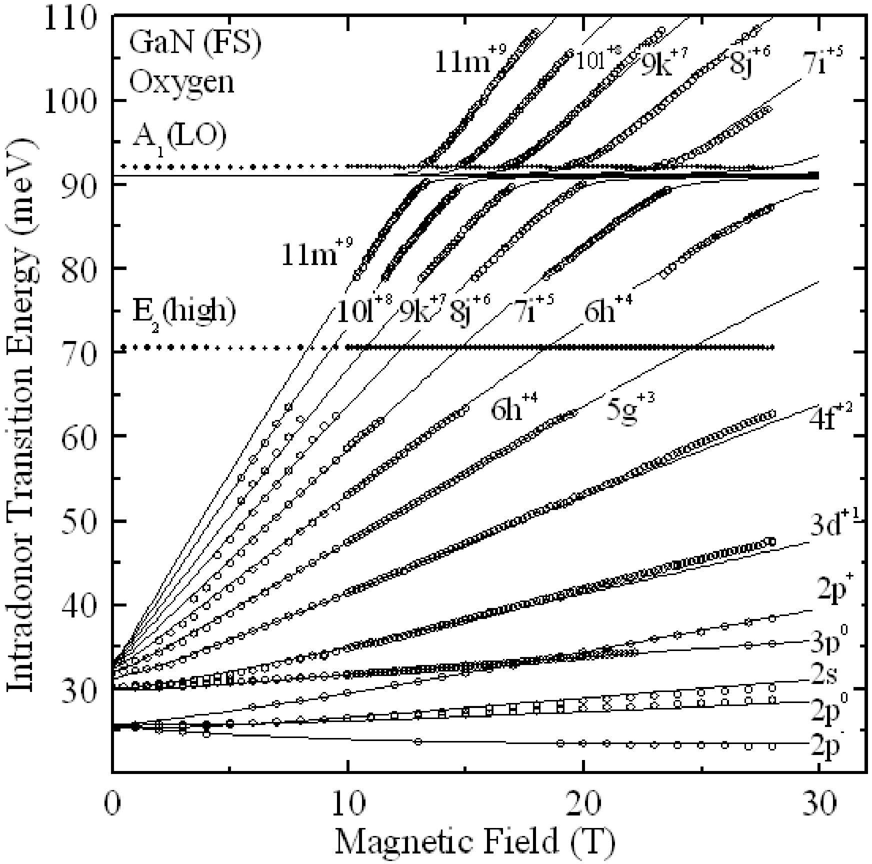


Silicon

R_y=30.28(5) meV

Far infrared spectroscopy



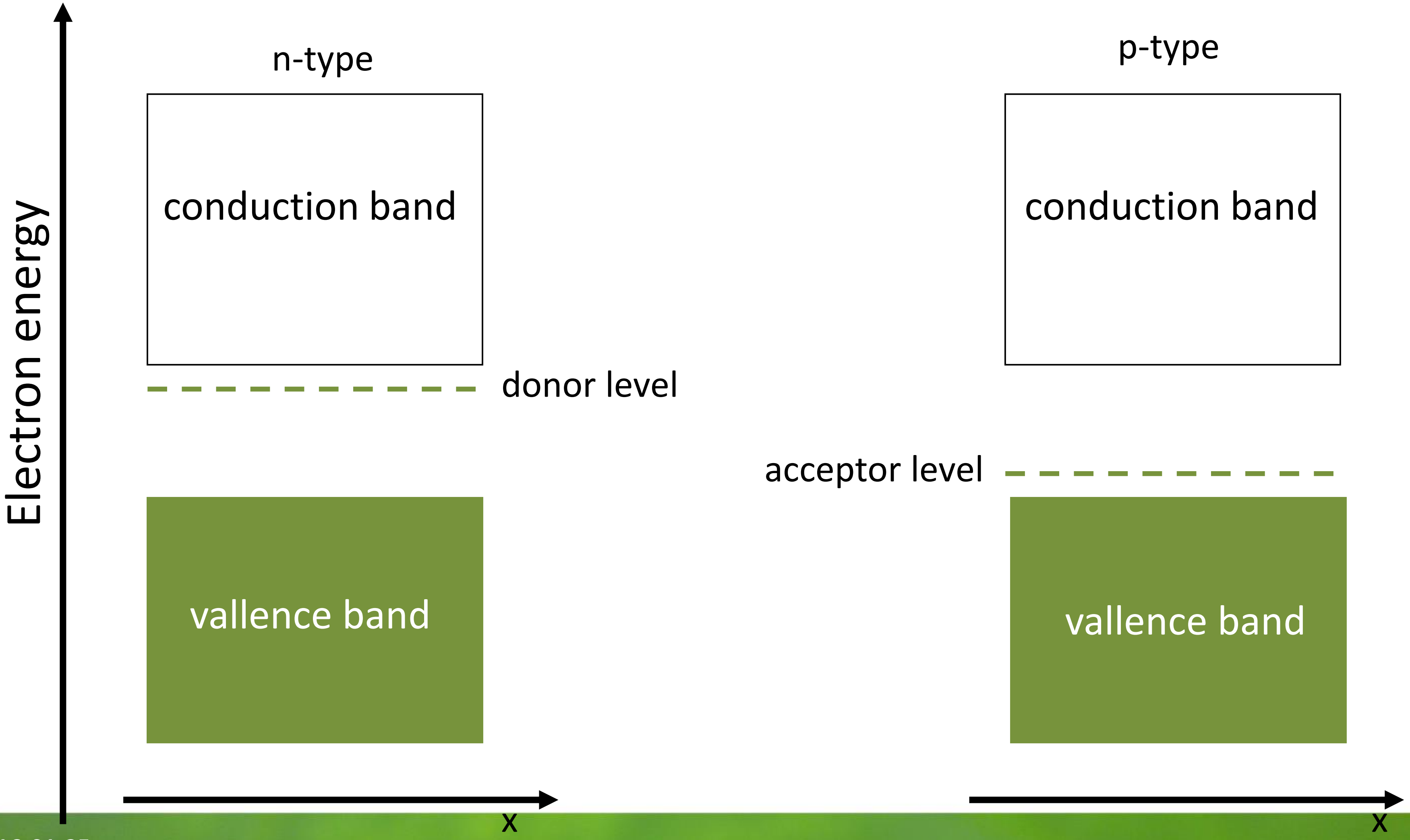


Oxygen

R_y=30.28(5) meV

Dopants, impurities and defects

Hydrogen-like model – ionization of the dopant



Electron energy

n-type

conduction band

donor level

valence band

x

p-type

conduction band

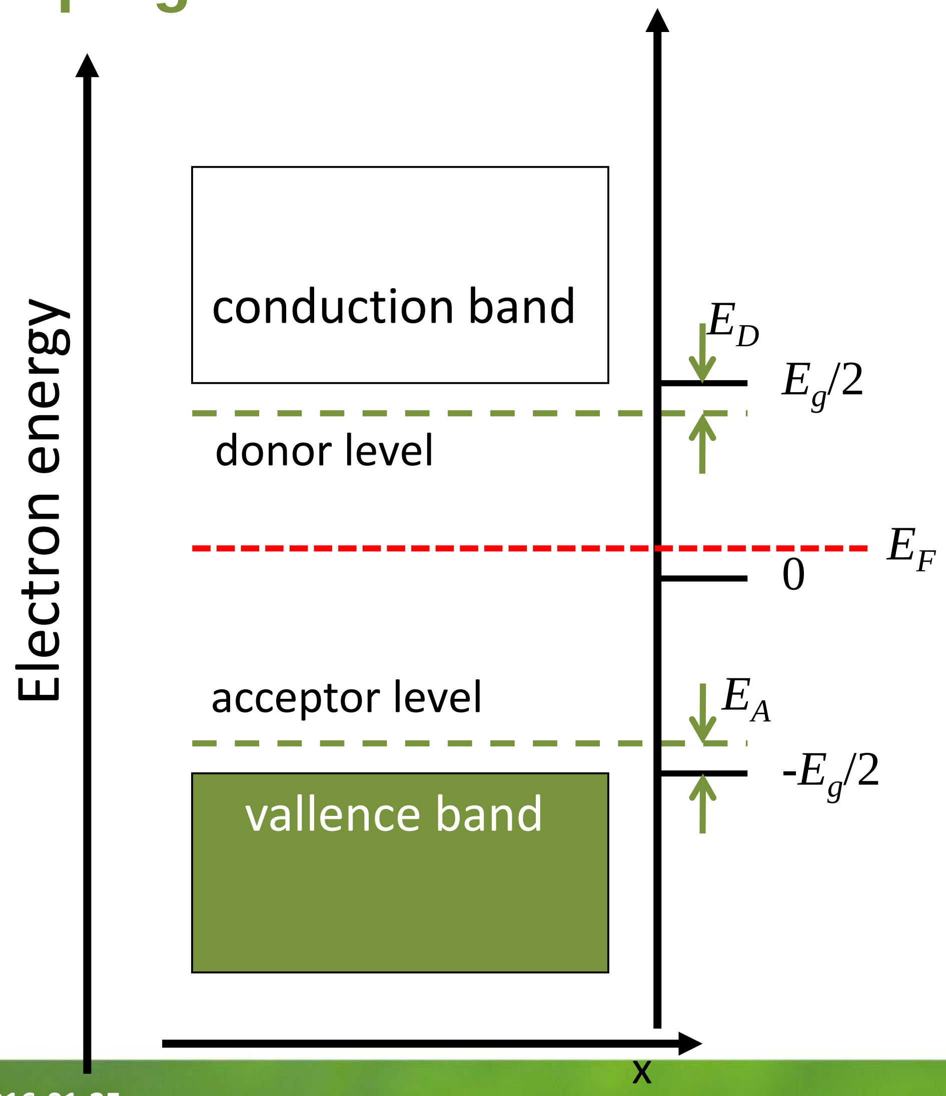
acceptor level

valence band

x

Dopants, impurities and defects

Doping



The carrier concentration in extrinsic semiconductor (*niesamoistny*)

Consider a semiconductor, in which:

N_A – concentration of acceptors

N_D – concentration of donors

p_A – concentration of neutral acceptors

n_D – concentration of neutral donors

n_c – concentration of electrons in conduction band

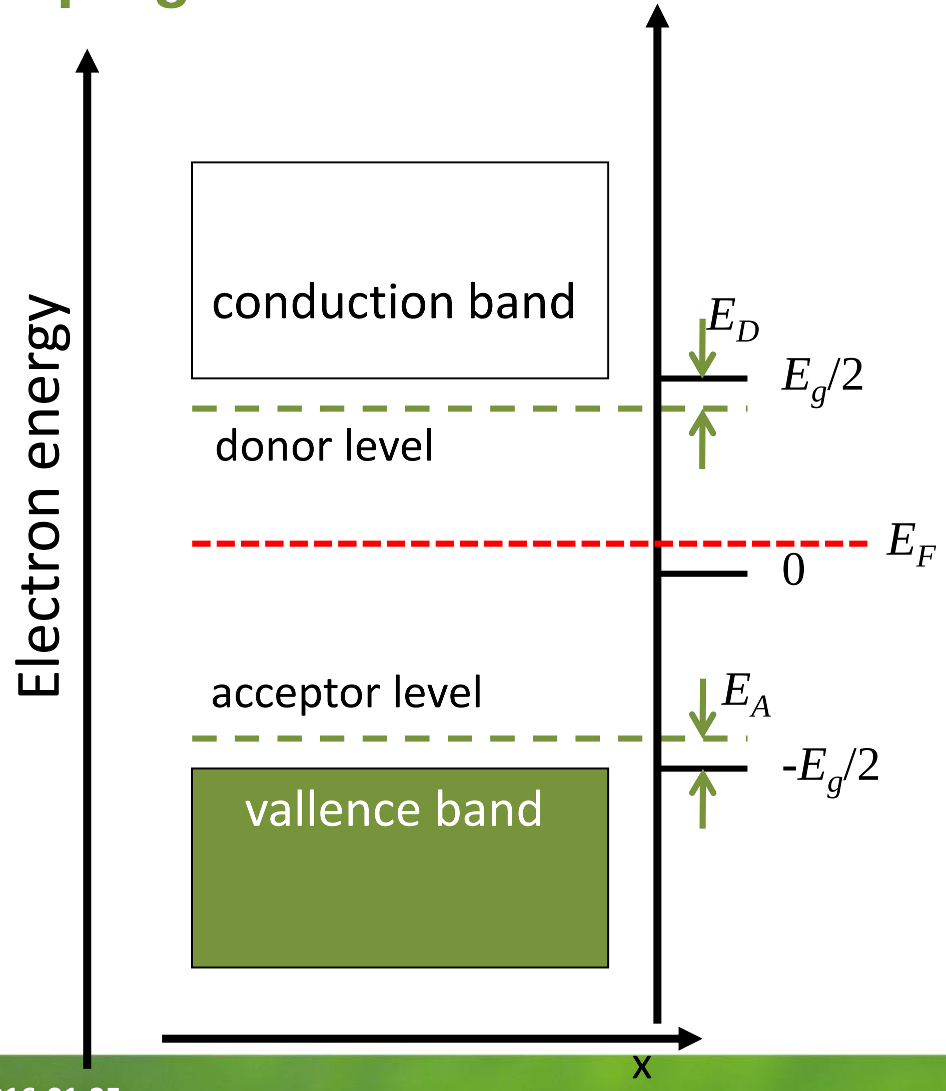
p_v – concentration of holes in valence band

From the charge neutrality of the crystal:

Blackboard!

Dopants, impurities and defects

Doping



The carrier concentration in extrinsic semiconductor (*niesamoistny*)

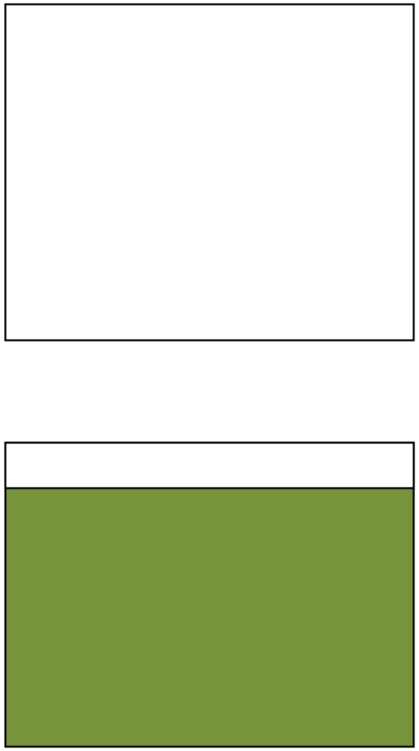
Consider a semiconductor, in which:

N_A – concentration of acceptors
N_D – concentration of donors
p_A – concentration of neutral acceptors
n_D – concentration of neutral donors
n_c – concentration of electrons in conduction band
p_v – concentration of holes in valence band

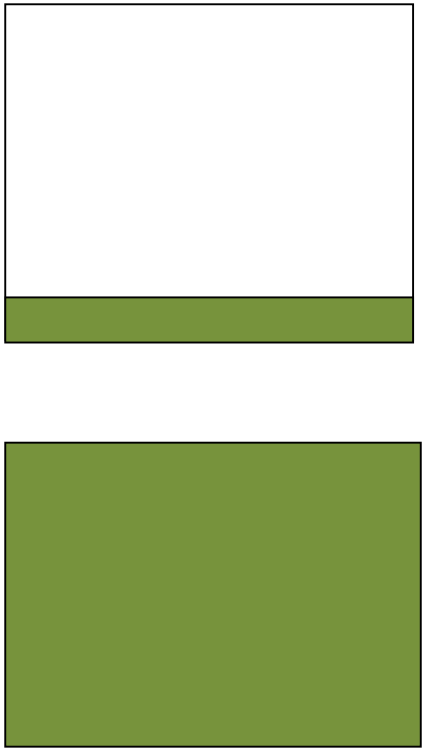
From the charge neutrality of the crystal:

$$n_c + (N_A - p_A) = p_v + (N_D - n_D)$$
$$n_c + n_D = (N_D - N_A) + p_v + p_A$$

Teoria pasmowa ciał stałych.



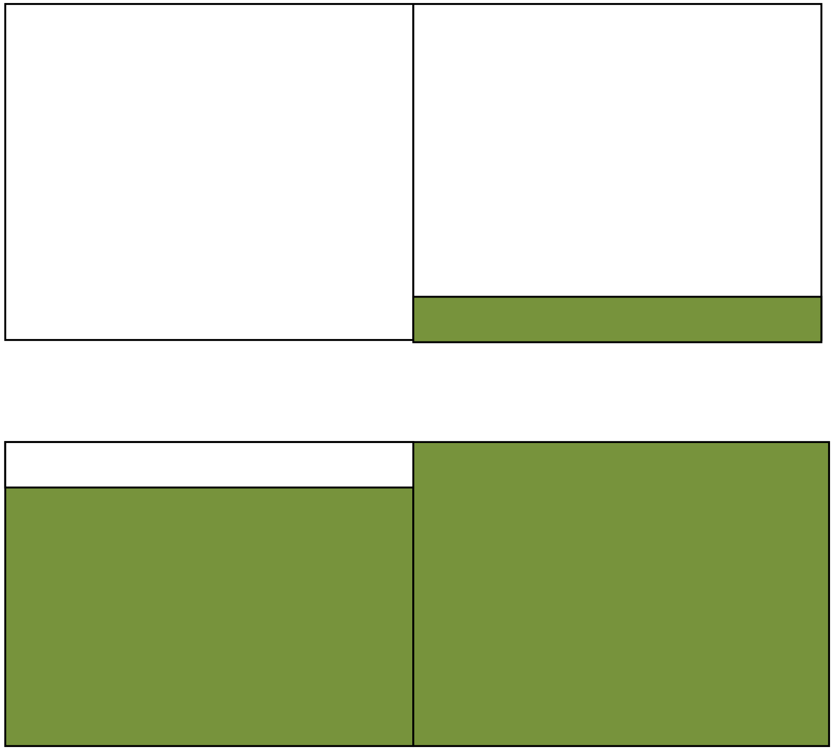
półprzewodnik typu p



półprzewodnik typu n

Teoria pasmowa ciał stałych.

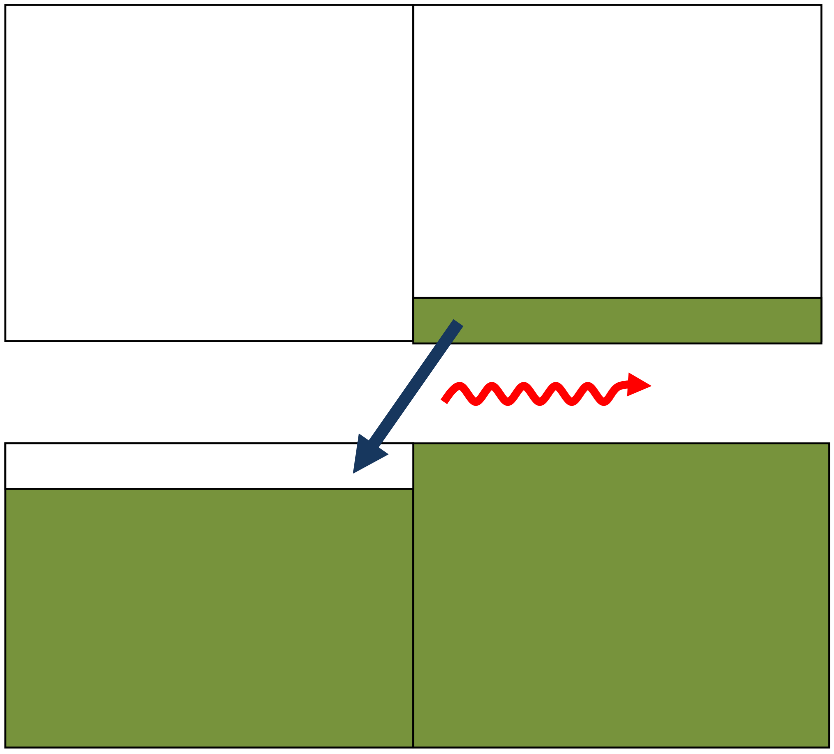
Dioda – czyli złącze *p-n*



Flat band

Teoria pasmowa ciał stałych.

Dioda – czyli złącze *p-n*



typ p

typ n

Flat band

The electronic band structure

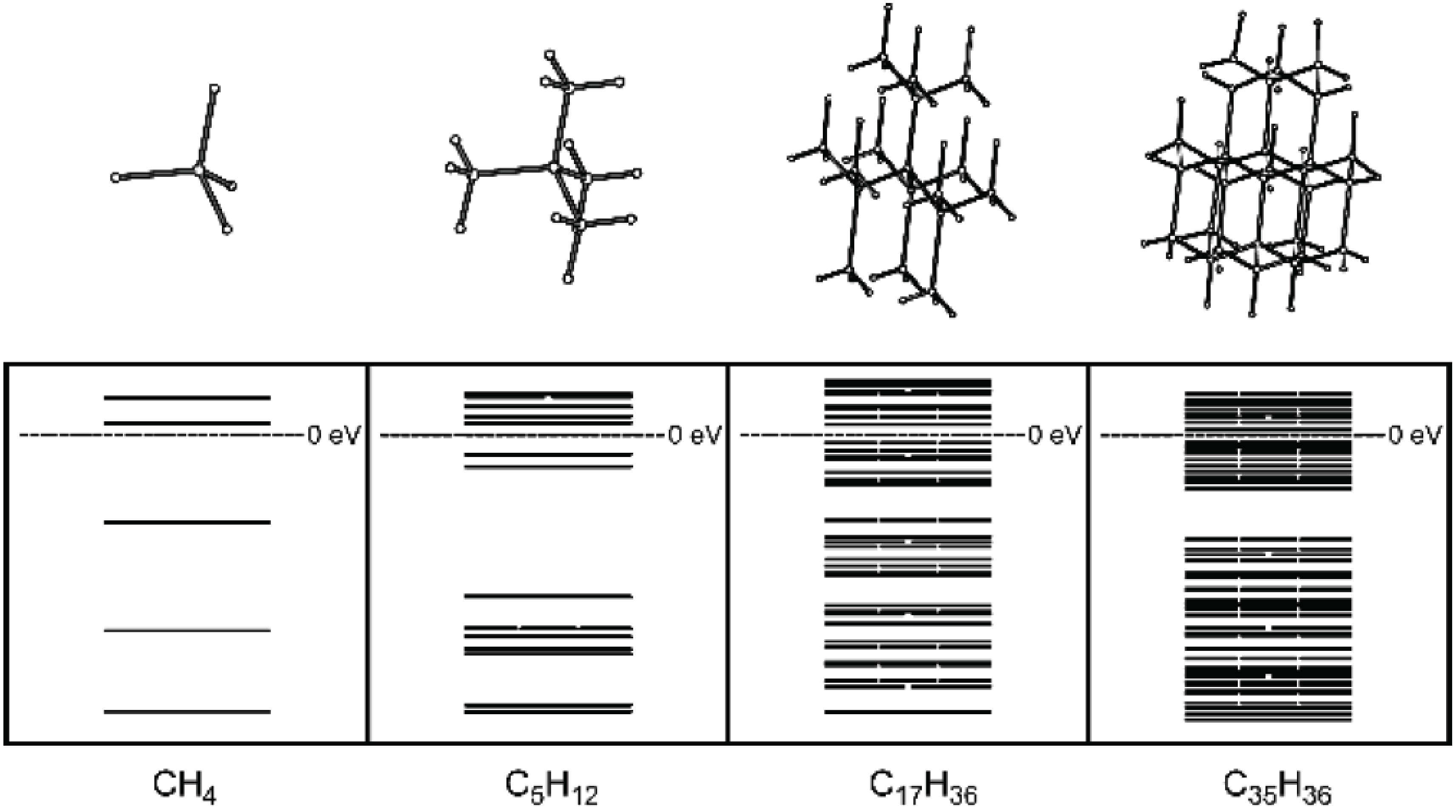


Fig. 2.3 Development of the diamond band gap

W. R. Fahrner (Editor) **Nanotechnology and Nanoelectronics**