Physics of Condensed Matter I

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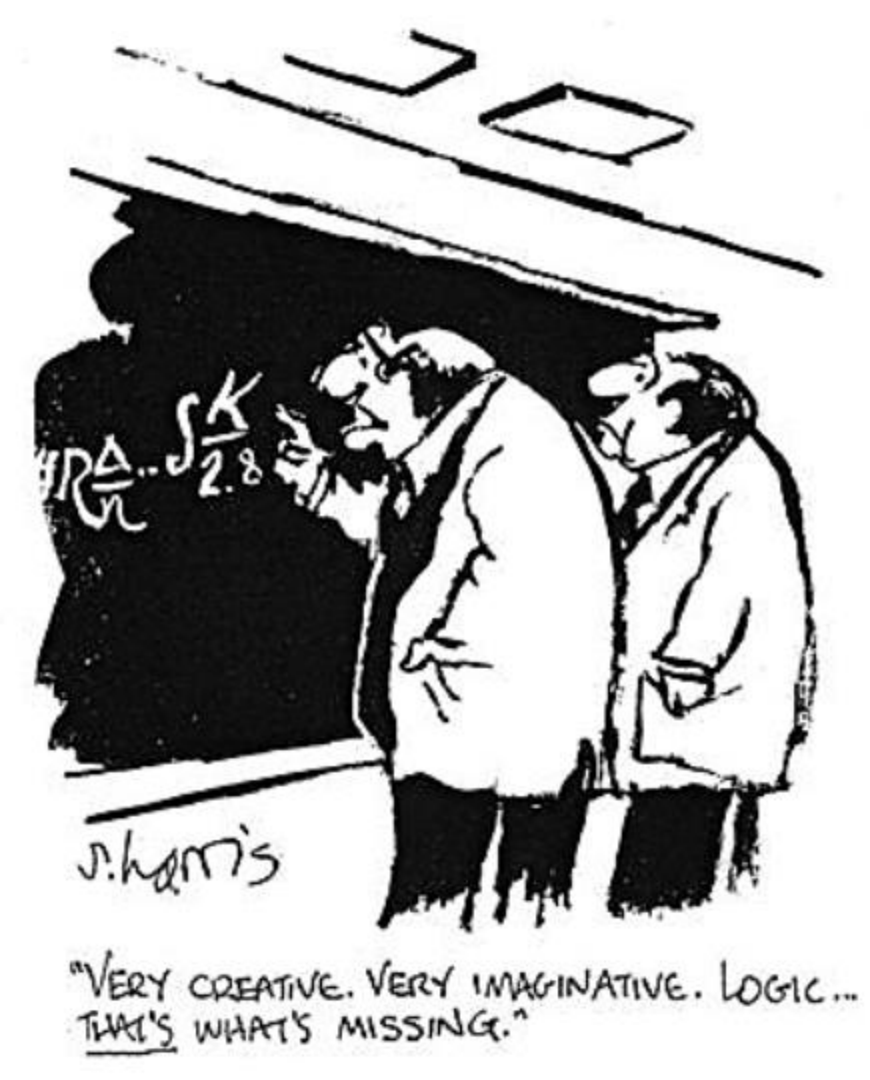

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Solid state 4

inżynieria nanostruktur

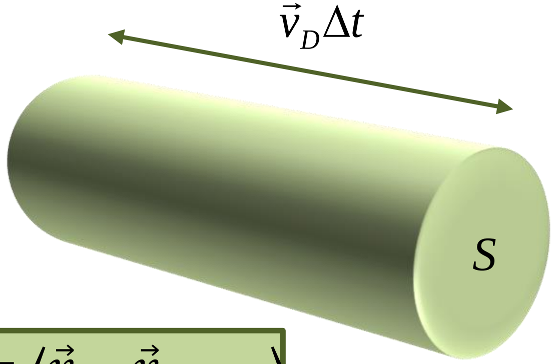
The classical model of electrical conduction

Electrical conductivity of plasma:

Paul Karl Ludwig Drude
1863-1906

Current density:

$$\vec{j} = \frac{1}{S}\frac{\Delta Q}{\Delta t} = \frac{1}{S}\frac{\Delta(-enV)}{\Delta t} = \frac{ne}{S}\frac{S\vec{v}_D\Delta t}{\Delta t}$$



$$\vec{j} = -en\vec{v}_D$$

Drift velocity $\vec{v}_D = \langle \vec{v} - \vec{v}_{therm} \rangle$

Drude model. Model of the conductivity of metals proposed by Drude approx. 1900, soon after the discovery of the electron.

$$m\frac{d\vec{v}}{dt} + \frac{m}{\tau}\vec{v} = -e\vec{E}$$

After switching off the electric field $\vec{v}$ returns to thermal velocity (exponentially: τ)

For the stationary case: $\frac{d\vec{v}}{dt} = 0 \Rightarrow \vec{v}_D = -\frac{e\tau}{m}\vec{E}$ Mobility: $\mu = \frac{e\tau}{m}$

$$\sigma = ne\mu = \frac{ne^2}{m}\tau \approx \frac{ne^2}{m}\frac{l}{\langle v \rangle}$$

The classical model of electrical conduction

Electrical conductivity of plasma:

Paul Karl Ludwig Drude
1863-1906

How can we calculate the average speed of electrons?

Drude: Ideal gas, Boltzman distribution

$$\frac{1}{2}\,m\langle v\rangle^2 = \frac{3}{2}k_BT$$

$$\langle v\rangle = \sqrt{\frac{3k_BT}{m}} = \;\dots 300K \dots = 1{,}2 \cdot 10^5\,\frac{m}{s}$$

Pure metals at T = 300 K $\langle l\rangle \approx$ 5 × 10^{-6} m,
at T = 4 K $\langle l\rangle \approx$1cm

Arnold Johannes
Wilhelm Sommerfeld
(1868 –1951)

Sommerfeld: degenerated Fermi gas (Fermi-Dirac distribution):

$$\langle v\rangle = \sqrt{\frac{2E_F}{m}} = \;1{,}6 \cdot 10^6\,\frac{m}{s} \qquad \langle l\rangle \approx 40\;nm$$

Theoretical description of condensed matter

Born – Oppenheimer approximation

Full non-relativistic Hamiltonian of the system of nuclei and electrons:

$$H(\vec{r},\vec{R})\Psi(\vec{r},\vec{R}) = E\Psi(\vec{r},\vec{R})$$

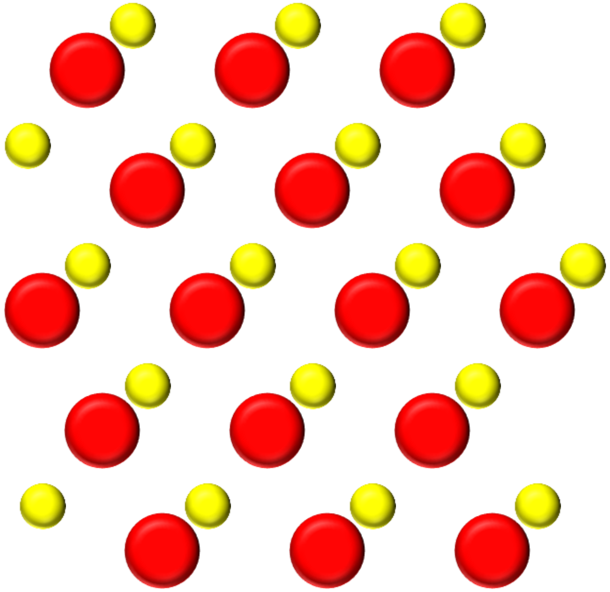
$$\begin{aligned} &H(\vec{r},\vec{R}) \\ &= -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 - \sum_N \frac{\hbar^2}{2M_N}\nabla_N^2 - -\frac{1}{4\pi\varepsilon_0}\sum_{N,i}\frac{Z_N e^2}{\left|\vec{r}_i - \vec{R}_N\right|} + \\ &+ \frac{1}{4\pi\varepsilon_0}\sum_{N<K}\frac{Z_N Z_K e^2}{\left|\vec{R}_N - \vec{R}_K\right|} + \frac{1}{4\pi\varepsilon_0}\sum_{i<j}\frac{e^2}{\left|\vec{r}_i - \vec{r}_j\right|} = \\ &= \hat{T}_e + \hat{T}_N + V(\vec{r},\vec{R}) + V_e(\vec{r}) + G(\vec{R}) \end{aligned}$$

Electron and nuclear (ions) subsystems coordinates are intermixed, separation of electronic and nuclear variables is impossible

Assumption: motion of atomic nuclei and electrons in a molecule can be separated
Born-Oppenheimer adiabatic approximation

Periodic potential

Hartree approximation (one-electron)



Assumptions:

Motionless atoms, crystal (periodic) lattice .

One-electron Hartree approximation

$$\Psi_{el}^{k}(\vec{r}_1,\vec{r}_2,\vec{r}_3,\dots) = \varphi_1(\vec{r}_1)\cdot\varphi_2(\vec{r}_2)\cdot\varphi_3(\vec{r}_3)\cdot\dots\cdot\varphi_n(\vec{r}_n)$$

or Hartree-Fock approximation (Slater determinant).

Self-consistent field method – the multi-electron issue is reduced to the solution of one-electron problem in a potential of all other electrons and atoms

$$\left(\frac{p^2}{2m}+V(\vec{r})\right)\varphi_n(\vec{r}_n) = E_n\varphi_n(\vec{r}_n)$$

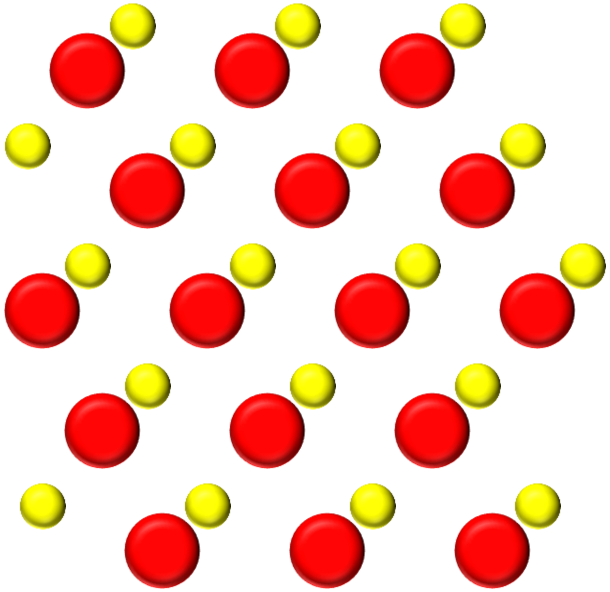
„One-electron” Schrödinger equation

Effective potential, periodic potential of the crystal lattice, the same for all electrons.

$$\boxed{V(\vec{r}) = V\left(\vec{r}+\vec{R}\right)}$$

Periodic potential

Bloch theorem



For every periodic potential $\boxed{V(\vec{r}) = V(\vec{r} + \vec{R})}$

The solutions of the Schrodinger equation:

$$\left(\frac{p^2}{2m} + V(\vec{r})\right)\psi_n(\vec{r}_n) = E_n\psi_n(\vec{r}_n)$$

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

Bloch wave,
Bloch function

Bloch amplitude,
Bloch envelope

The solution of the one-electron Schrödinger equation for a periodic potential has a form of modulated plane wave:

$$u_{n,\vec{k}}(\vec{r}) = u_{n,\vec{k}}(\vec{r} + \vec{R})$$

Periodic potential

Bloch theorem

Bloch function:

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

Bloch wave,
Bloch function

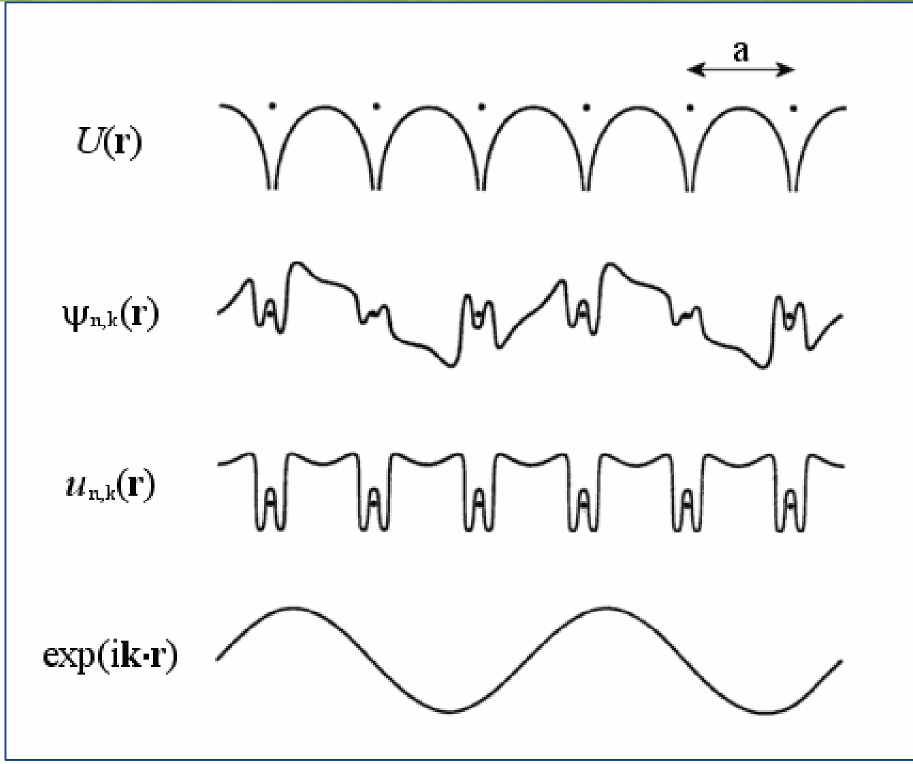
Bloch amplitude,
Bloch envelope

Example:
Motion of the electron in a periodic potential

$$V(\vec{r}) = V\left(\vec{r} + \vec{R}\right)$$

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

the Fourier series expansion

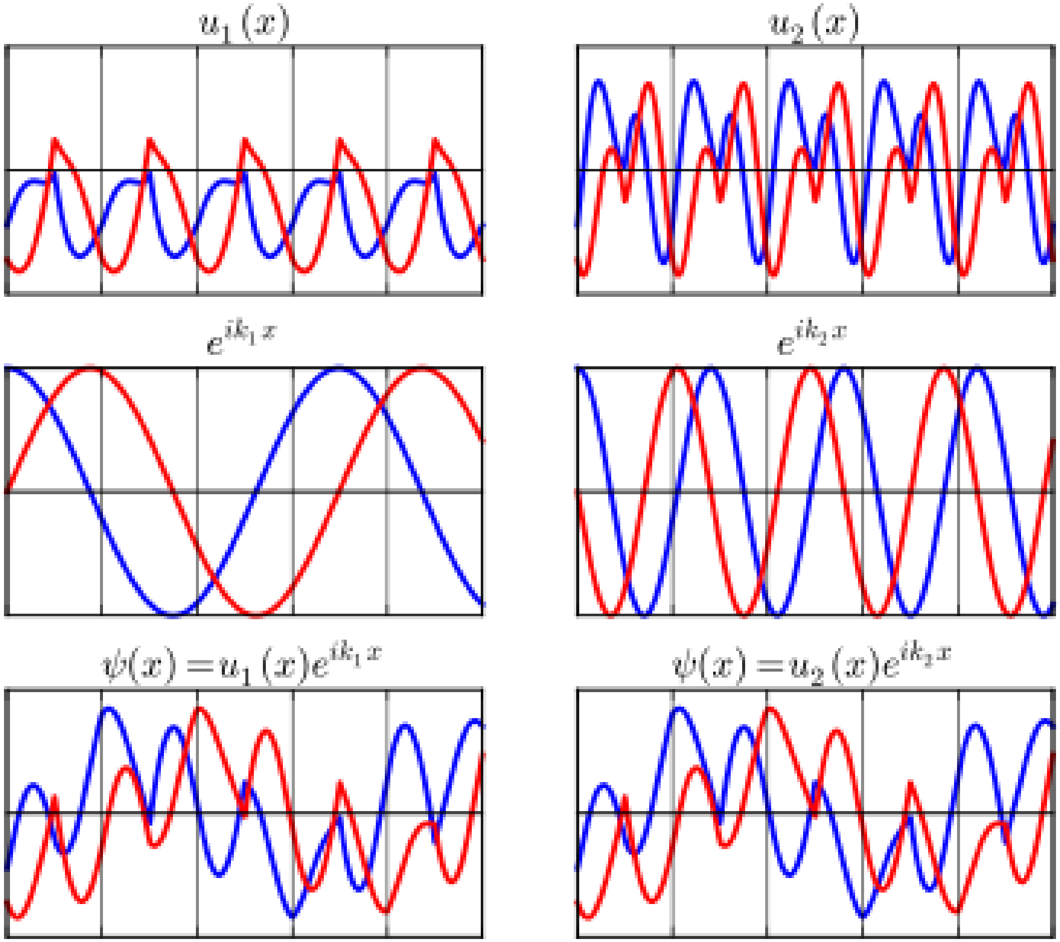


Periodic potential

Bloch theorem

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

Bloch waves whose wave vectors differ by a reciprocal lattice vector are IDENTICAL!



$$\vec{k}_1 - \vec{k}_2 = \vec{G}$$

Periodic potential

Bloch theorem

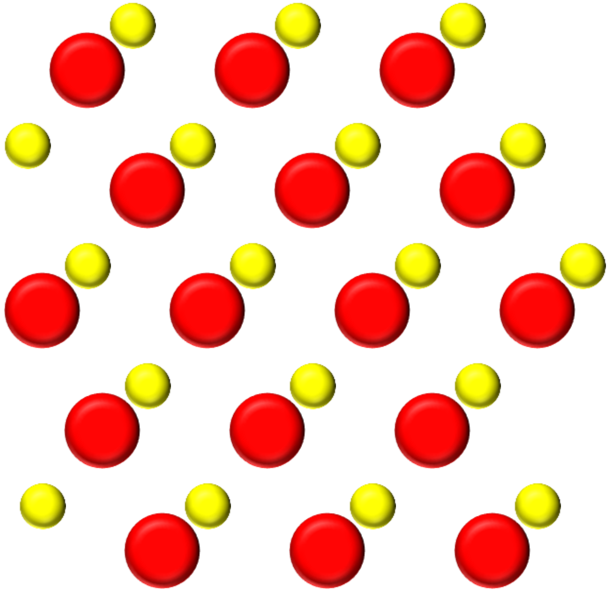
Crystal lattice:

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

For periodic functions with the lattice period $\vec{R}$

$f(\vec{r}) = f(\vec{r} + \vec{R})$ a good base in the Fourier series expansion are functions $g(\vec{r}) = \exp(i\vec{G}\vec{r})$ which depend on the reciprocal lattice vectors:

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



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

$$\exp[i\vec{G}(\vec{r} + \vec{R})] =$$

$$= \exp[i\vec{G}\vec{r}] \cdot \exp[i\vec{G}\vec{R}] = \exp[i\vec{G}\vec{r}]\exp[2\pi\,(n_1m_1 + n_2m_2 + n_3m_3)] = \exp(i\vec{G}\vec{r})$$

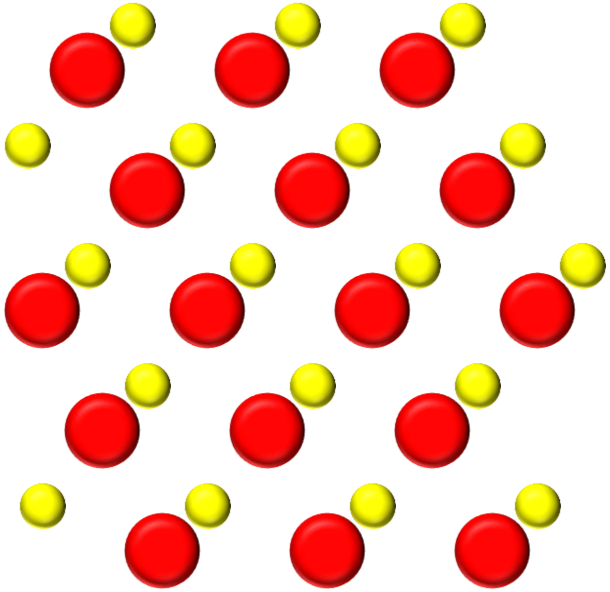
therefore $g(\vec{r}) = g(\vec{r} + \vec{R})$ and finally we get:

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

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

Periodic potential

Bloch theorem



Periodic potenetial we can expand as a Fourier series:

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

The wavefunction can be represented as a sum of plane waves of different wavelengths satisfying periodic boundary conditions :

$$\psi(\vec{r}) = \sum_{\vec{k}} C_{\vec{k}} \exp\left(i\vec{k}\vec{r}\right)$$

Schrödinger equation:

$$\left(\frac{\hat{p}^2}{2m} + V(\vec{r})\right)\psi(\vec{r}) = E\psi(\vec{r})$$

$$\sum_{\vec{k}} \frac{\hbar^2\vec{k}^2}{2m} C_{\vec{k}} \exp\left(i\vec{k}\vec{r}\right) + \sum_{\vec{k},\vec{G}} C_{\vec{k}}\, V_{\vec{G}} \exp\left[i\left(\vec{k}+\vec{G}\right)\vec{r}\right] = E\sum_{\vec{k}} C_{\vec{k}} \exp\left(i\vec{k}\vec{r}\right)$$

This is an equation for E and $C_{\vec{k}}$ for all vectors $\vec{k}, \vec{r}$ and $\vec{G}$.

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

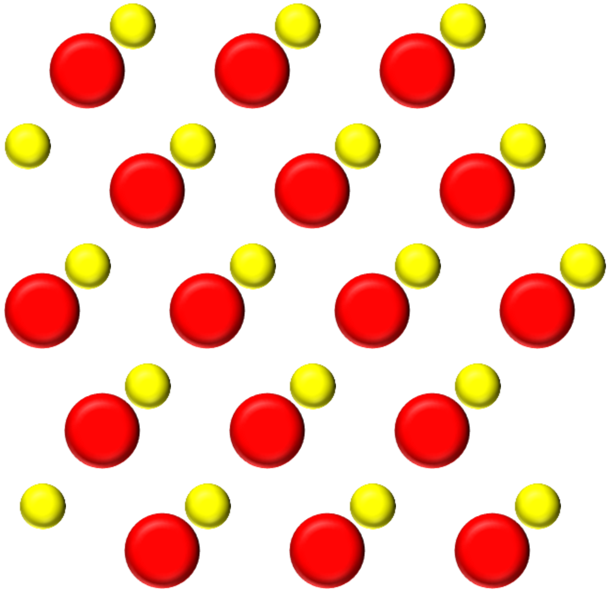
Periodic potential

Bloch theorem

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

Bloch wave,
Bloch function

Bloch amplitude,
Bloch envelope



The solution of the one-electron Schrödinger equation for a periodic potential has a form of modulated plane wave:

$$u_{n,\vec{k}}(\vec{r}) = u_{n,\vec{k}}(\vec{r} + \vec{R})$$

We introduced coefficient n for different solutions corresponding to the same $\vec{k}$ (*index*). $\vec{k}$-vector is an element of the *first Brillouin zone.*

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

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

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

Periodic potential

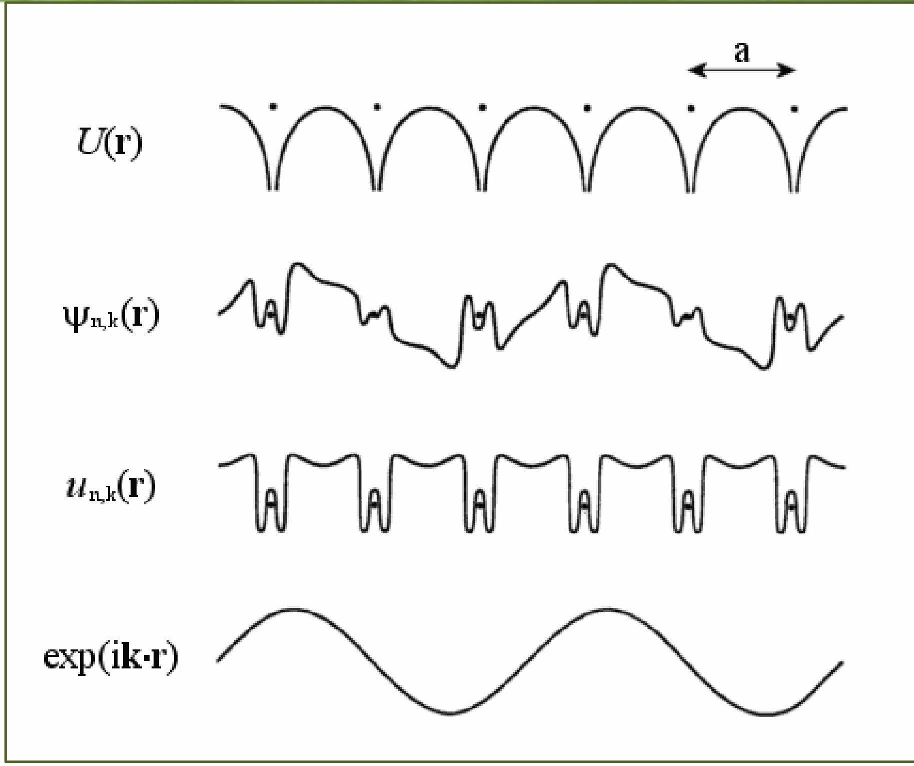
Bloch theorem

Bloch function has a form:

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

Generally non-periodic function

Periodic function, so-called *Bloch factor*



Example: electron in a constant potential

$$H = -\frac{\hbar^2}{2m}\Delta + V$$

substituting $\varphi_{n,\vec{k}}(\vec{r}) = 1\, e^{i\vec{k}\vec{r}}$

The solution is $E = \frac{\hbar^2 k^2}{2m} + V$

The momentum operator $\hat{p} = -i\hbar\nabla$ acting on $\varphi_{n,\vec{k}}(\vec{r})$

$\hat{p}\varphi_{n,\vec{k}}(\vec{r}) = \hbar k\;\; \varphi_{n,\vec{k}}(\vec{r})$. The solutions of the Schrödinger equation with a constant potential are eigenfunctions of the momentum operator. The momentum is well defined, the eigenvalue of the momentum operator is $\hat{p} = \hbar k$ (this defines the sense of $\vec{k}$-vector).

Periodic potential

Bloch theorem

Example:

Electron motion in a periodic potential.

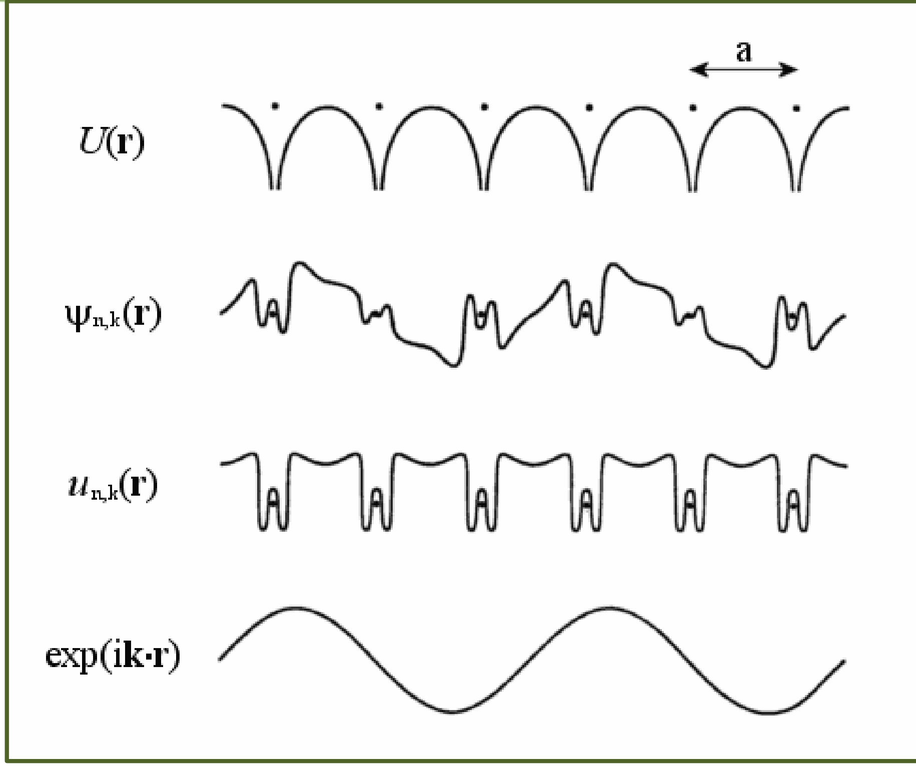
$$V(\vec{r}) = \sum_{\vec{G}} V_{\vec{G}} \exp\left(i\vec{G}\vec{r}\right)$$

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*):

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



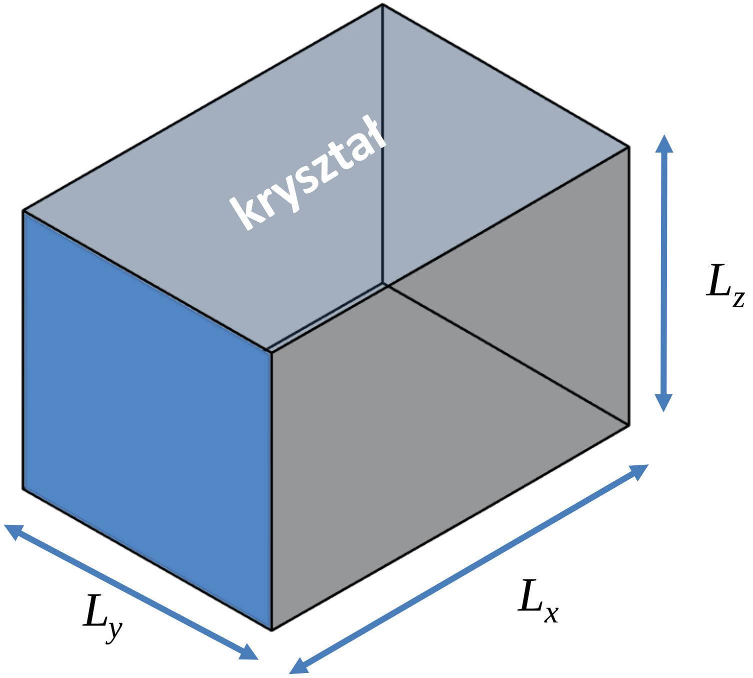
Applying $\hat{p} = -i\hbar\nabla$ we get $\hat{p}\psi(\vec{r}) = -i\hbar\left(i\,\vec{k} + \nabla u_{n,\vec{k}}\right)e^{i\vec{k}\vec{r}} \neq \hbar\vec{k}\psi(\vec{r})$.

Momentum of the Bloch function is not well defined!

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

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:

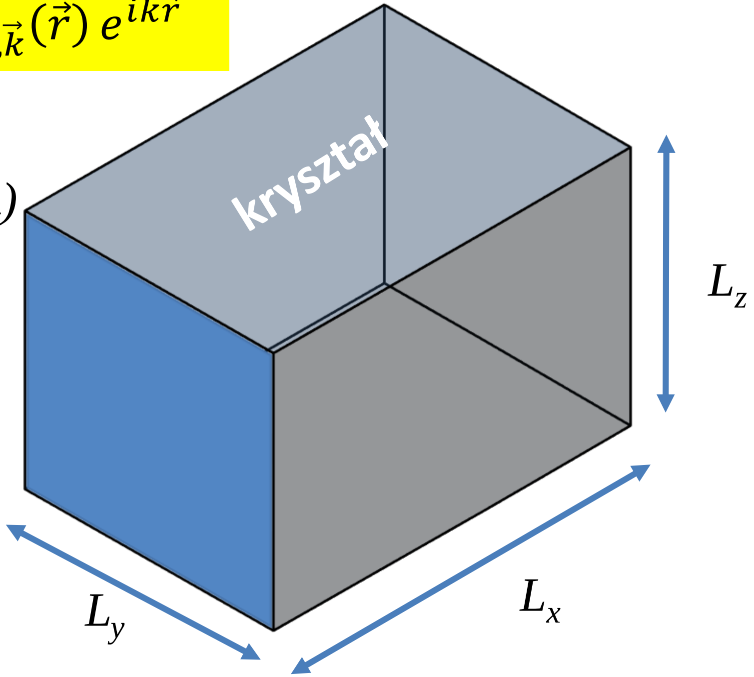
Born- von Karman boundary conditions

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

Finite size of the crystal L_x, L_y, L_z

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

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



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

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

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

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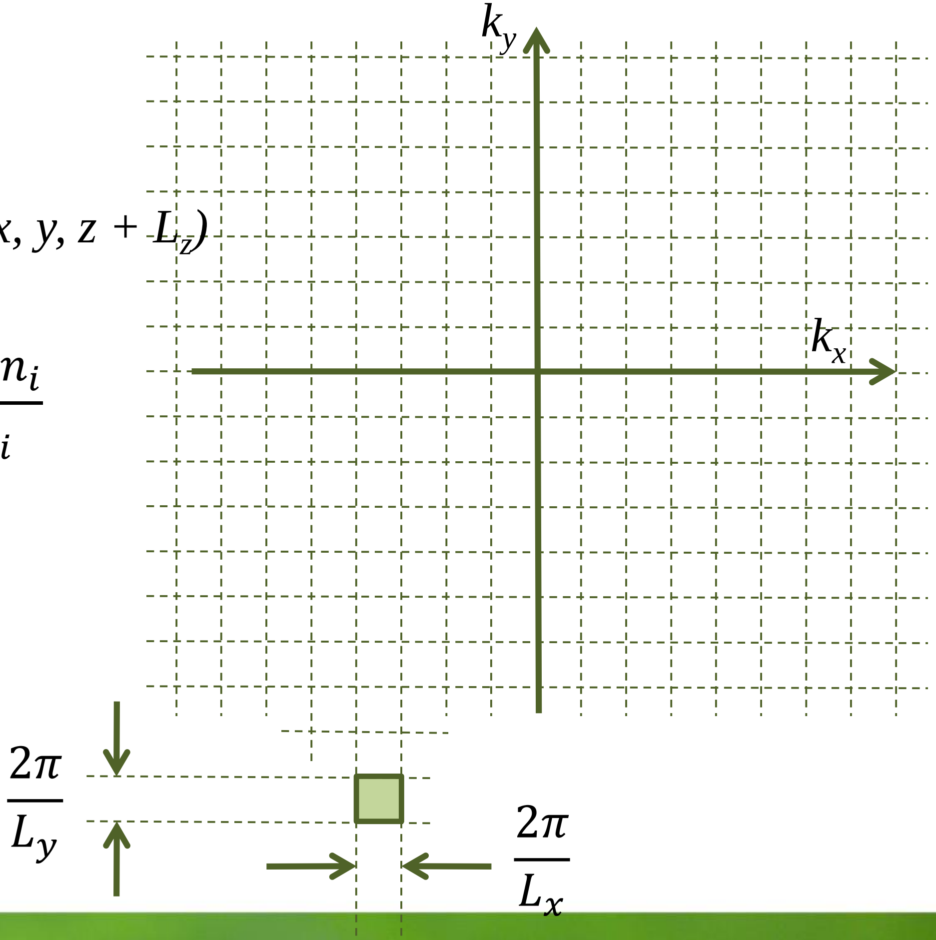
$$\boxed{\begin{aligned} e^{ik_xL_x} &= 1 \\ e^{ik_yL_y} &= 1 \\ e^{ik_zL_z} &= 1 \end{aligned}}$$

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

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



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:

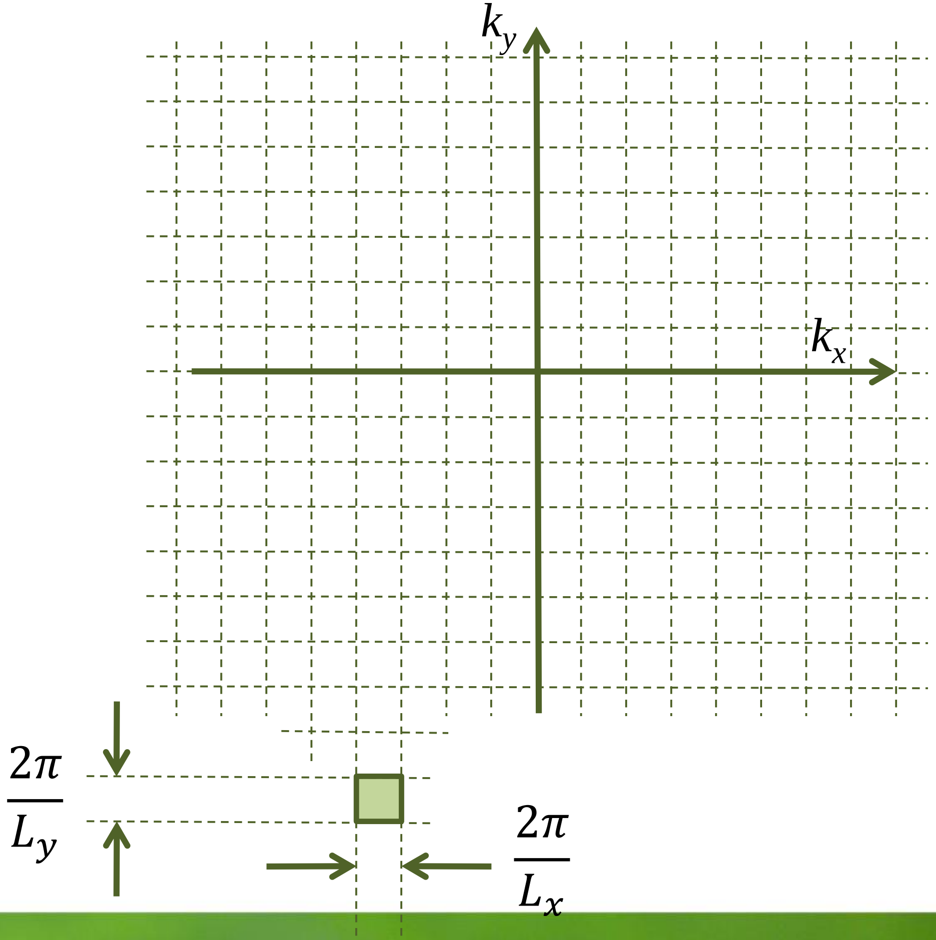
The density of states in k-space of n dimension (and the unite volume)

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 $$= \frac{2}{\frac{2\pi}{L_x}\times\frac{2\pi}{L_y}\times\frac{2\pi}{L_z}} = \frac{2V}{(2\pi)^3}$$



Periodic potential

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:

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

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

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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Periodic potential

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Proof:

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

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What about energies?

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

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

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

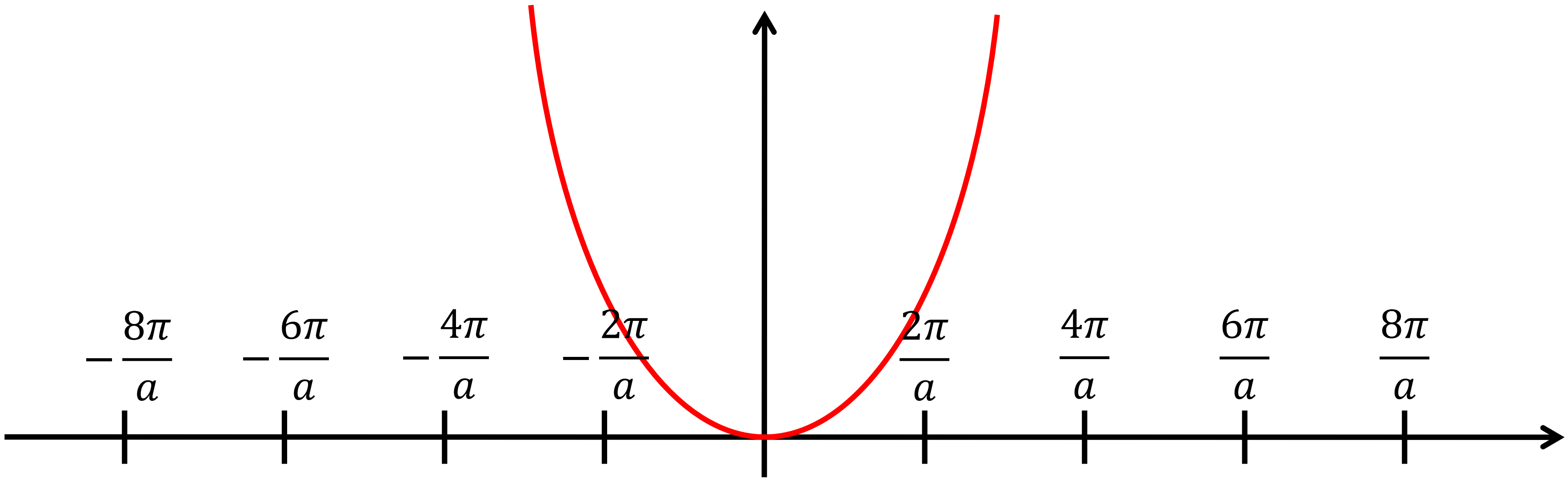
Energy eigenvalues are a periodic function of $\vec{k}$ (wave vectors of Bloch function).

Periodic potential

The nearly free-electron approximation

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

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

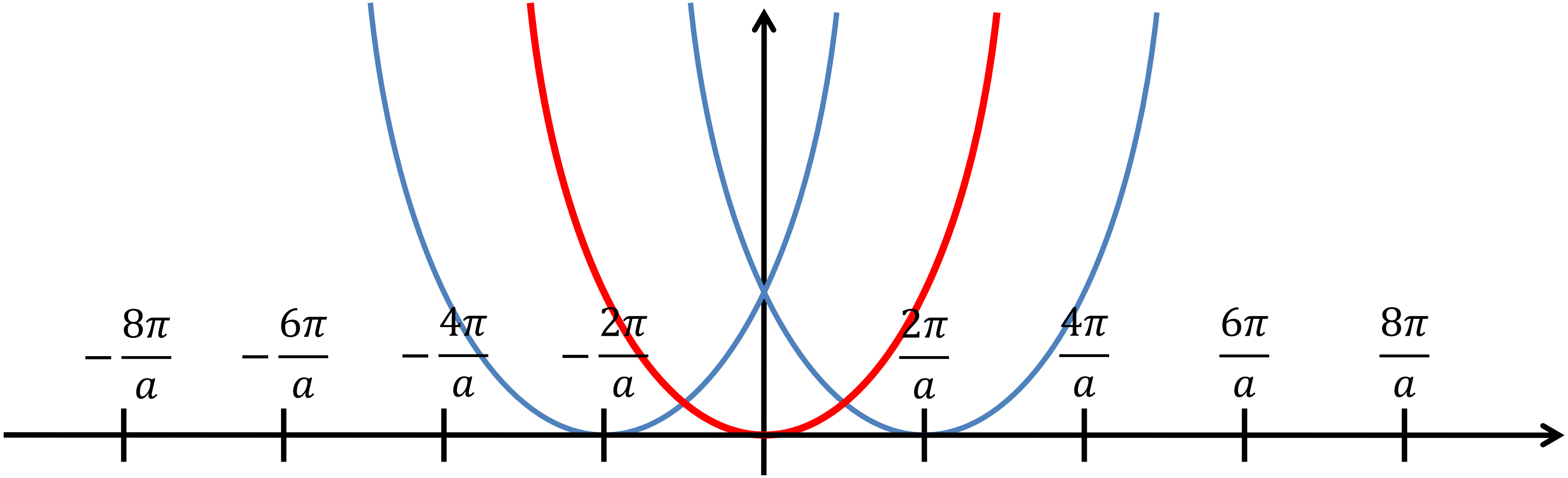


Periodic potential

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

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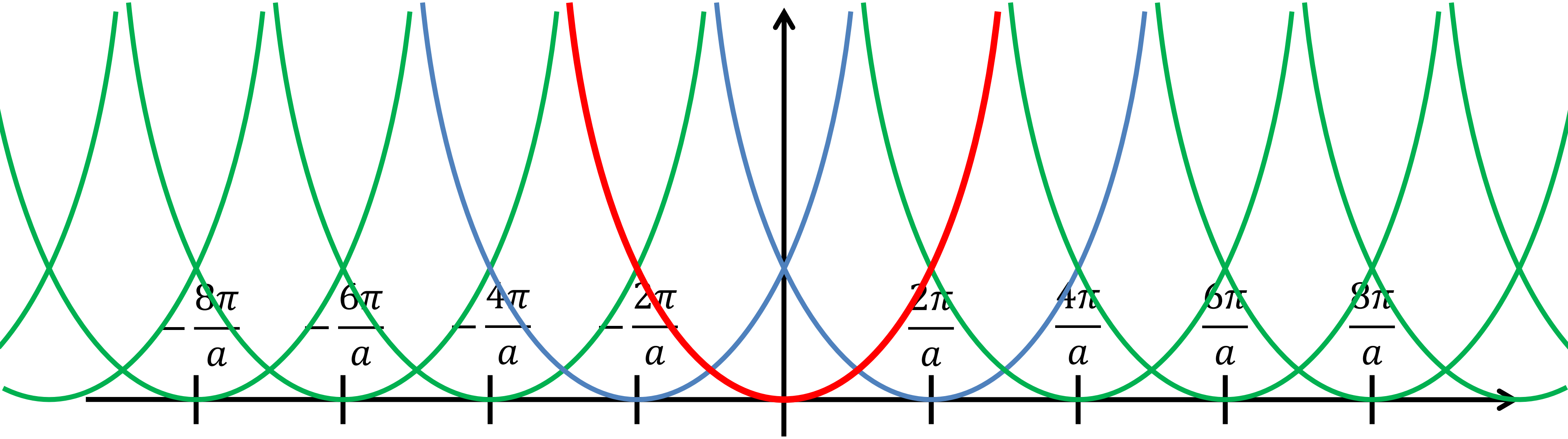
Energy of the plane wave in empty space as the function of wave vector:

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



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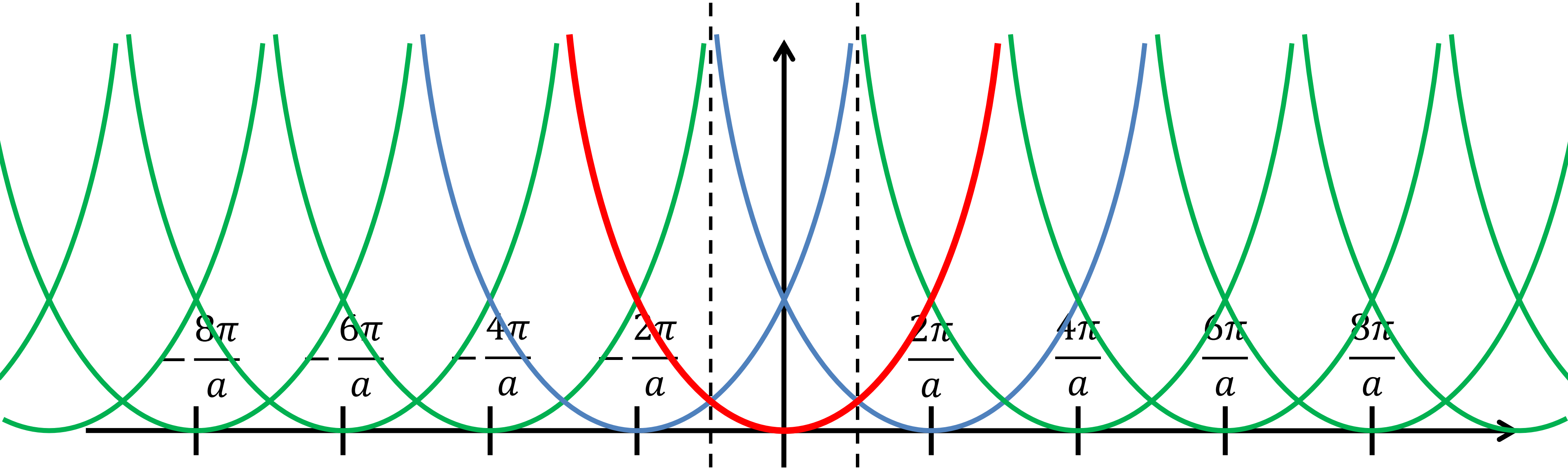

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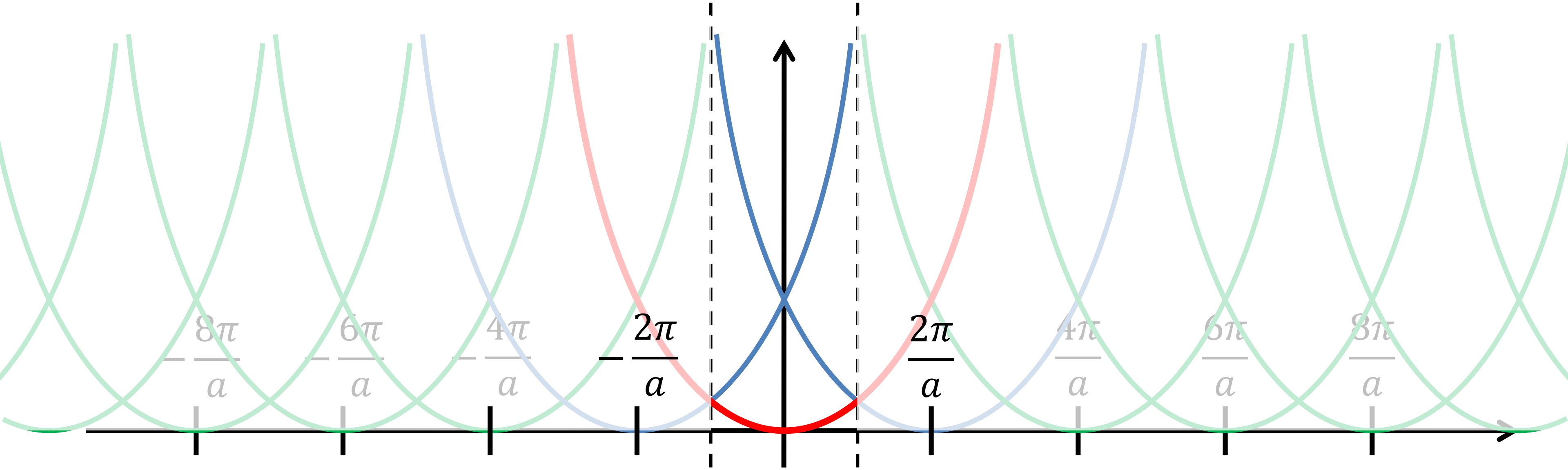


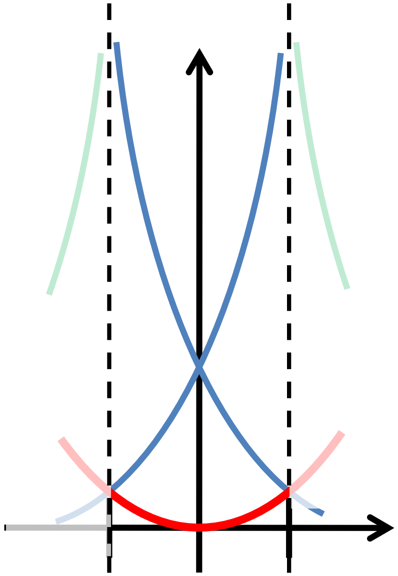
Periodic potential

The nearly free-electron approximation

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

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

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



Periodic potential

The nearly free-electron approximation

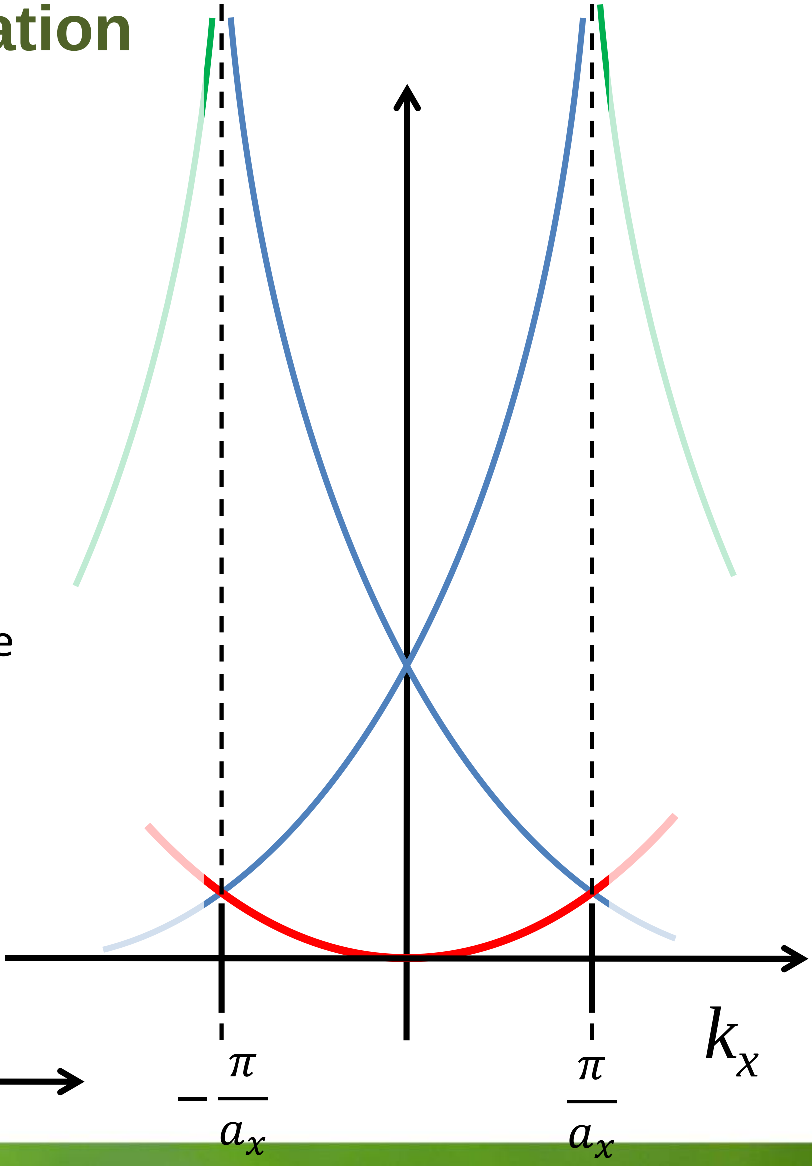
$$E(n,\vec{k}) = E(n,\vec{k}+\vec{G}) = \frac{\hbar^2(\vec{k}+\vec{G})^2}{2m}$$

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

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

The band structure of nearly free-electron cubic lattice

$[hkl]$=
000,
100, $\bar{1}00$, 200, $\bar{2}00$,



Periodic potential

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

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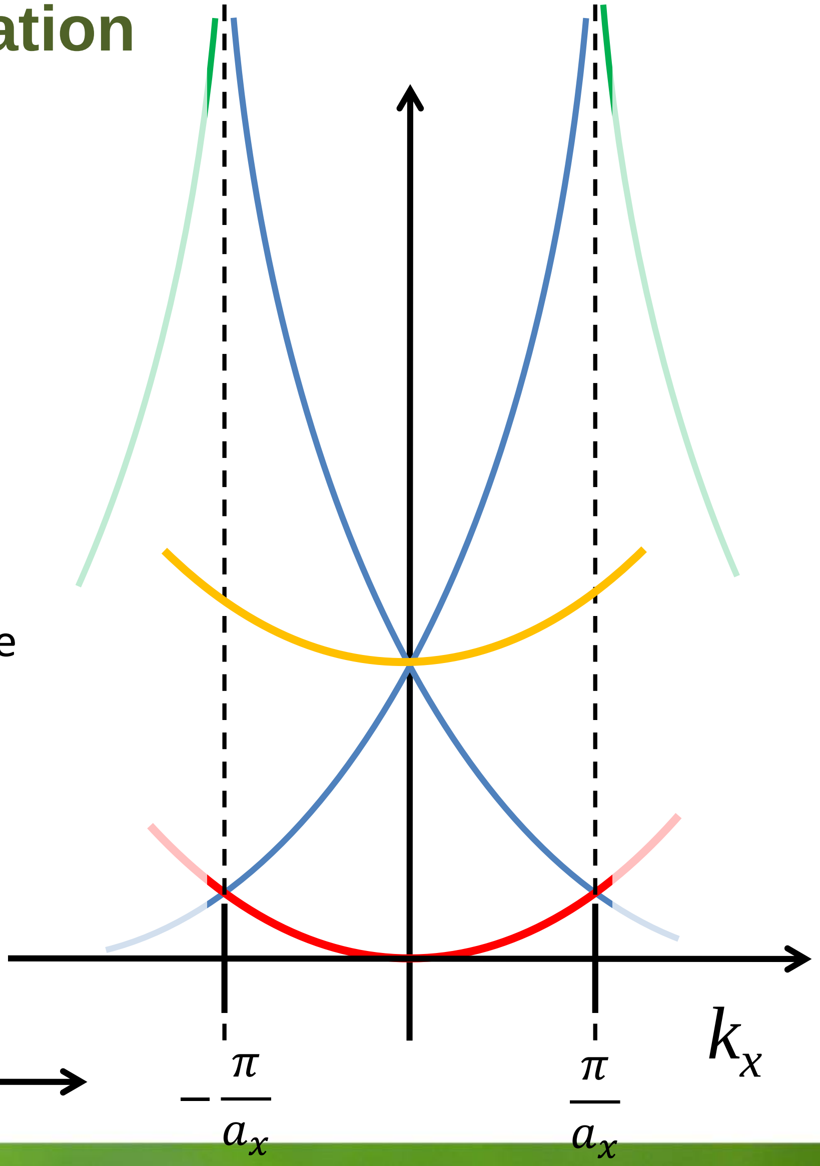
$[hkl]$=

000,

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

010,010,001,001,



Periodic potential

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

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

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

The band structure of nearly free-electron cubic lattice

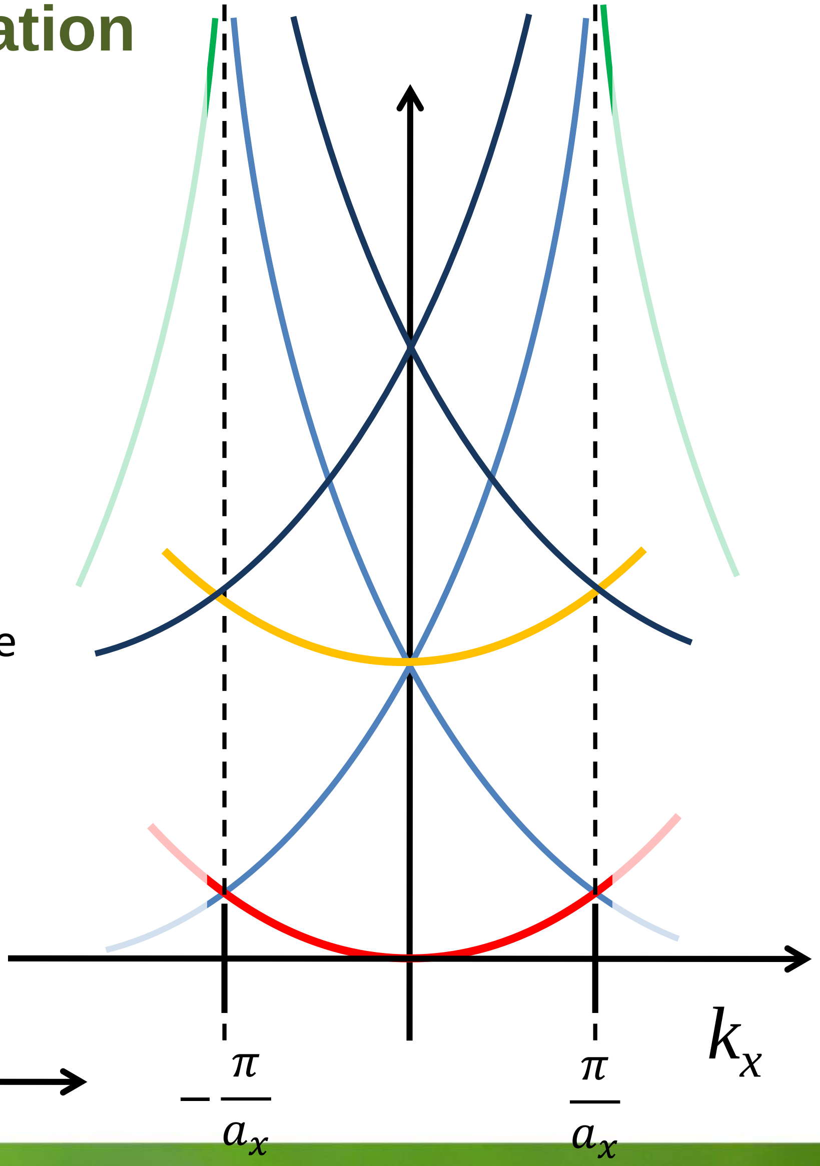
$[hkl]$=

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

The nearly free-electron approximation

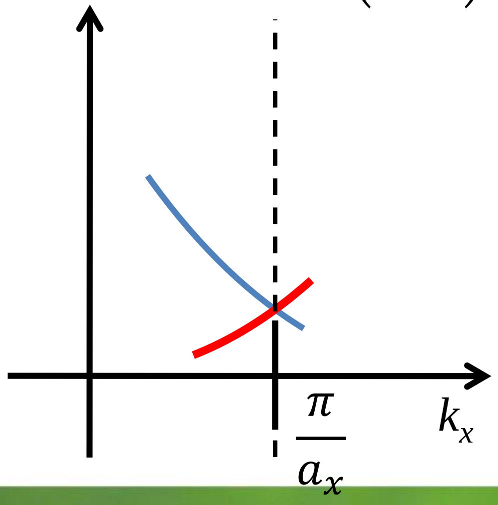
The appropriate expresions for a perturbation calculation of the influence of a small potential

$$V(x) = V_0 \cos\left(\frac{2\pi}{a}x\right) \qquad \text{(1D)}$$

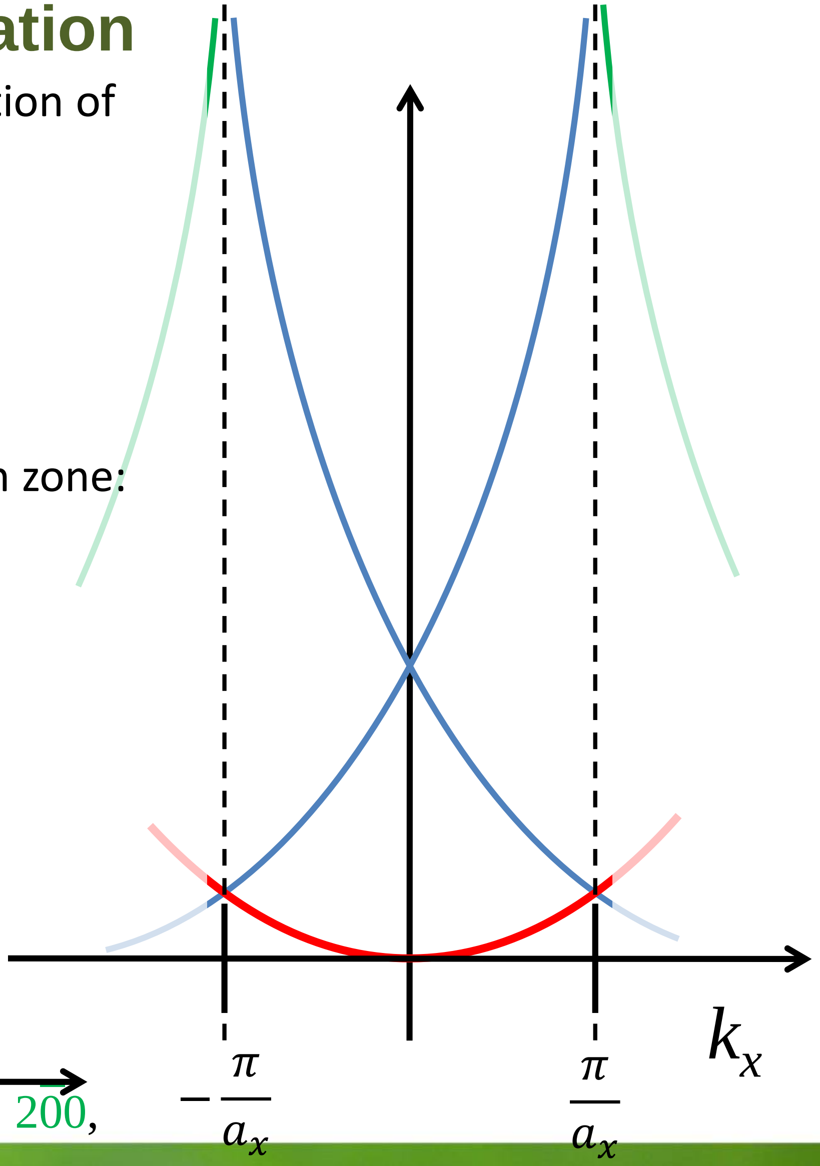
„small potetntial”

Small potential inluence on the borders of the Brilloun zone:

$$V(x) = V_0 \cos\left(\frac{2\pi}{a}x\right) = \frac{V_0}{2}\left(e^{i\frac{2\pi}{a}x} + e^{-i\frac{2\pi}{a}x}\right)$$



$hkl = 000, 100, \bar{1}00, 200, \bar{2}00,$



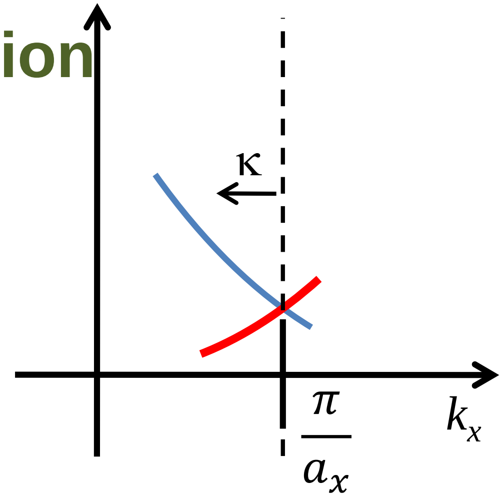
Periodic potential

The nearly free-electron approximation

$$\psi_+ \sim (e^{iGx/2} + e^{-iGx/2}) \sim \cos \pi \frac{x}{a} ,$$

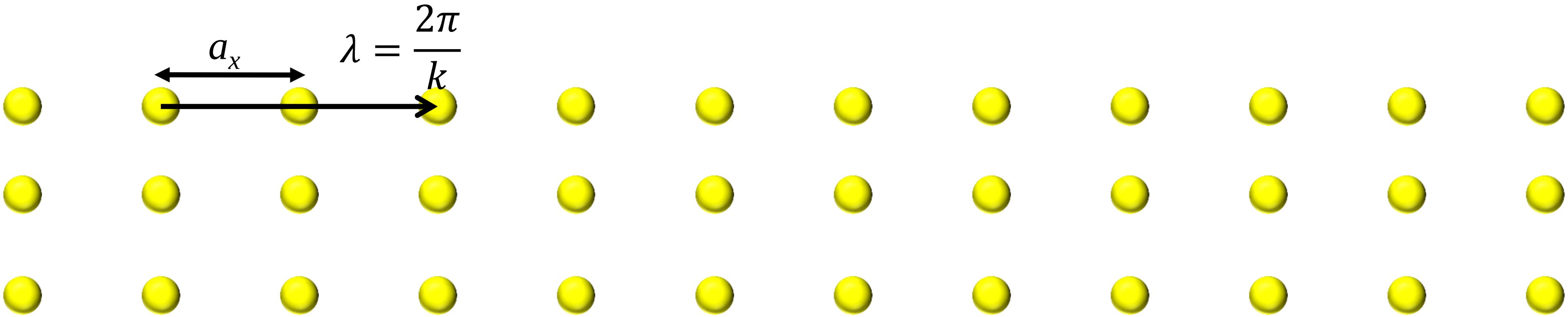
$$\psi_- \sim (e^{iGx/2} - e^{-iGx/2}) \sim \sin \pi \frac{x}{a} .$$

Plane waves of the same k-vector



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

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



Periodic potential

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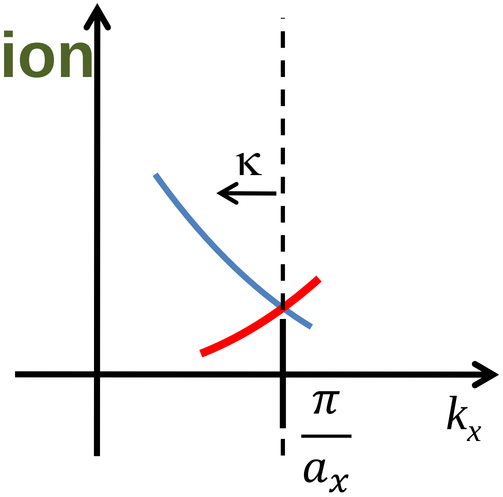
Plane waves of the same *k*-vector



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

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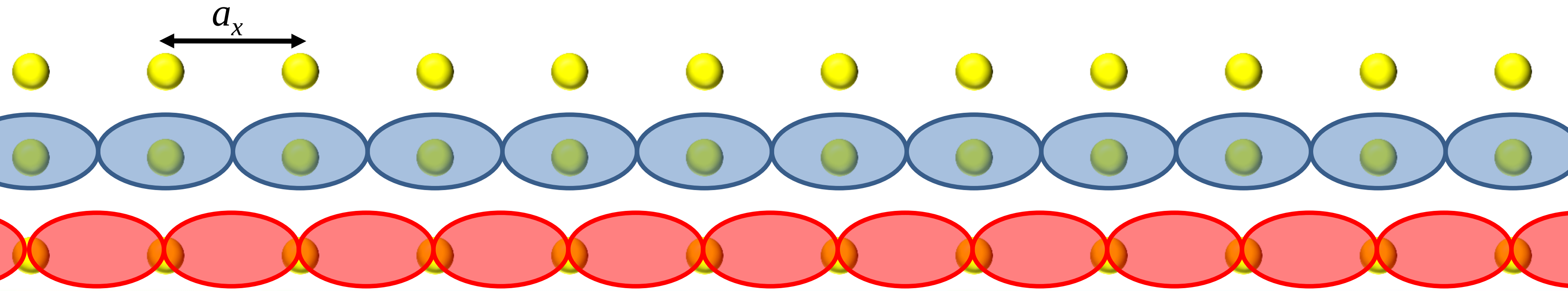
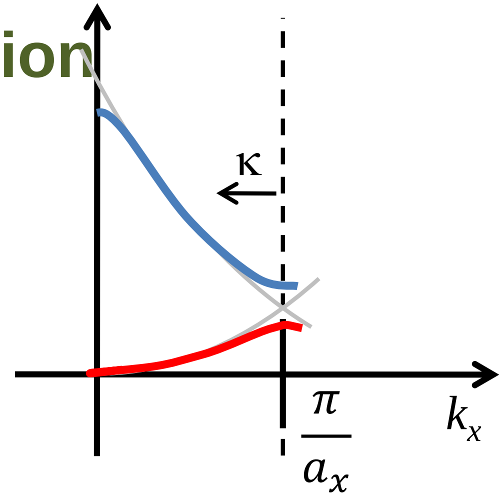


Periodic potential

The nearly free-electron approximation



$$\psi_+ \sim \left(e^{iGx/2} + e^{-iGx/2}\right) \sim \cos \pi \frac{x}{a}\ ,$$

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Plane waves of the same k-vector

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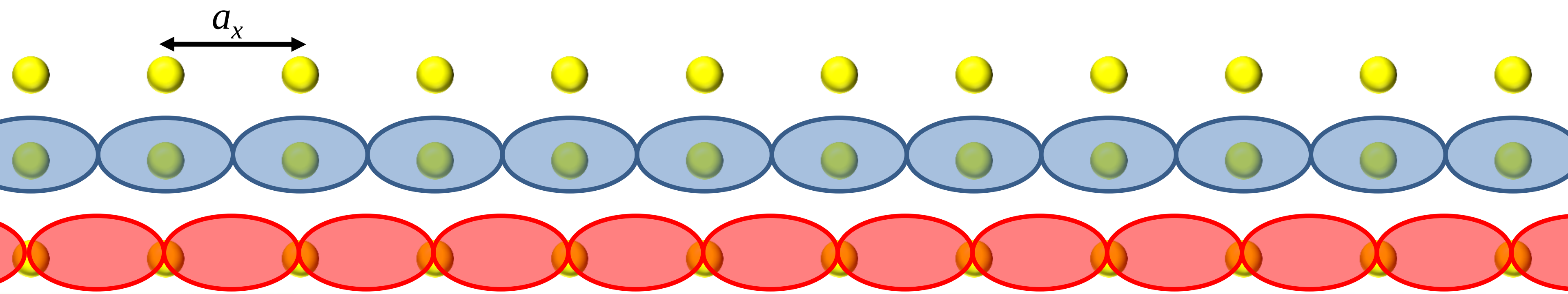

Periodic potential

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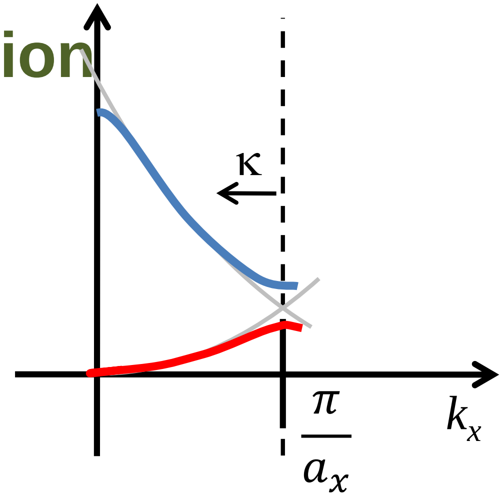
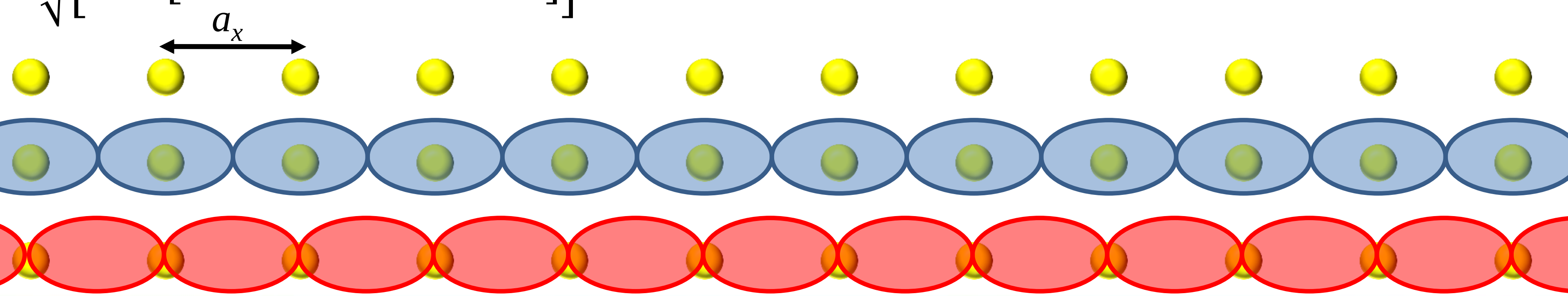


Plane waves of the same k-vector

$$E_\pm = \frac{1}{2}\frac{\hbar^2}{2m_0}\left[\left(\frac{G}{2}-\kappa\right)^2 + \left(\frac{G}{2}+\kappa\right)^2\right] \pm \sqrt{\left[\frac{\hbar^2}{2m_0}\left[\left(\frac{G}{2}-\kappa\right)^2 + \left(\frac{G}{2}+\kappa\right)^2\right]\right]^2 + 4V_0}$$

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

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



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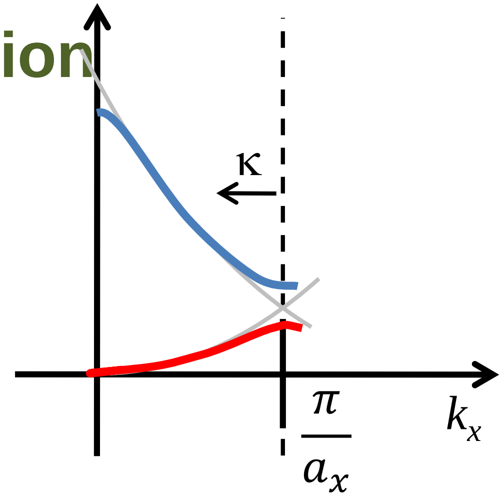
Plane waves of the same k-vector



$$E^{\pm} = \frac{1}{2}(E^0_{k-G} + E^0_k) \pm \left[\frac{1}{4}(E^0_{k-G} - E^0_k)^2 + |V_G|^2\right]^{1/2}$$

see Ibach, Lutch

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

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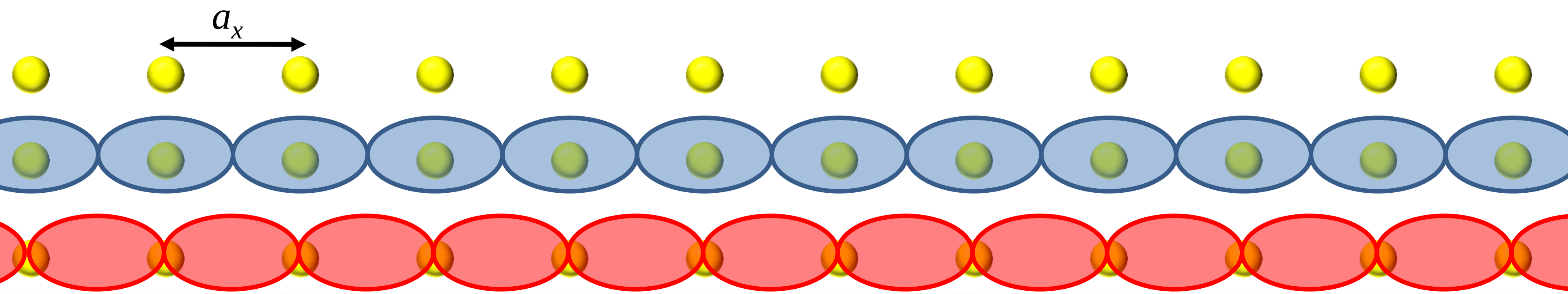
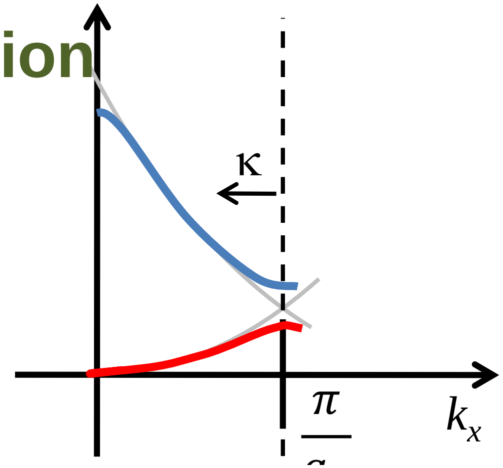
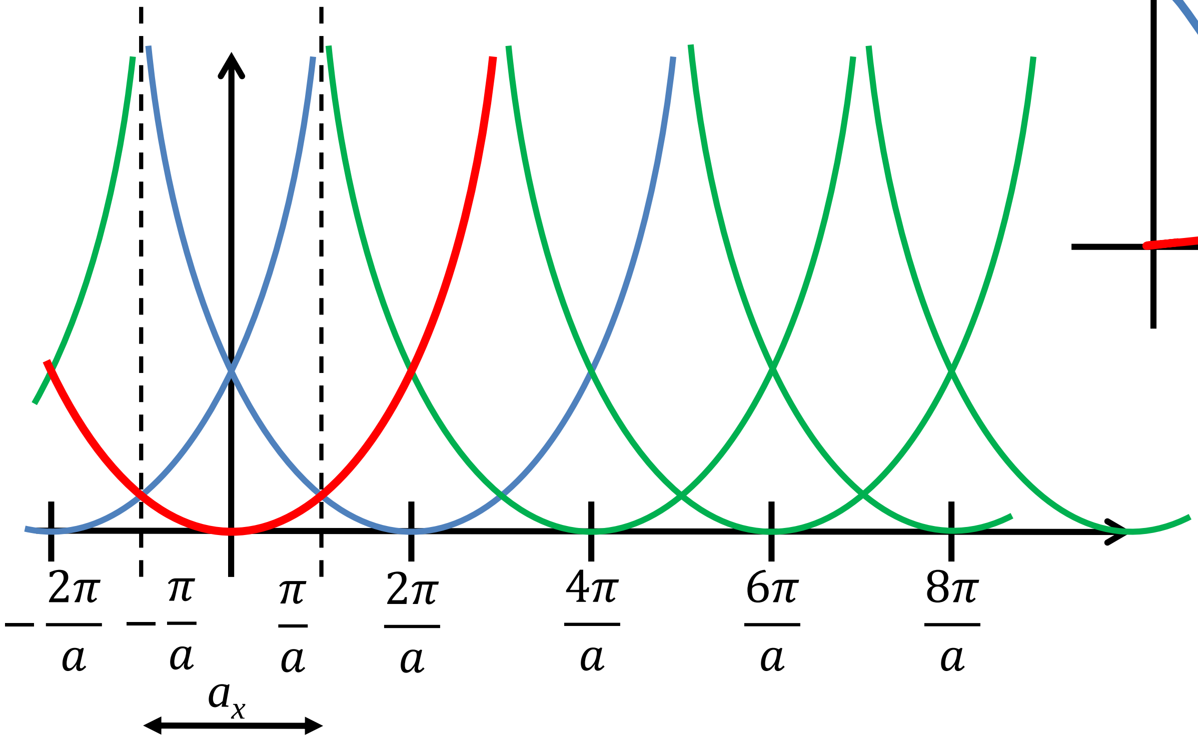


Periodic potential

The nearly free-electron approximation





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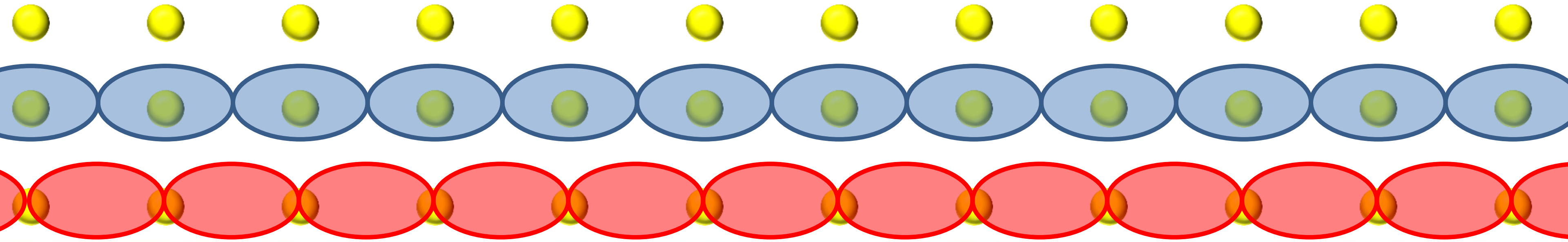
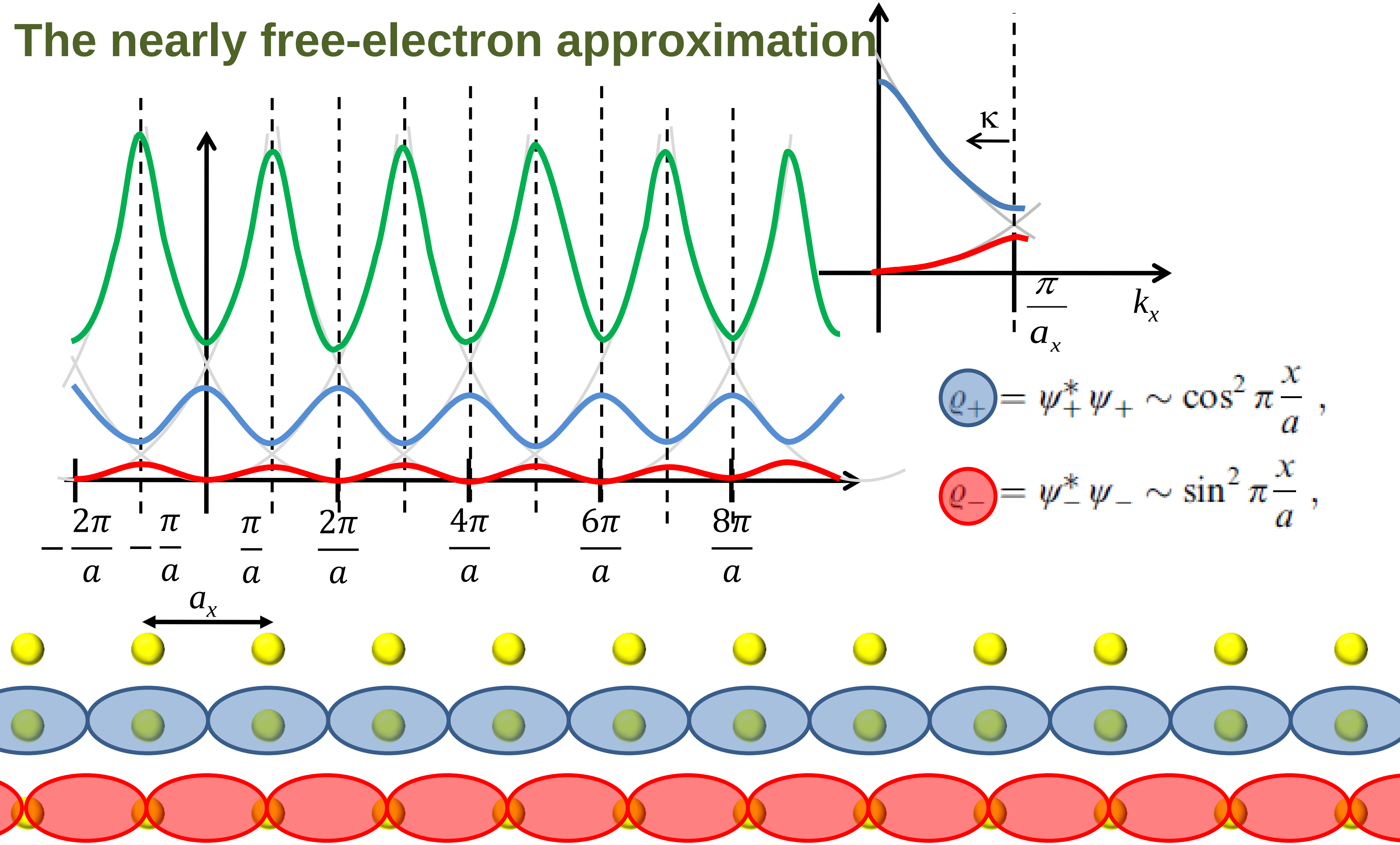


Periodic potential

The nearly free-electron approximation



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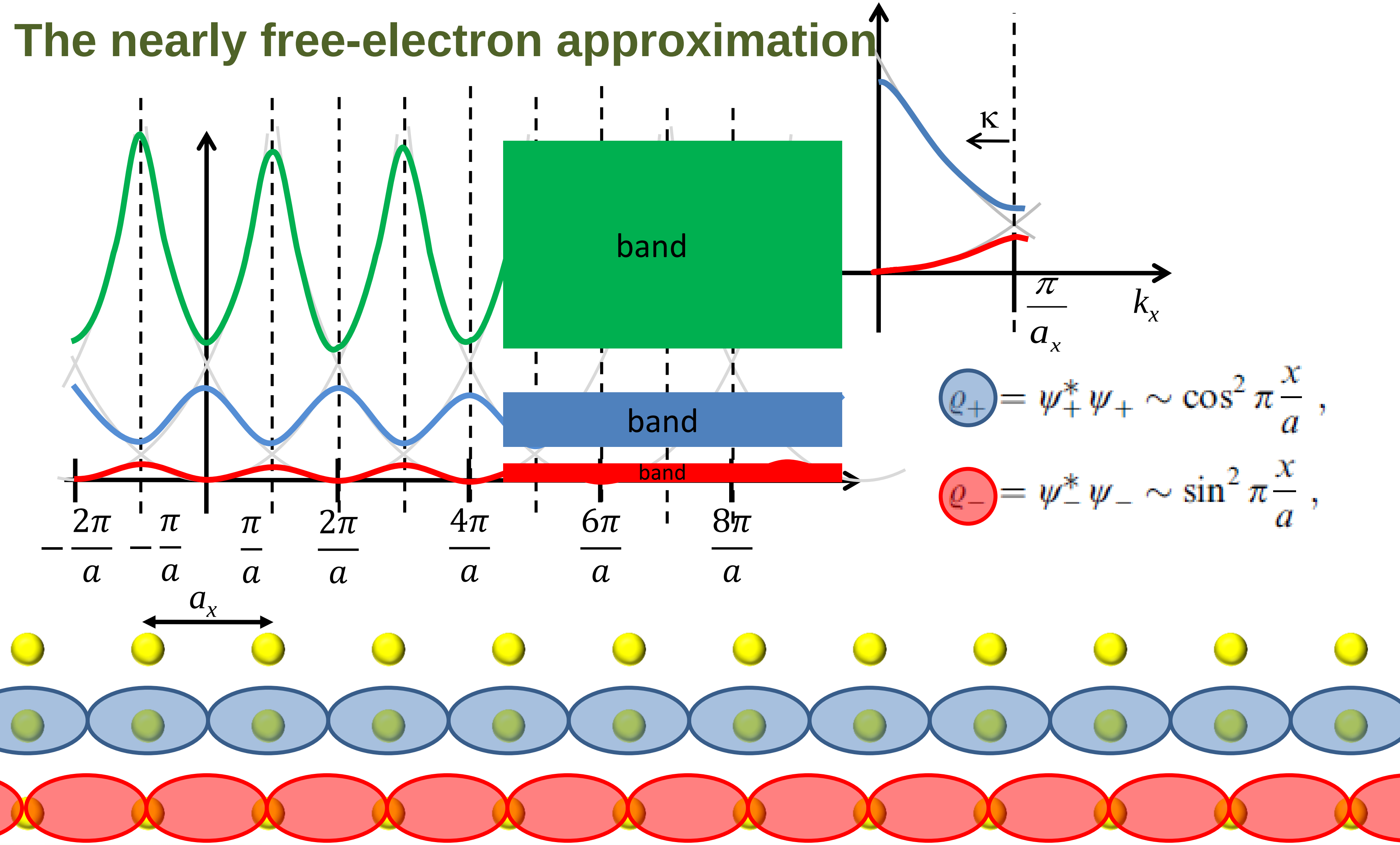
Periodic potential

The nearly free-electron approximation



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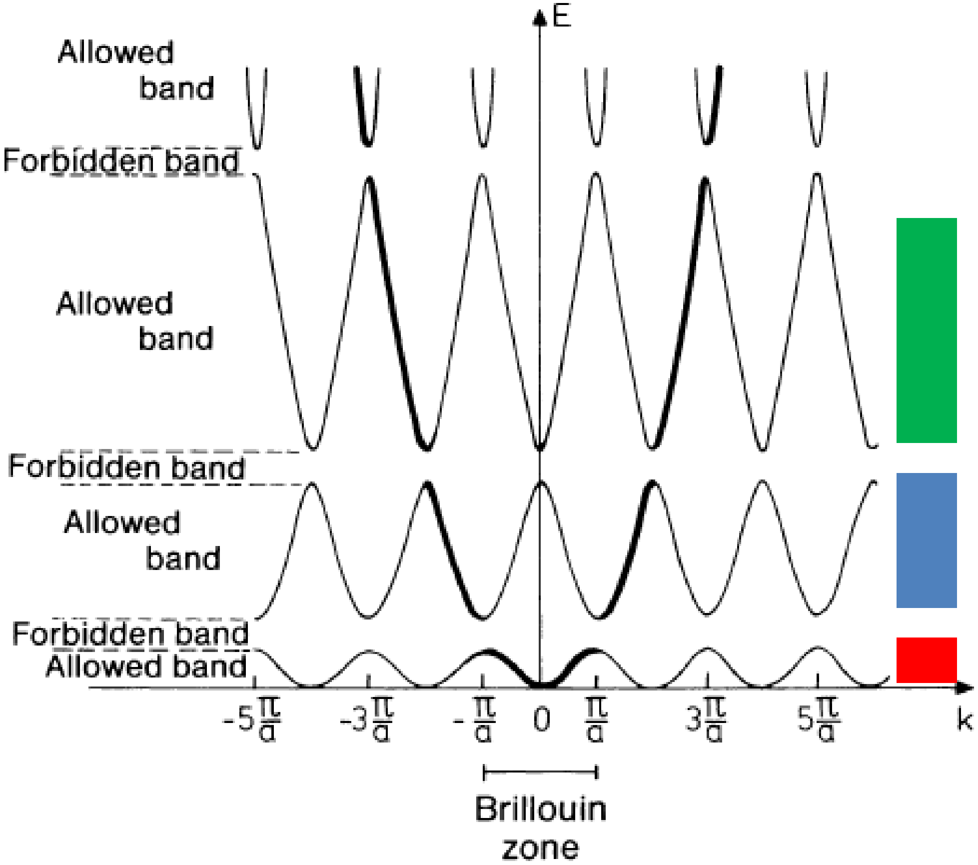
$$\varrho_- = \psi_-^* \psi_- \sim \sin^2 \pi \frac{x}{a} \ ,$$

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.



Fermi surfaces of metals

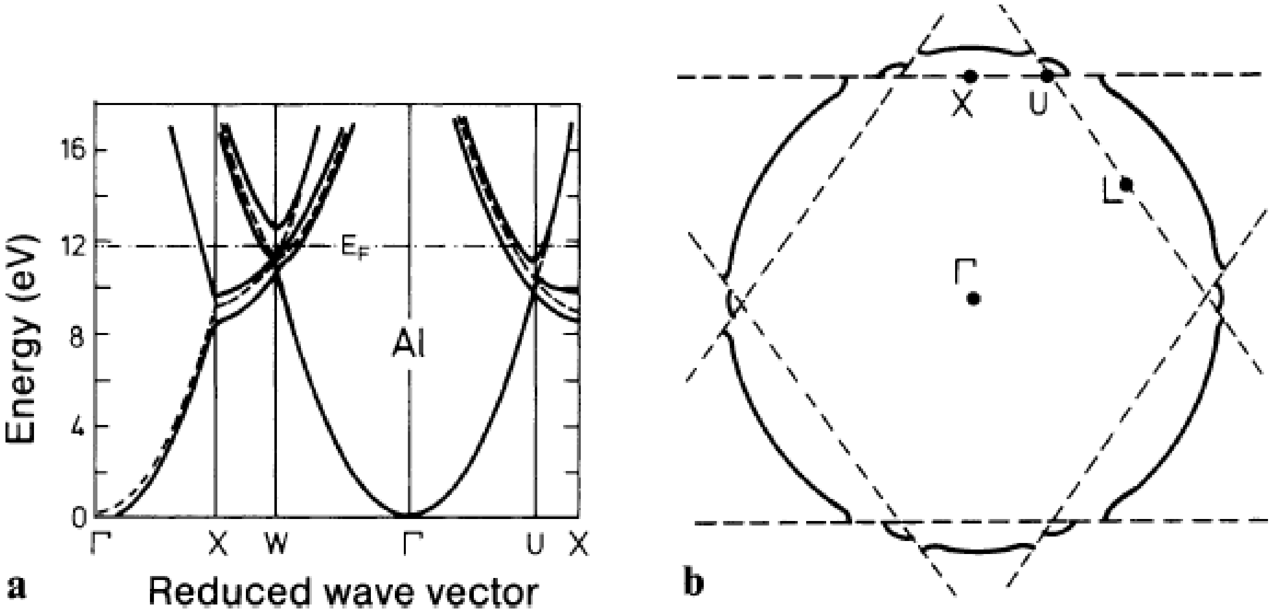


Fig. 7.11. (a) Theoretical bandstructure $E(\boldsymbol{k})$ for Al along directions of high symmetry (Γ is the center of the Brillouin zone). The dotted lines are the energy bands that one would obtain if the *s*- and *p*-electrons in Al were completely free ("empty" lattice). After [7.3]. (b) Cross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

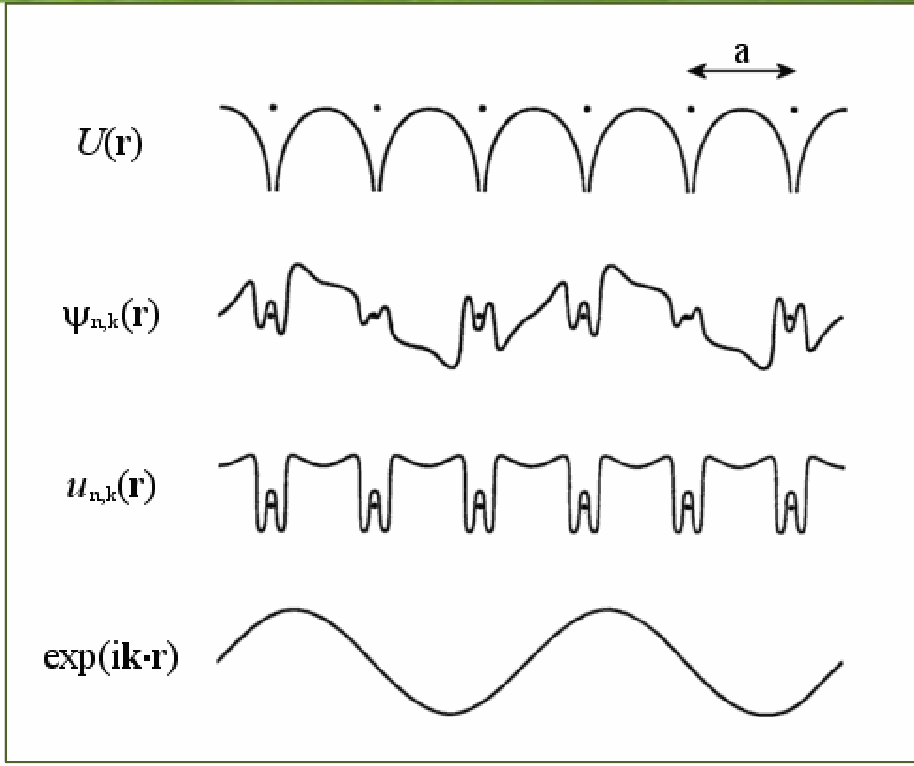
Bloch theorem

Bloch function has a form:

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

Generally non-periodic function

Periodic function, so-called *Bloch factor*



Example: electron in a constant potential

$$H = -\frac{\hbar^2}{2m}\Delta + V$$

substituting $\varphi_{n,\vec{k}}(\vec{r}) = 1\, e^{i\vec{k}\vec{r}}$

The solution is $E = \dfrac{\hbar^2 k^2}{2m} + V$

The momentum operator $\hat{p} = -i\hbar\nabla$ acting on $\varphi_{n,\vec{k}}(\vec{r})$

$\hat{p}\varphi_{n,\vec{k}}(\vec{r}) = \hbar k\ \varphi_{n,\vec{k}}(\vec{r})$. The solutions of the Schrödinger equation with a constant potential are eigenfunctions of the momentum operator. The momentum is well defined, the eigenvalue of the momentum operator is $\hat{p} = \hbar k$ (this defines the sense of $\vec{k}$-vector).

Periodic potential

Bloch theorem

Example:

Electron motion in a periodic potential.

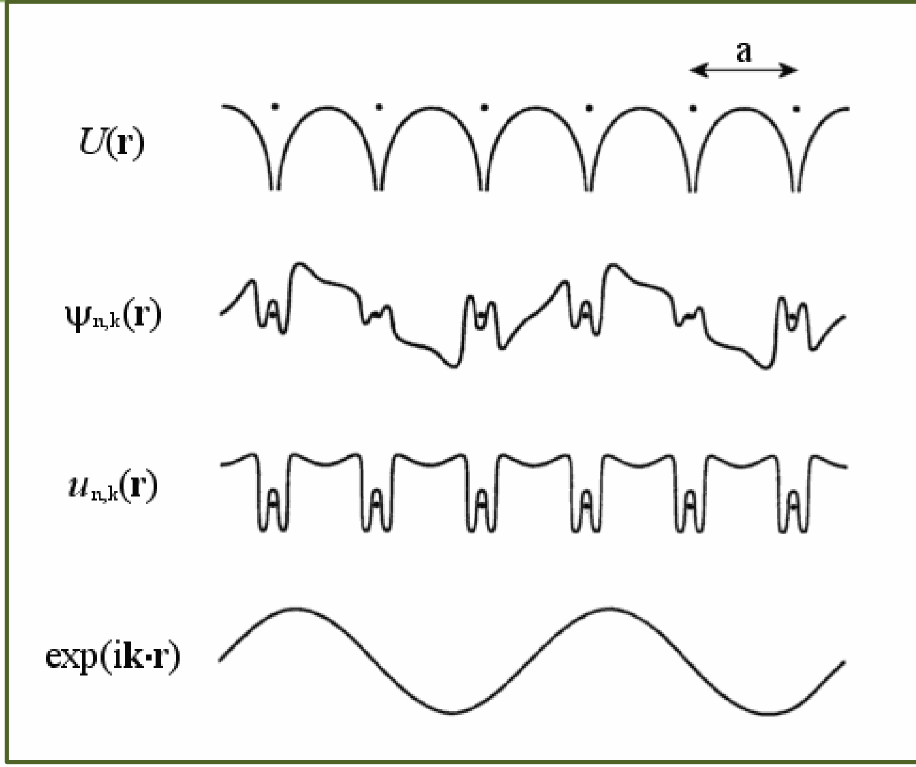
$$V(\vec{r}) = \sum_{\vec{G}} V_{\vec{G}} \exp\left(i\vec{G}\vec{r}\right)$$

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*):

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



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

Momentum of the Bloch function is not well defined!

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

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

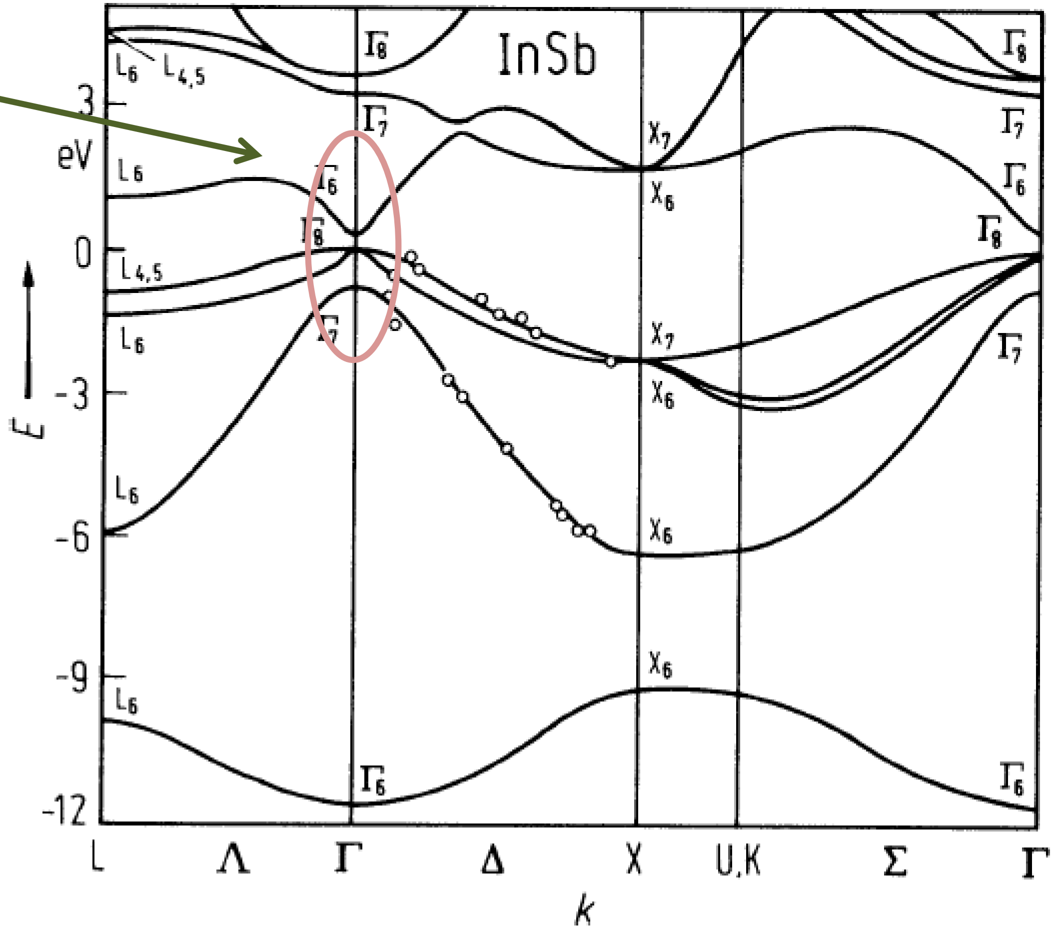
$$\hat{H}_{\vec{k}}u_{n,\vec{k}}(\vec{r}) = \left(\hat{H}_{\vec{k}_0} + \hat{H}'\right)u_{n,\vec{k}}(\vec{r}) = E_n(\vec{k})u_{n,\vec{k}}(\vec{r})$$

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 $E_n(\vec{k})$.

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.

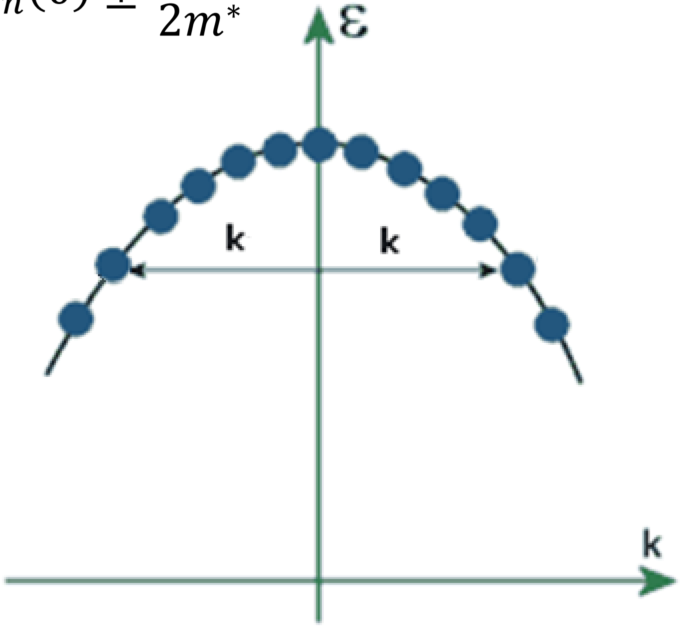
k·p perturbation theory – effective mass

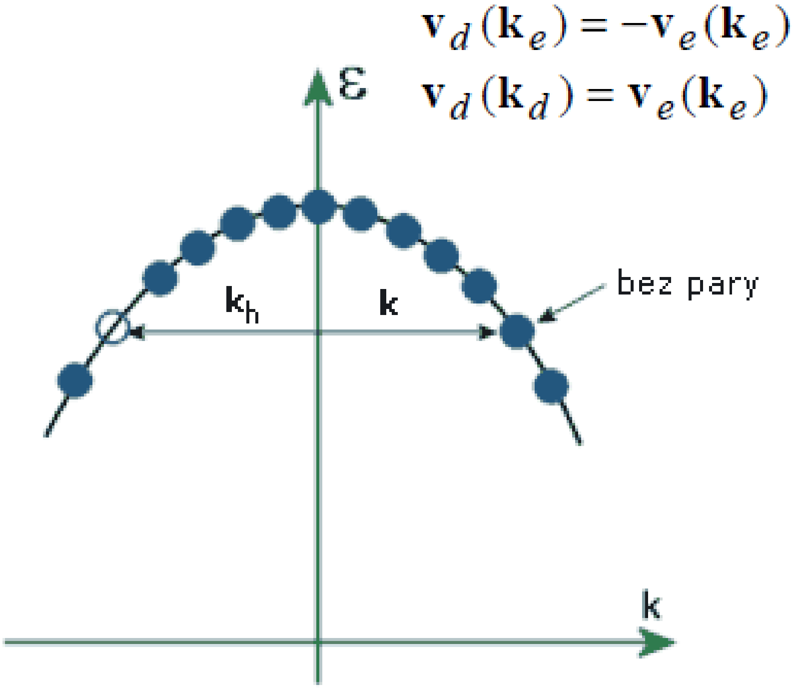
The energy $E_n(\boldsymbol{k})$ around extremum for the uniaxial crystal (np. GaN):

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

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

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

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

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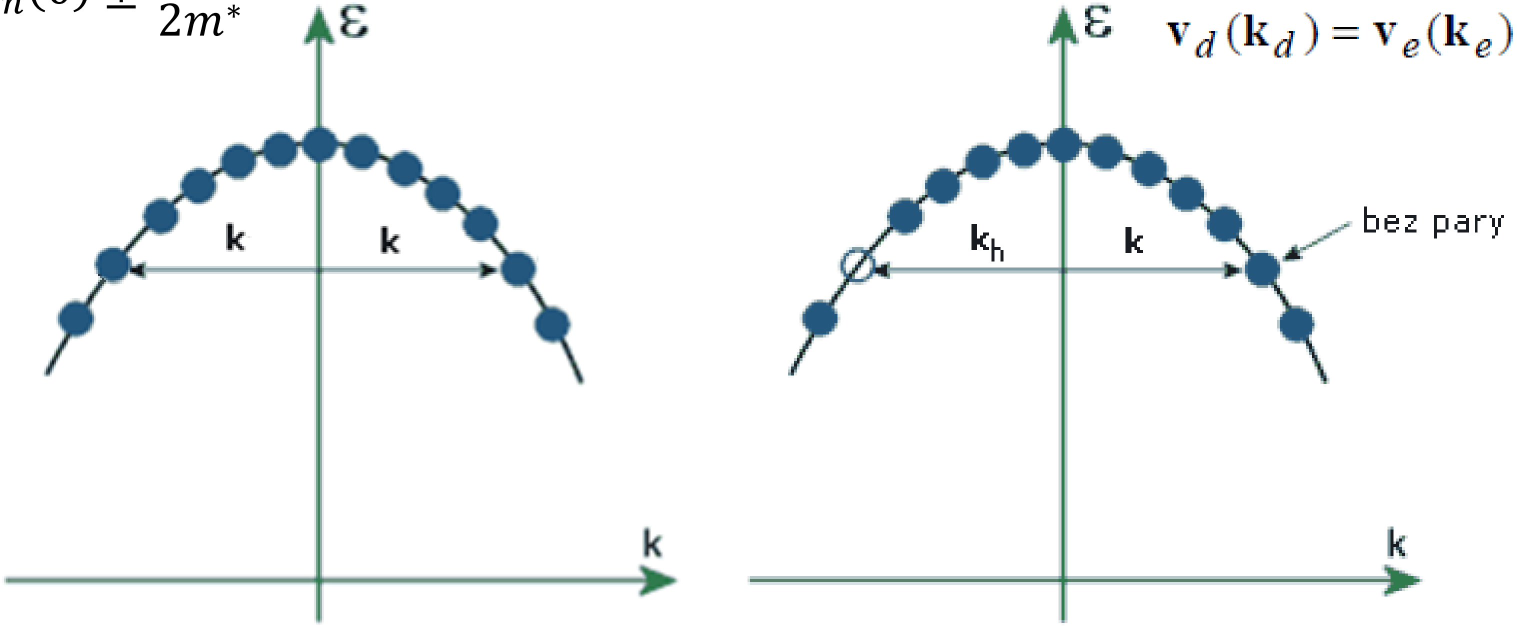

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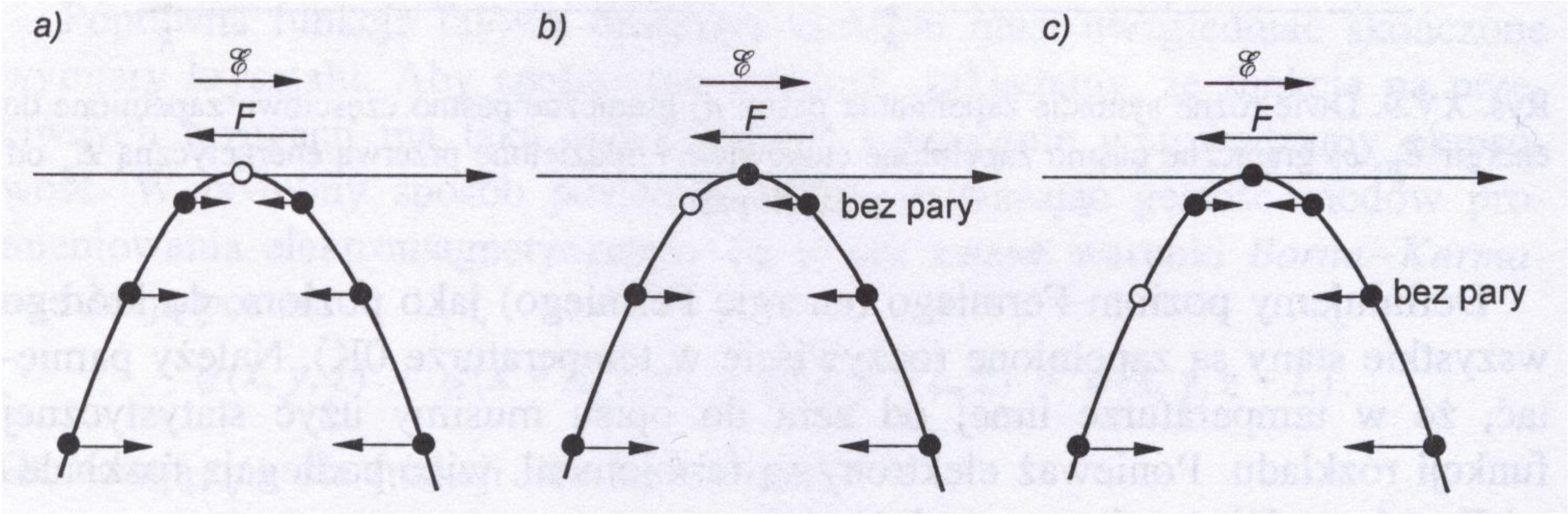
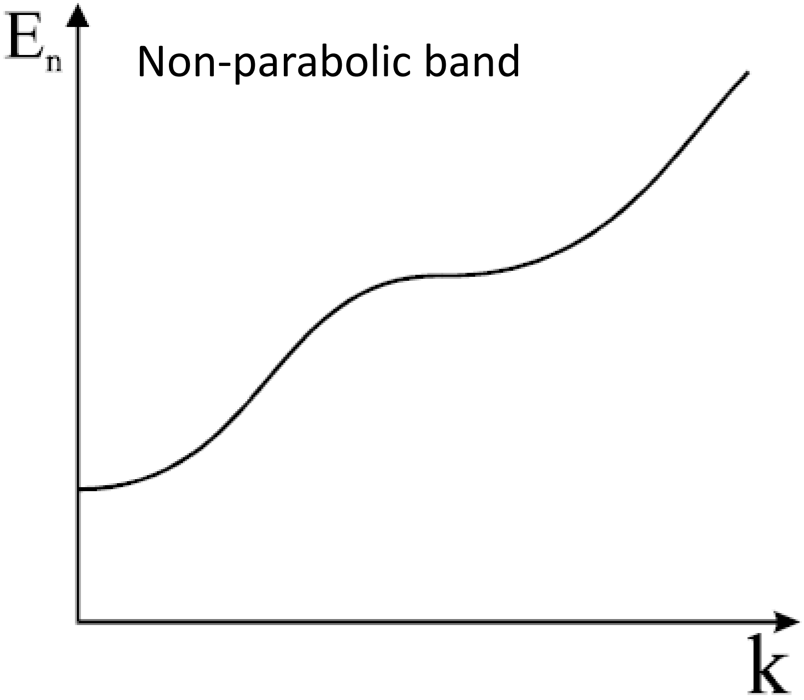


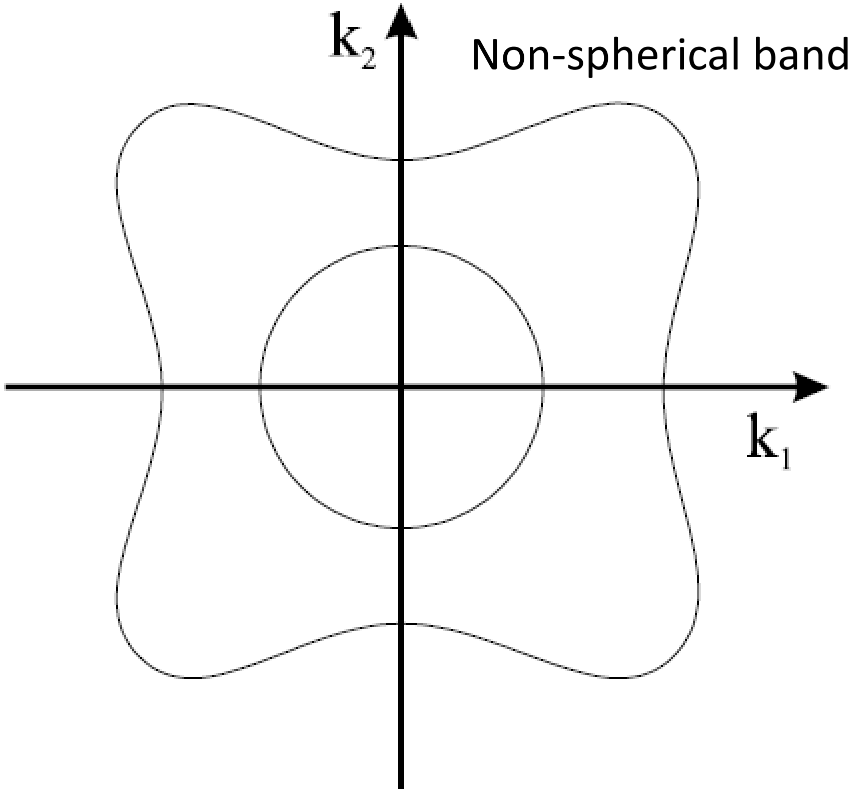
k·p perturbation theory – effective mass

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



Non-parabolic band

Przykładowa zależność energii stanów pasma n od wektora falowego k.



Non-spherical band

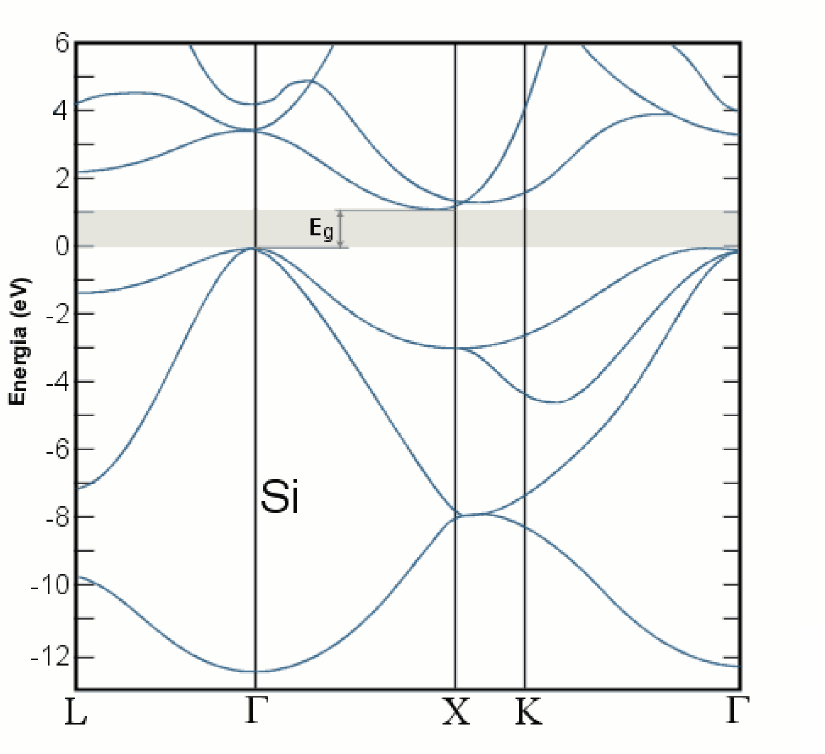
Przykładowe powierzchnie stałej energii w dwuwymiarowej przestrzeni k.

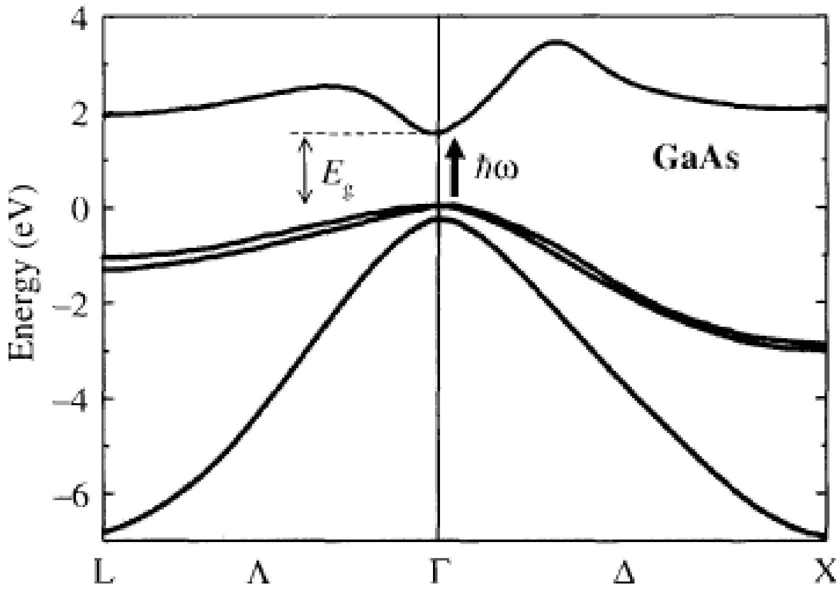
R. Stępniewski

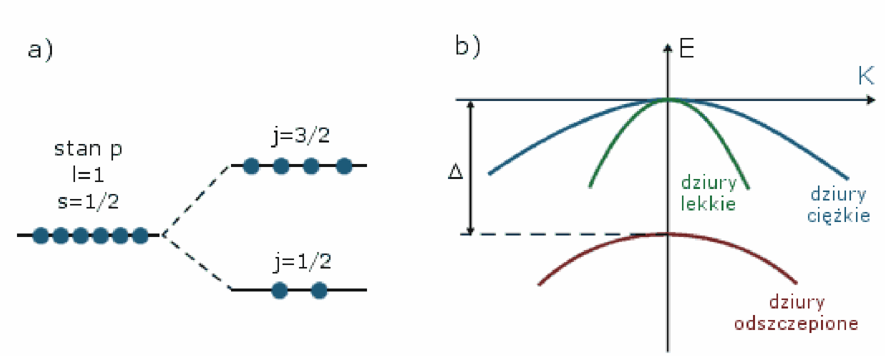
k·p perturbation theory – effective mass

The band theory of solids

Examples:







D. Wasik.

The band theory of solids.

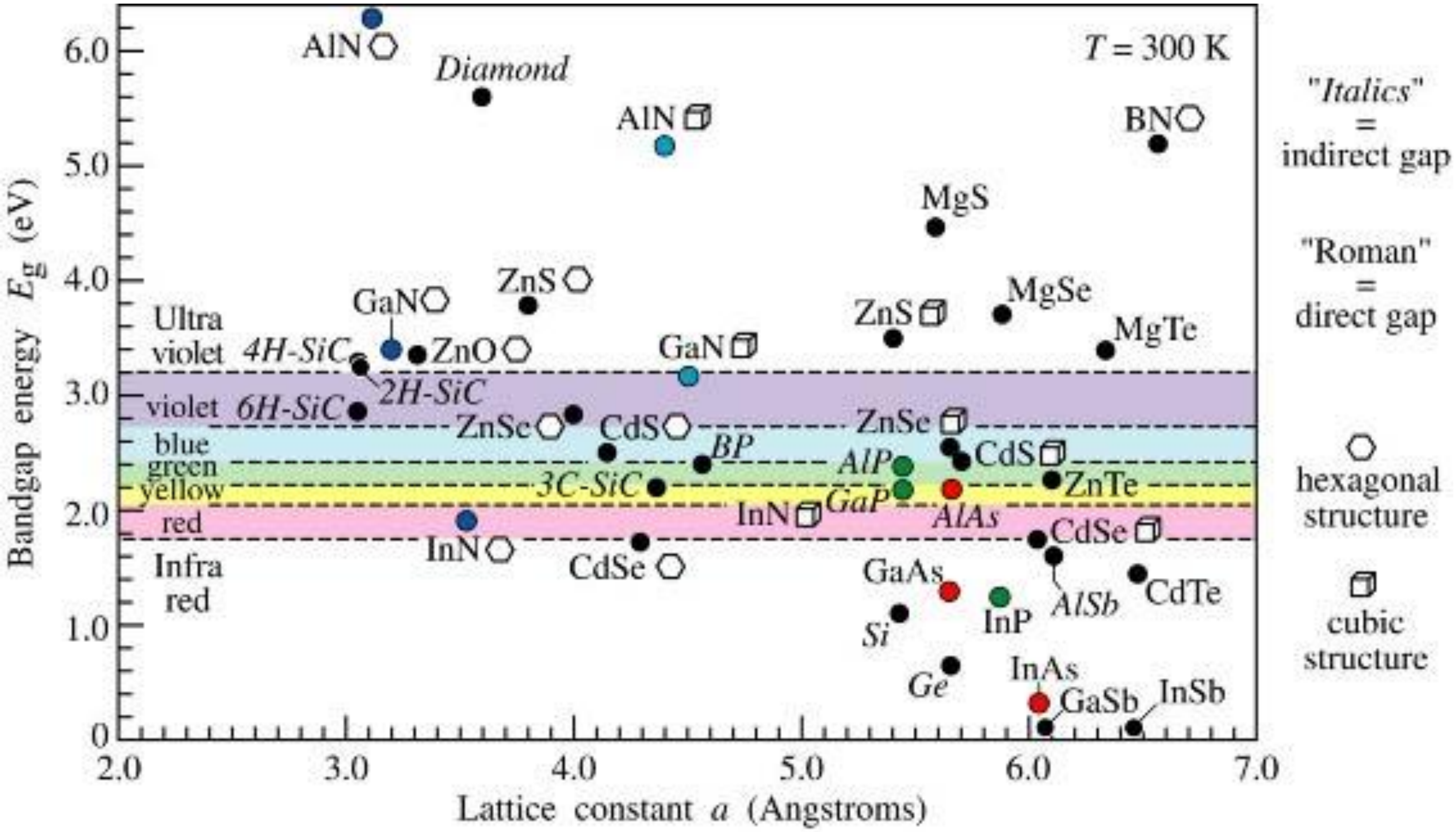


Fig. 11.4. Room-temperature bandgap energy versus lattice constant of common elemental and binary compound semiconductors.

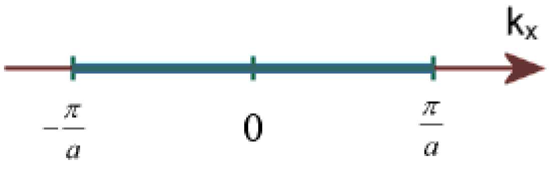
Periodic potential

Brillouin zones

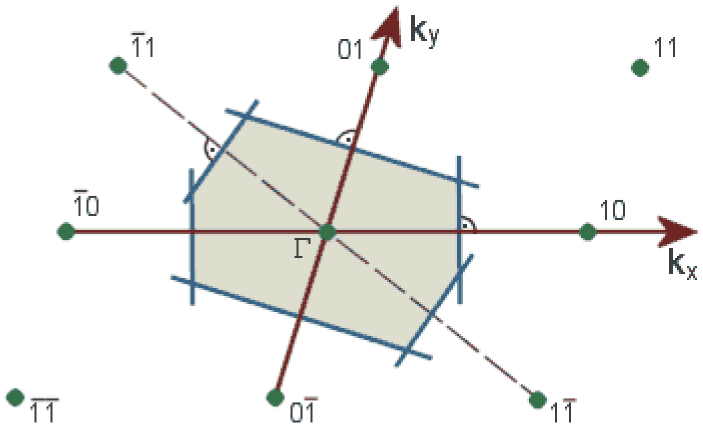
$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3, \qquad n_i \in \mathbb{Z}$$

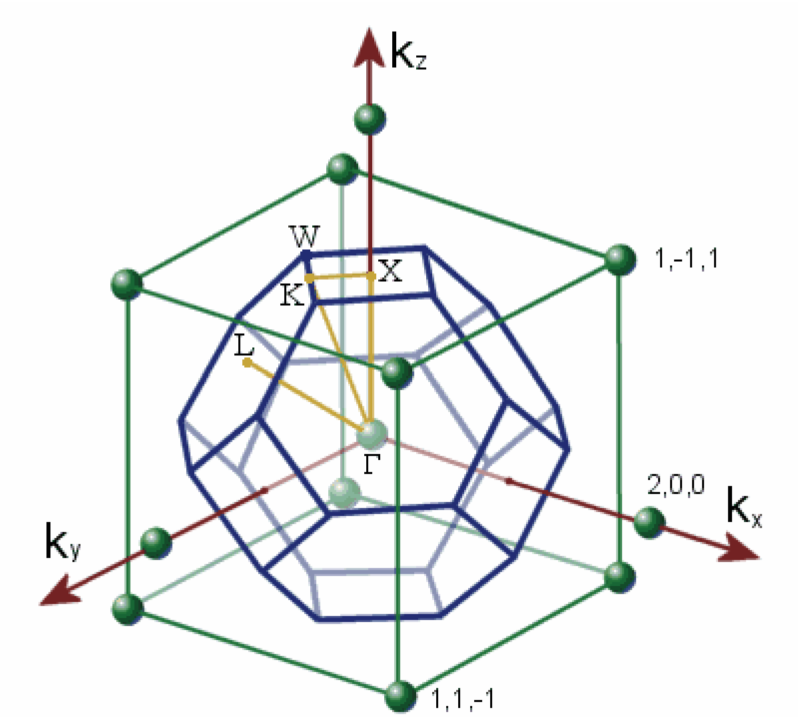
$$\vec{G} = m_1\vec{a}_1^* + m_2\vec{a}_2^* + m_3\vec{a}_3^*, \qquad m_i \in \mathbb{Z}$$

Brillouin zone in 1D



Brillouin zone in 2D, oblique lattice.

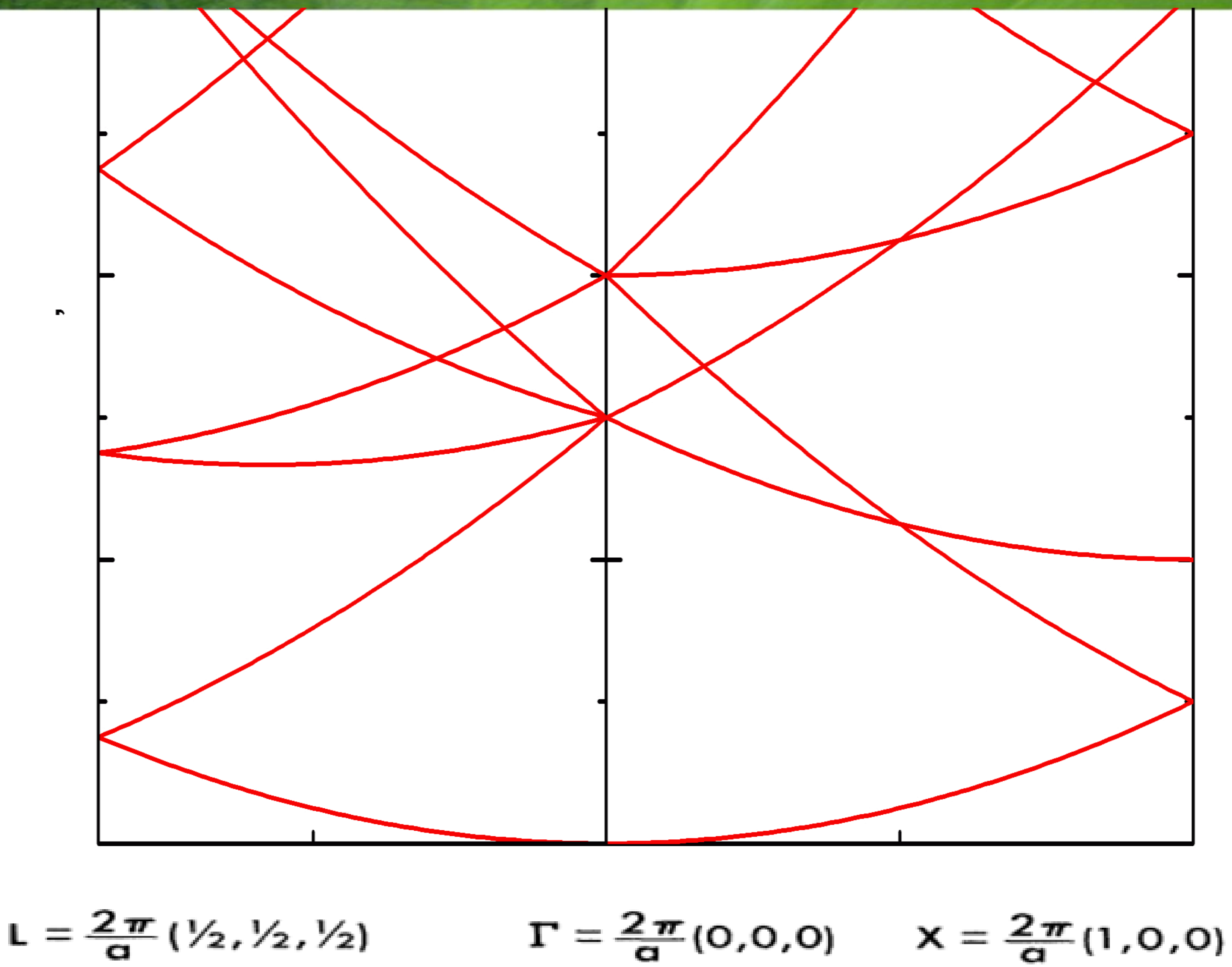




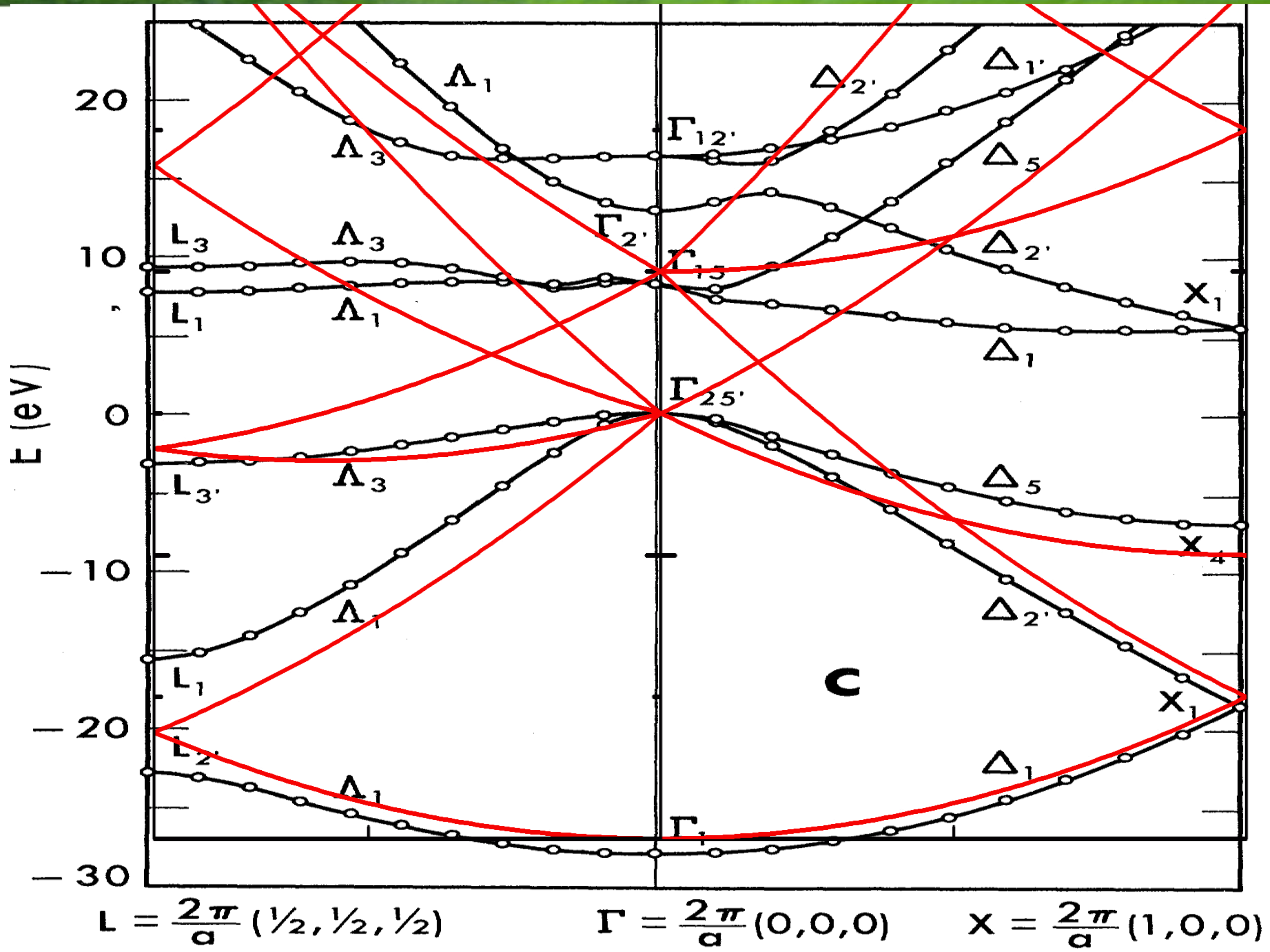
Brillouin zone for face centered cubic (fcc) lattice. The limiting zone walls comes from reciprocal lattice points (2,0,0) square and (1,1,1) hexagonal.

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

Periodic potential



Periodic potential



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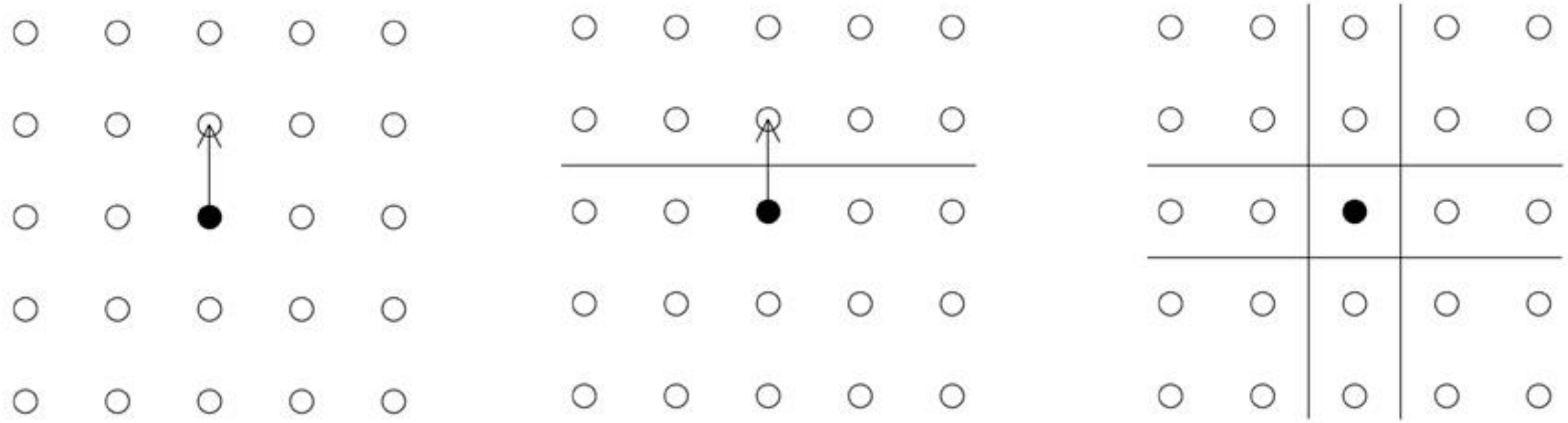
2-D square lattice

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



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

Periodic potential

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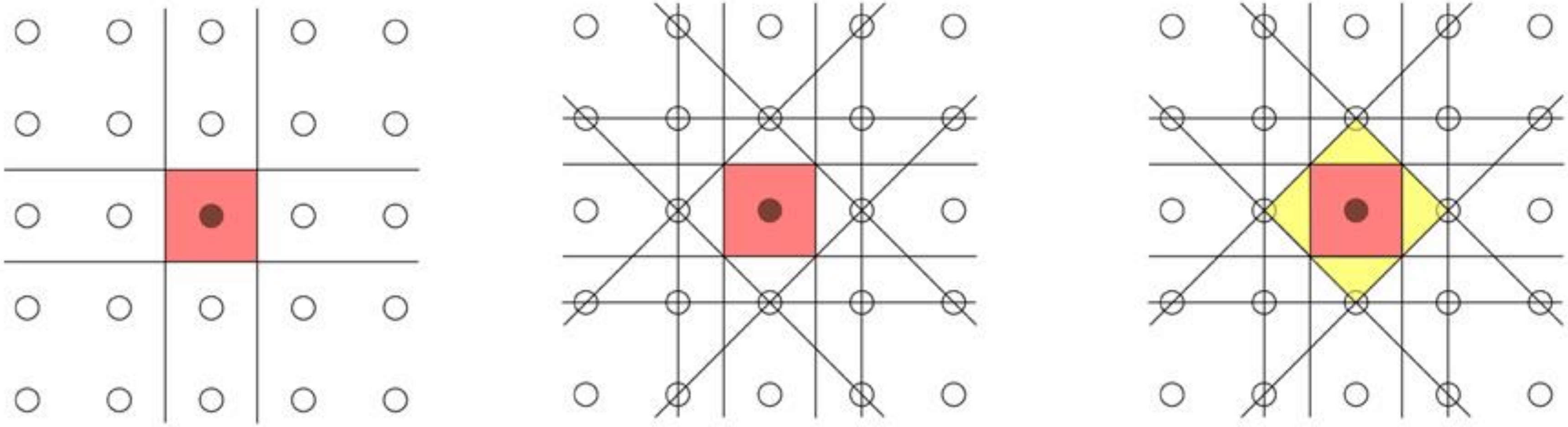

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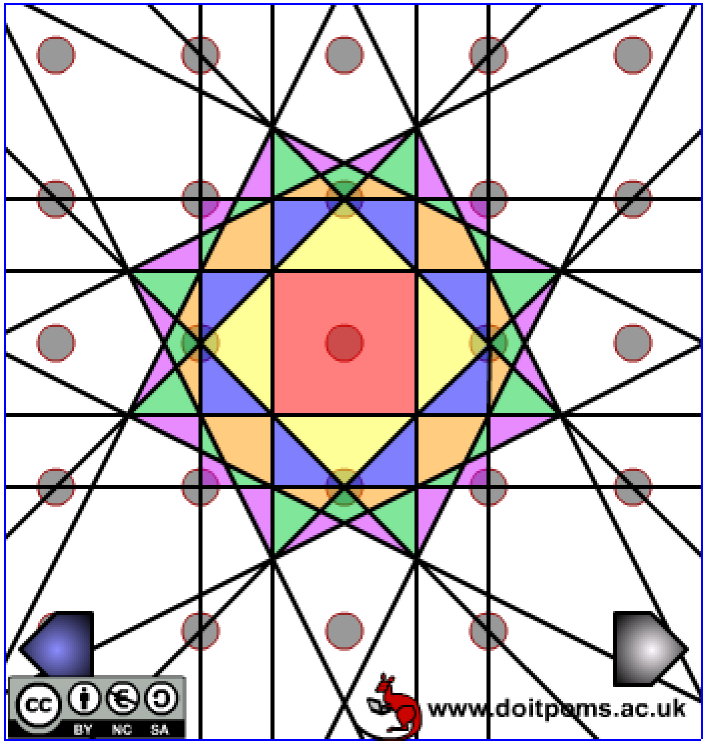

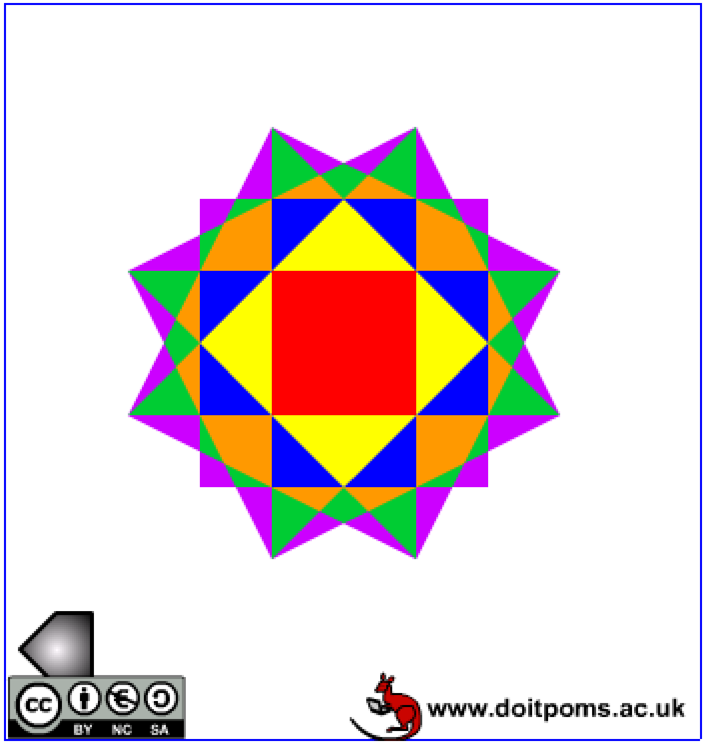

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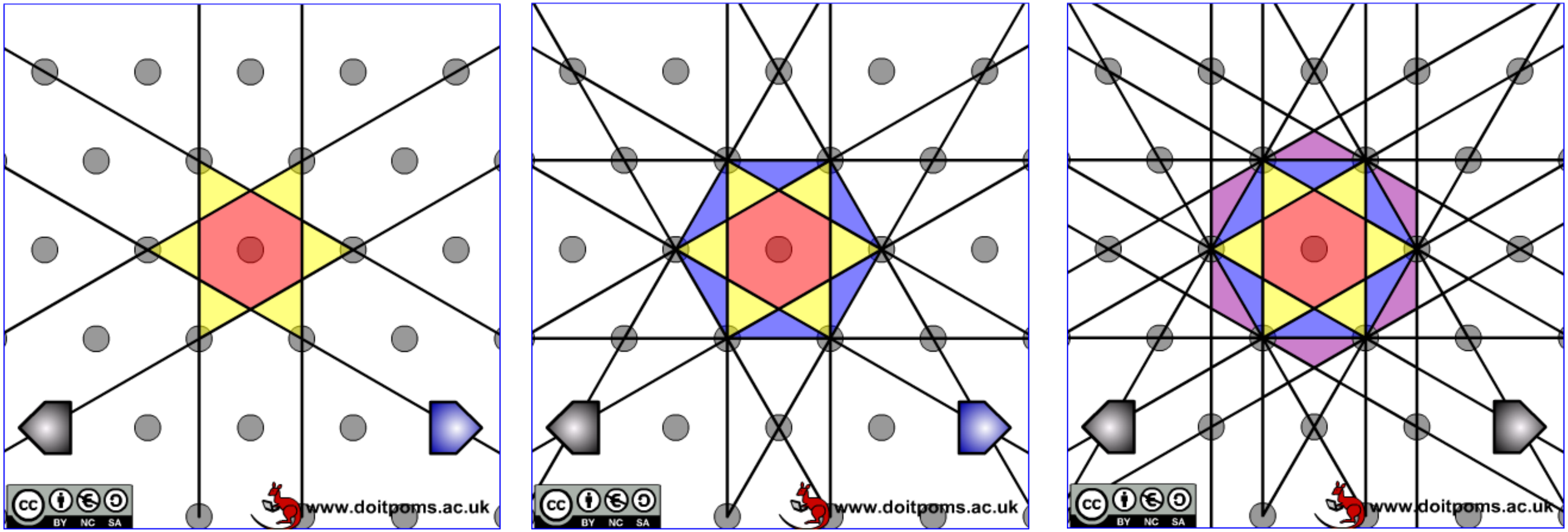
2-D hexagonal lattice



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Periodic potential

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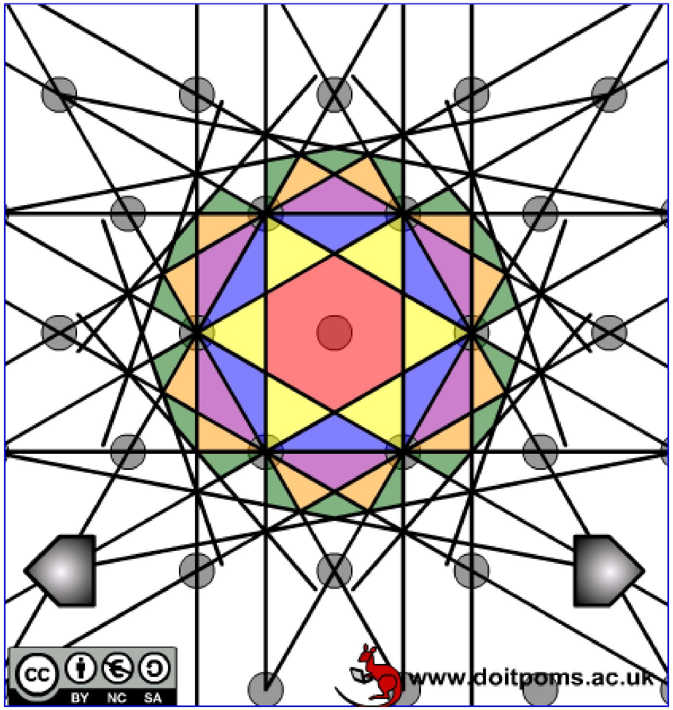
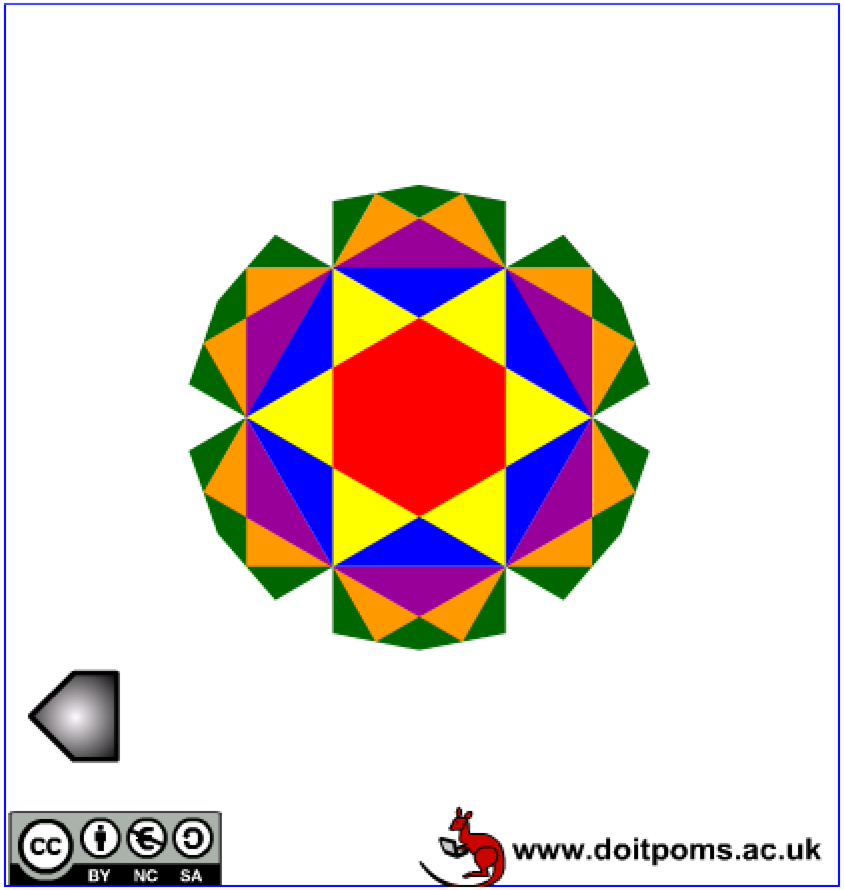




http://www.doitpoms.ac.uk/tlplib/brillouin_zones/zone_construction.php

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:

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

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

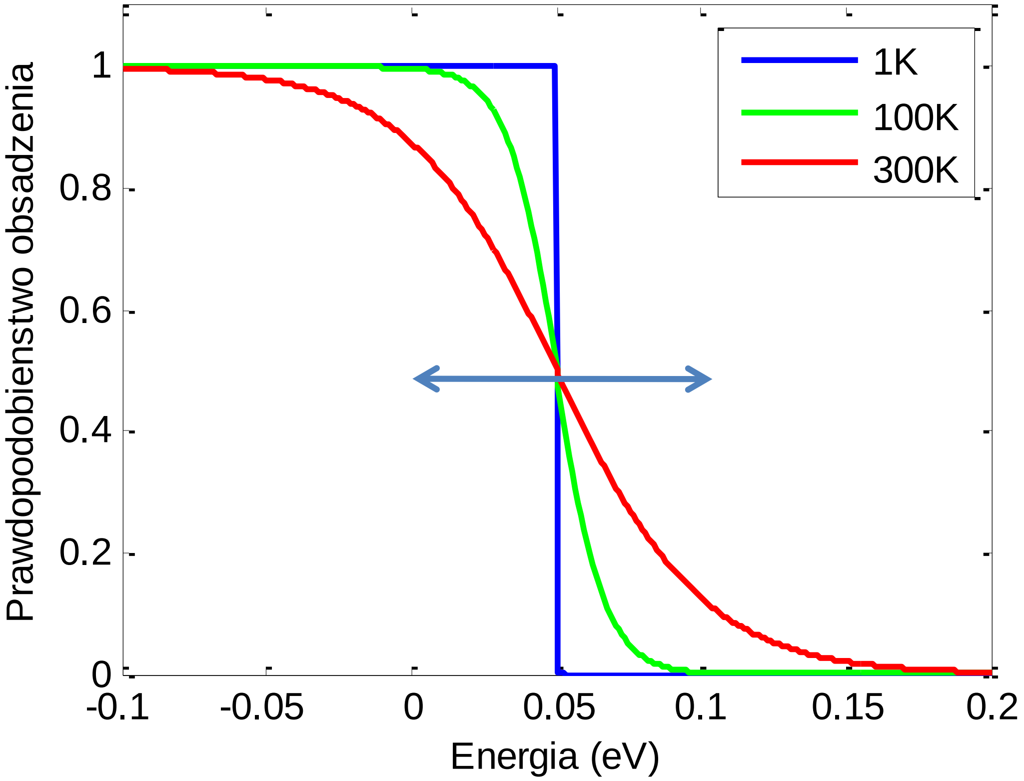
$$F = U - TS$$

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

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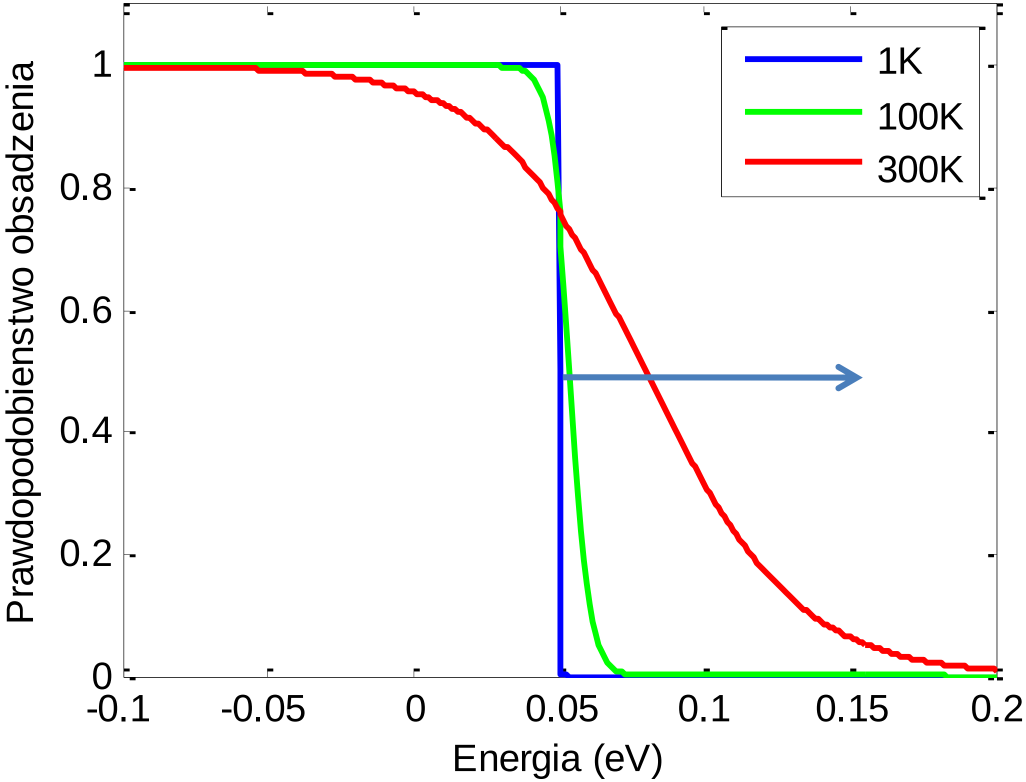

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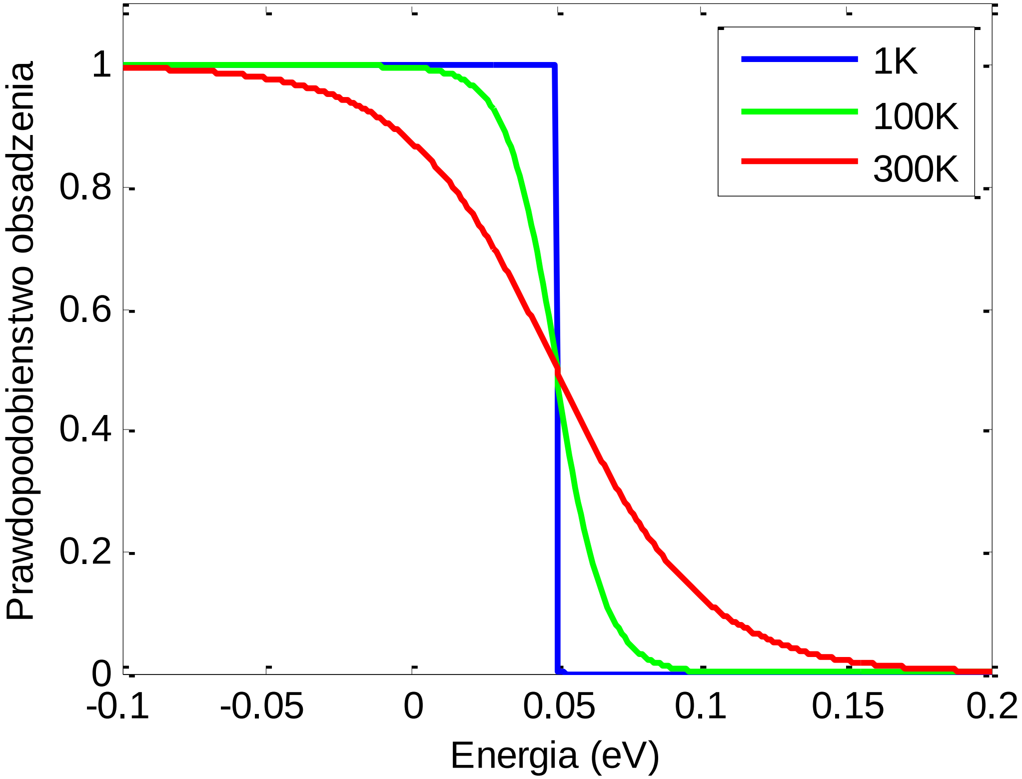

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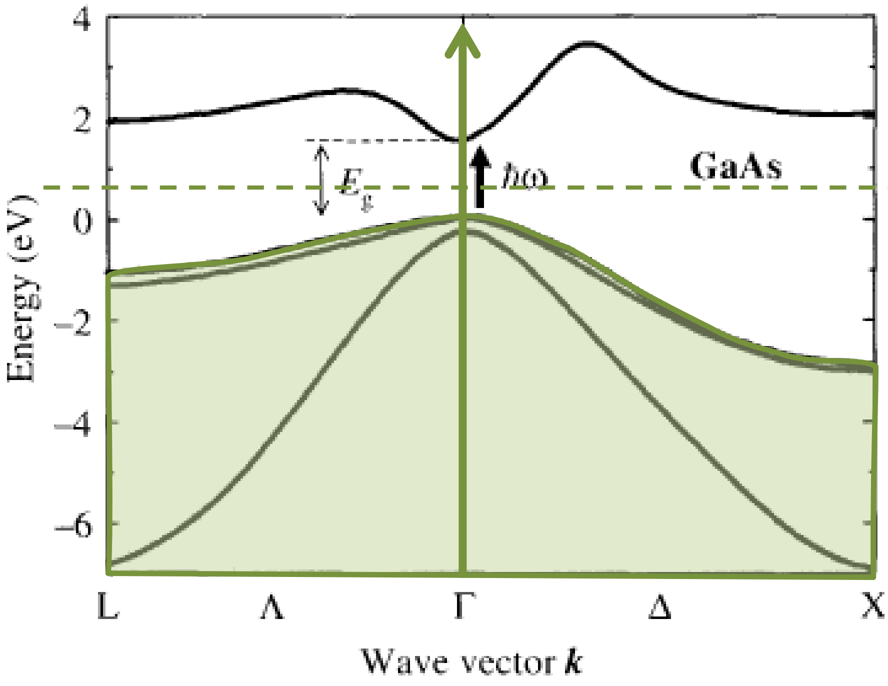

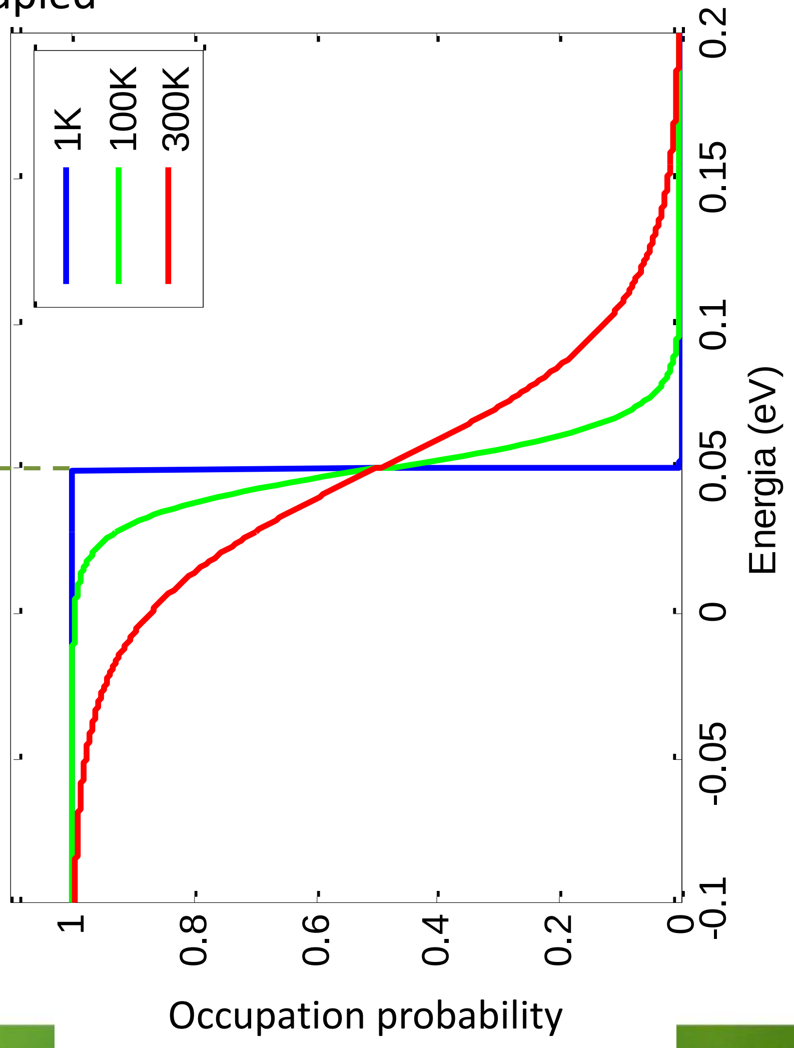

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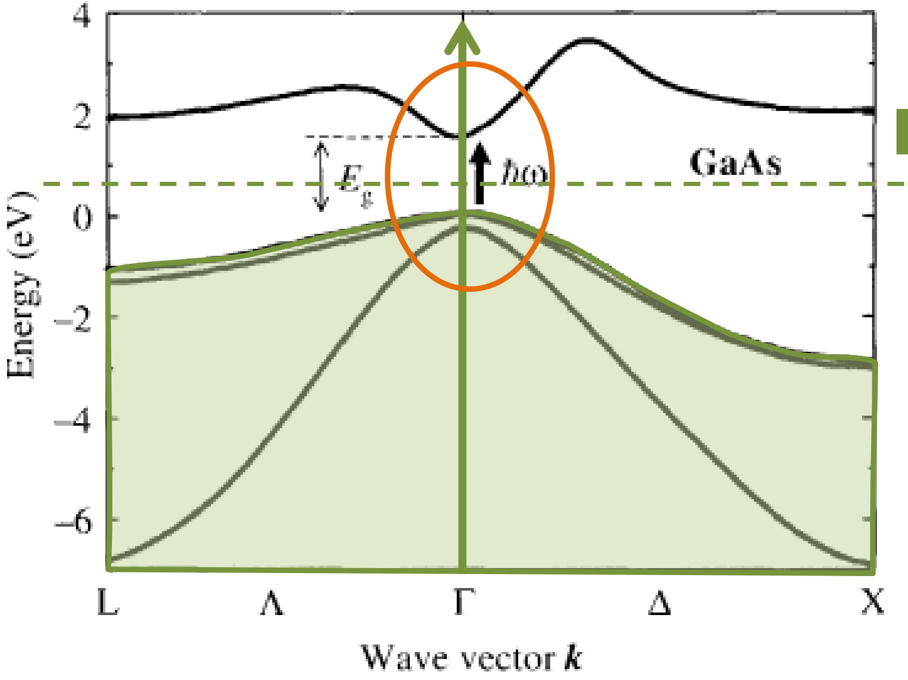

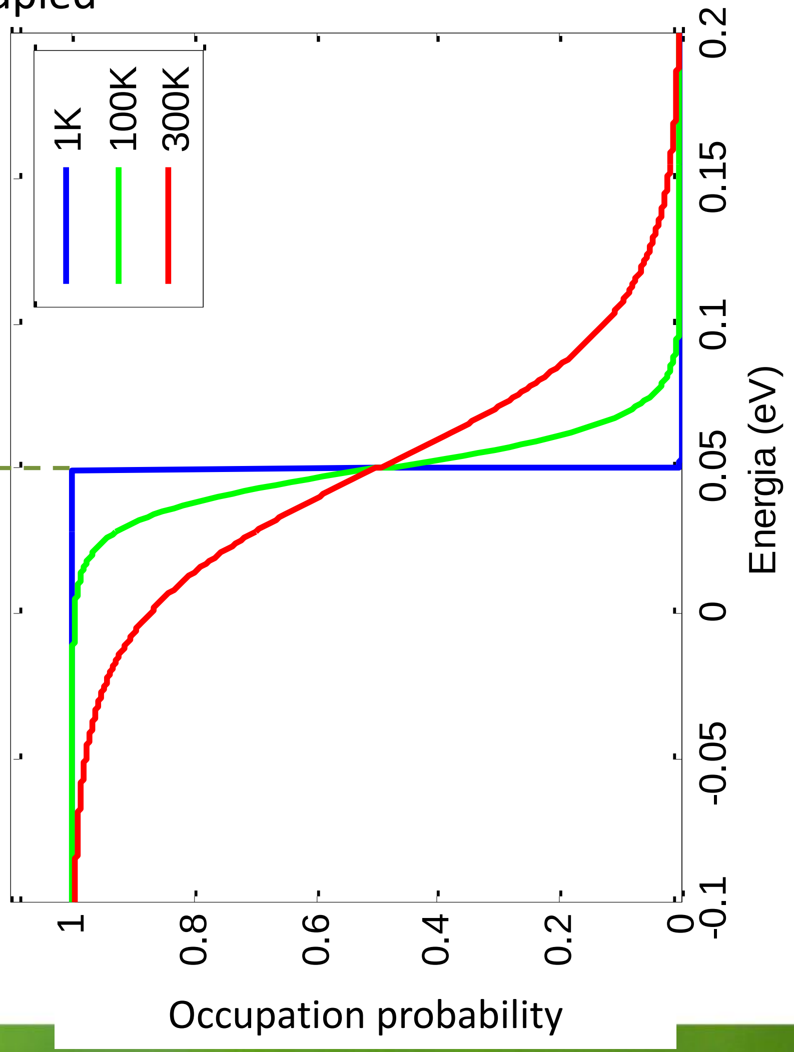

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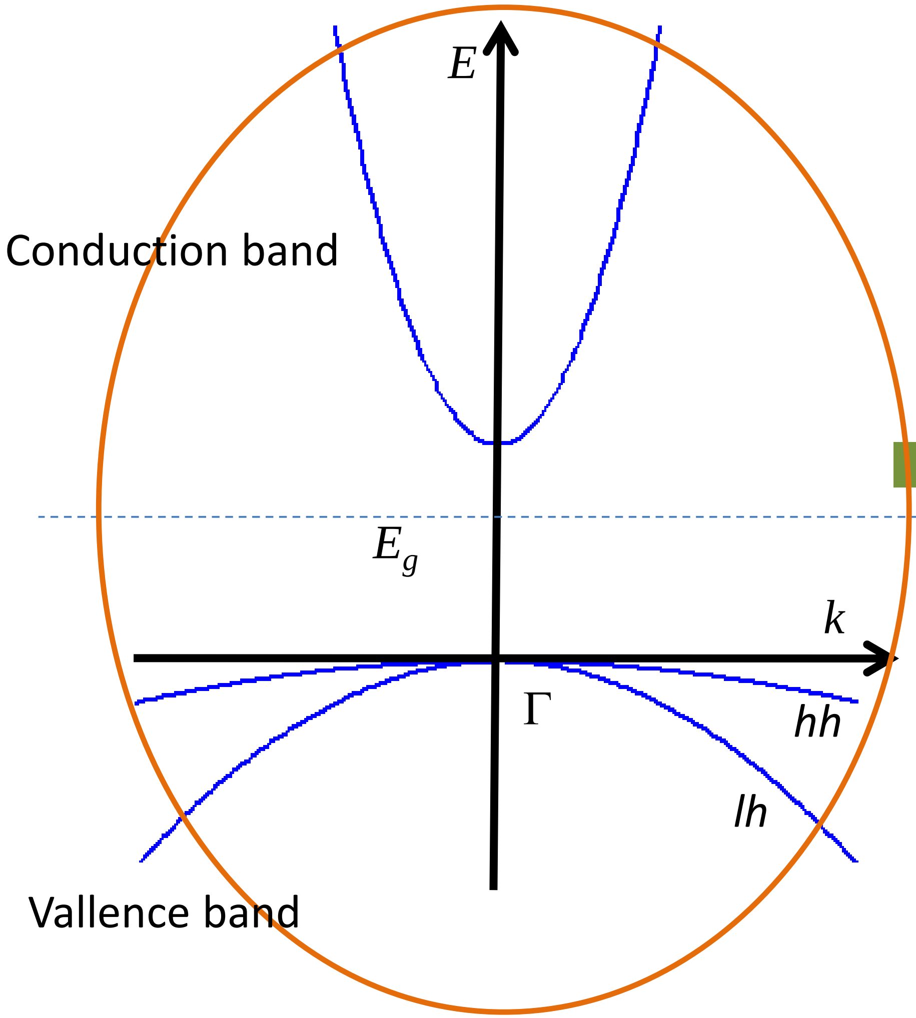
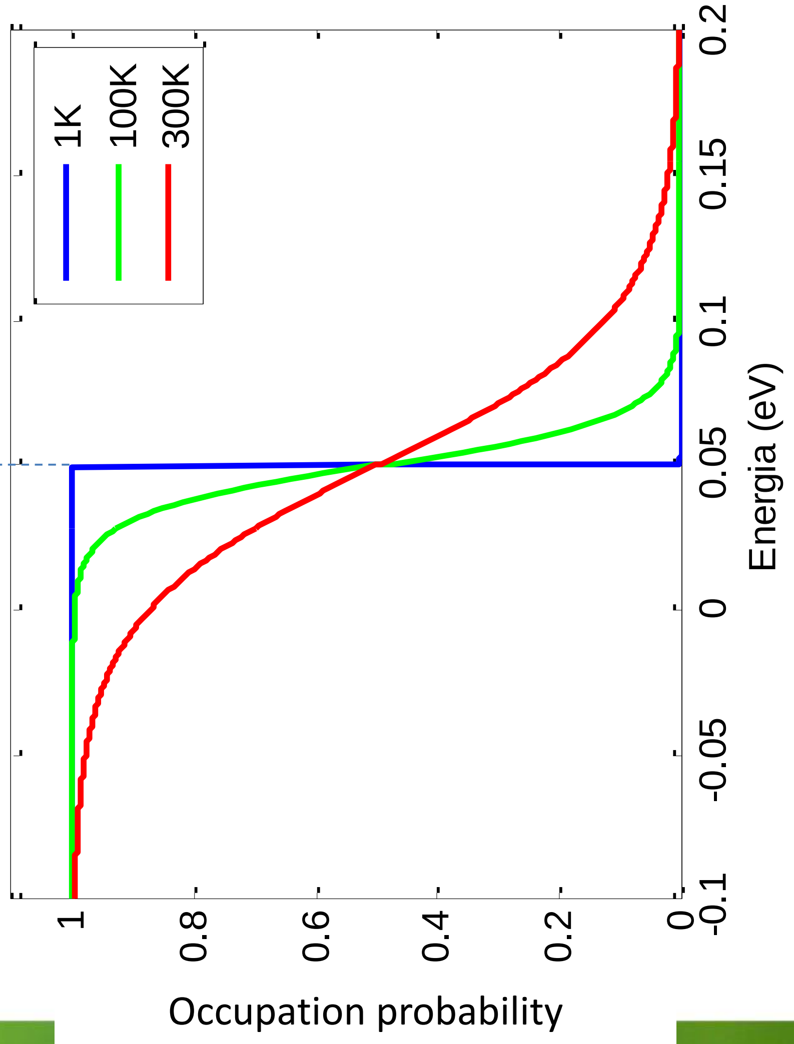




Density of states

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

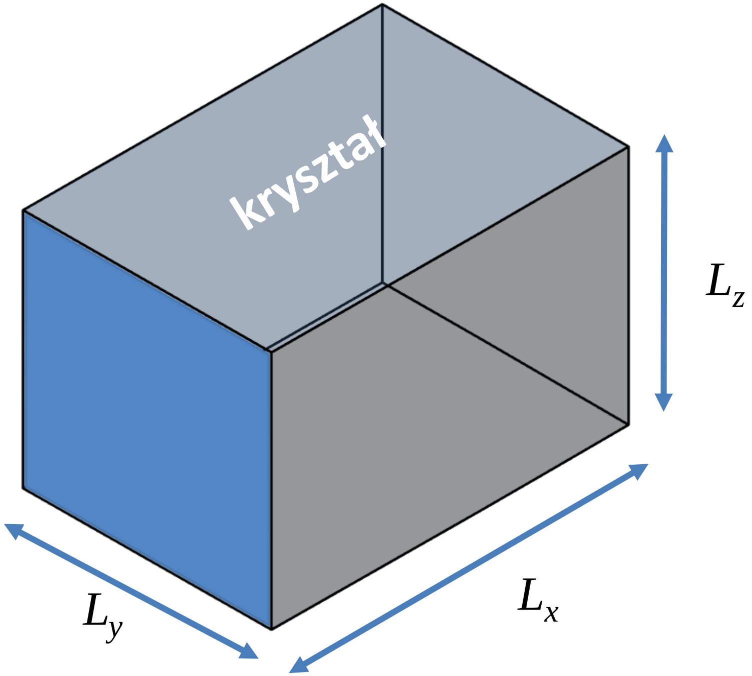
Finite size of the crystal L_x, L_y, L_z

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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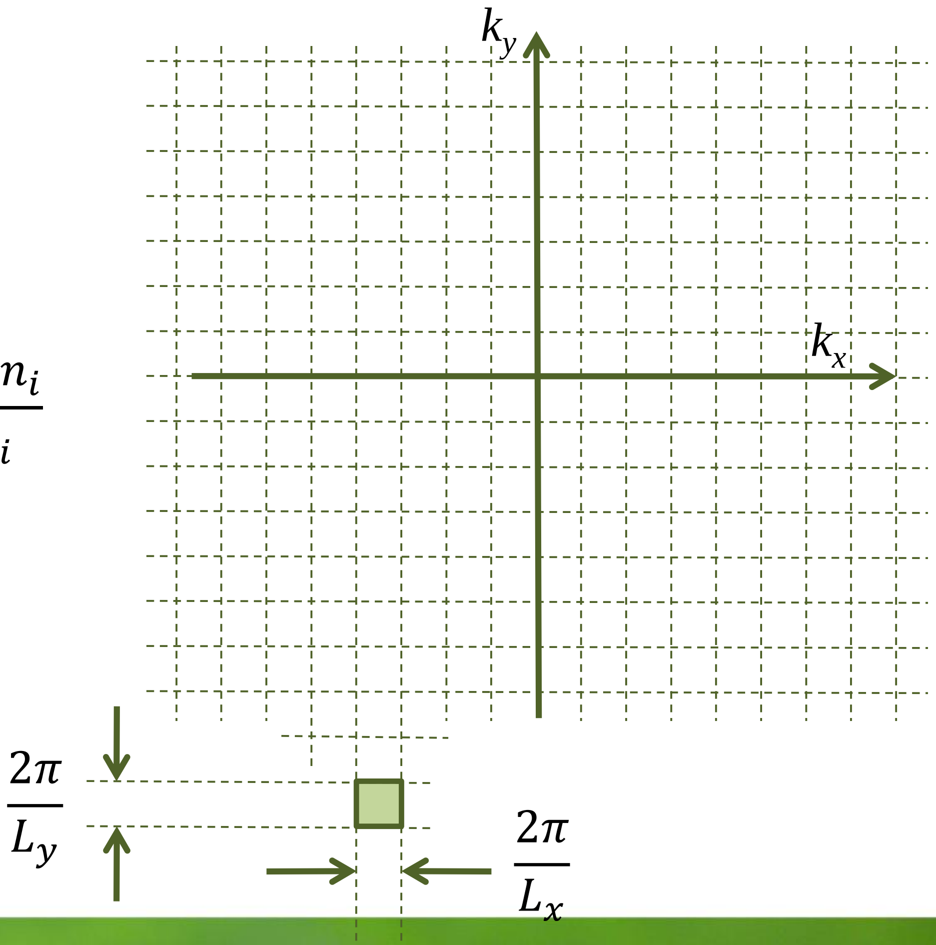

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The density of states in k-space of n dimension (and the unite volume)

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

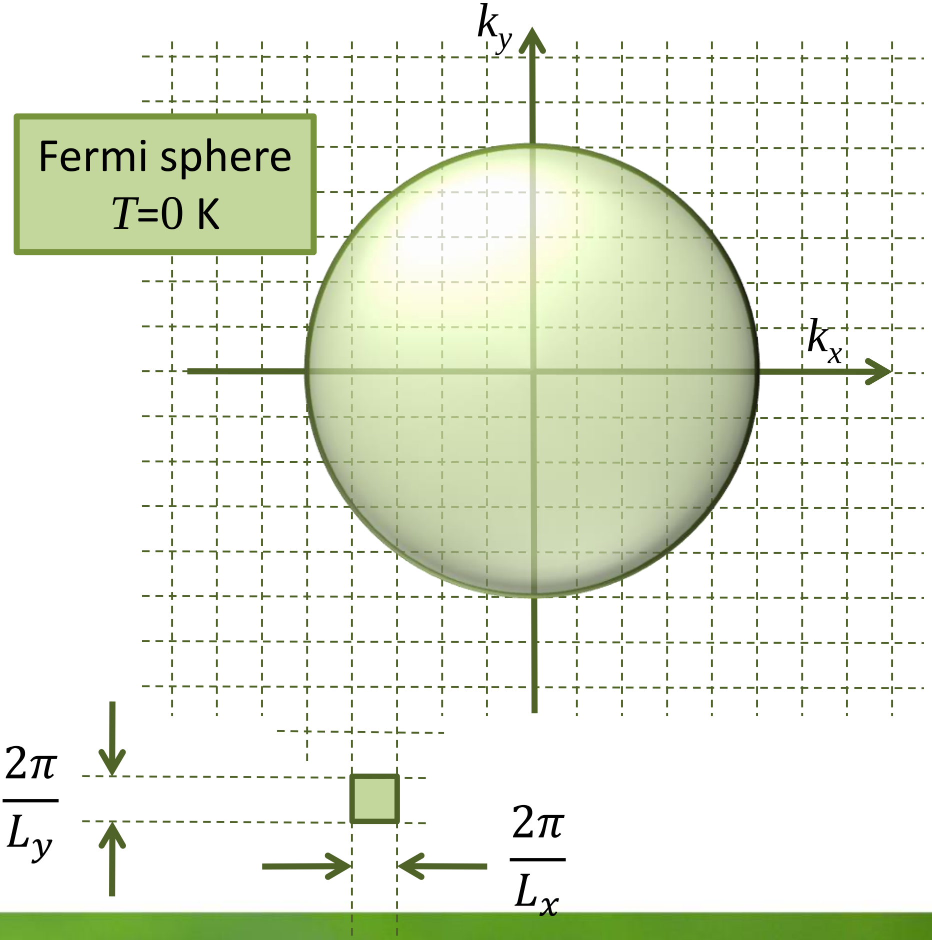
3D case

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

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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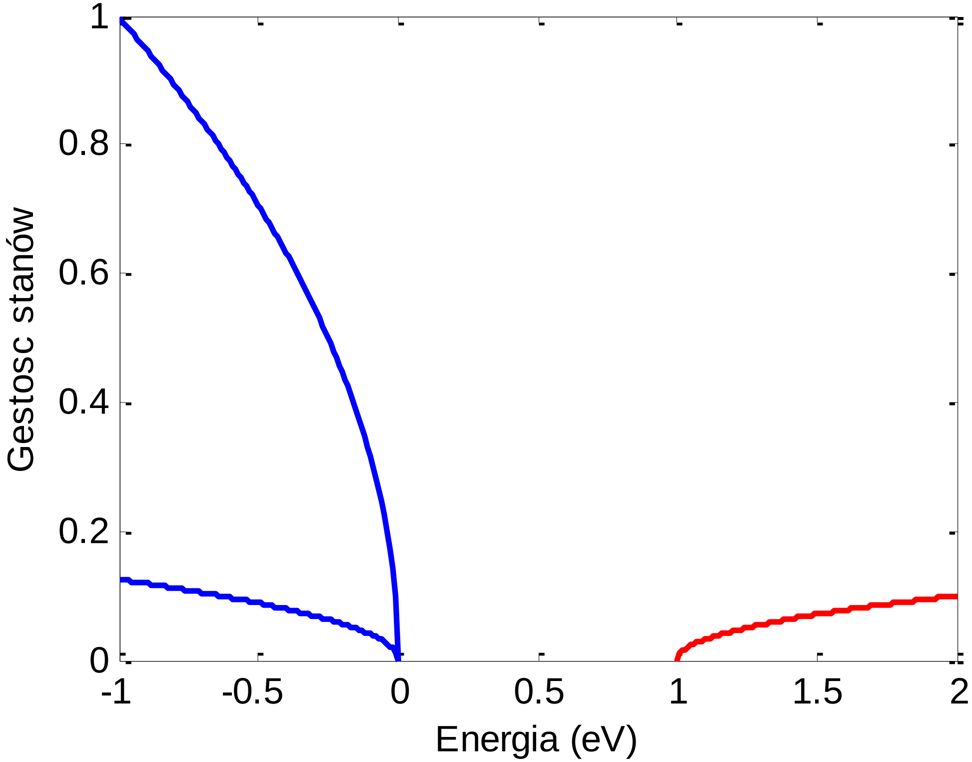

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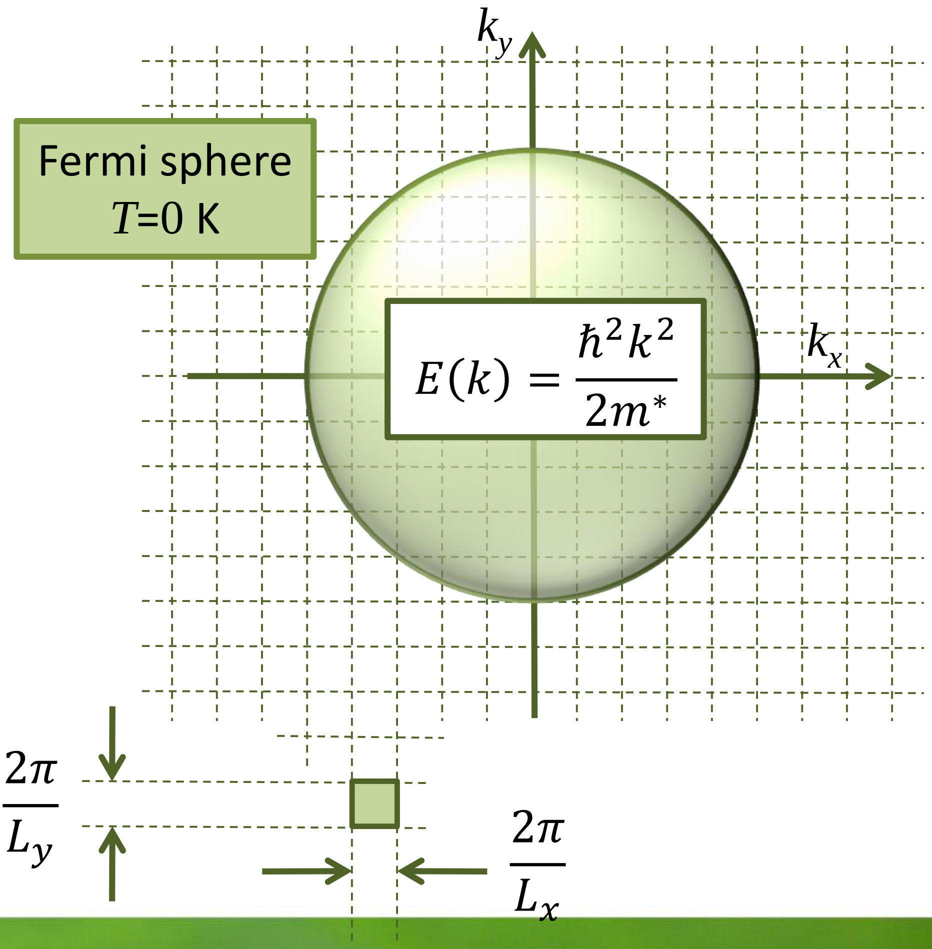
2D case

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

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

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

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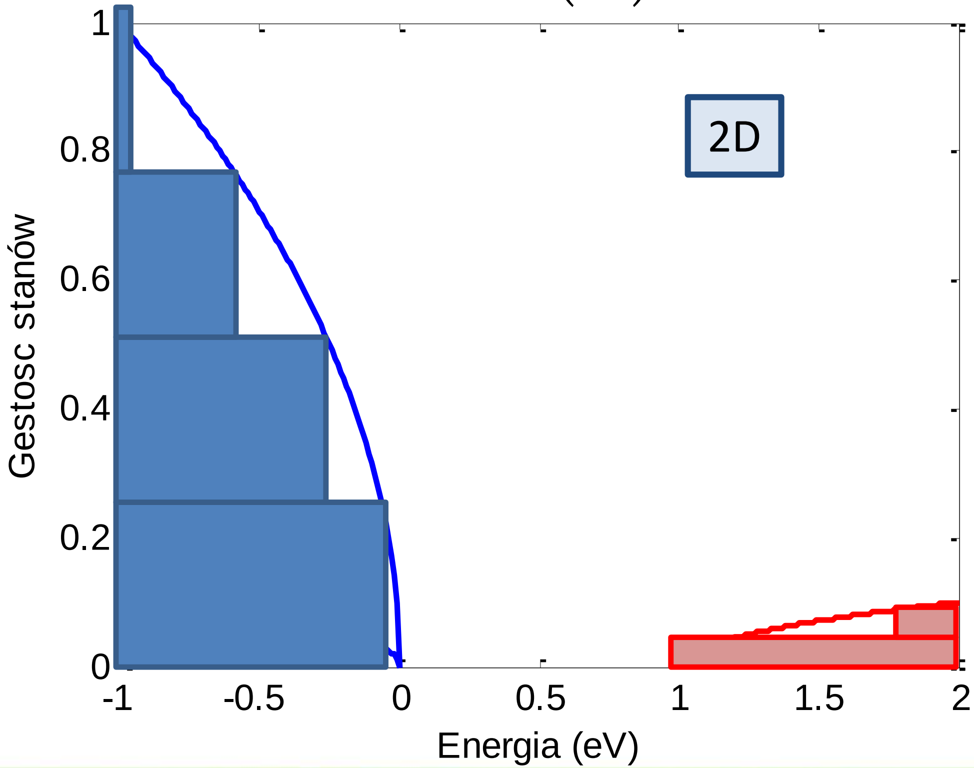
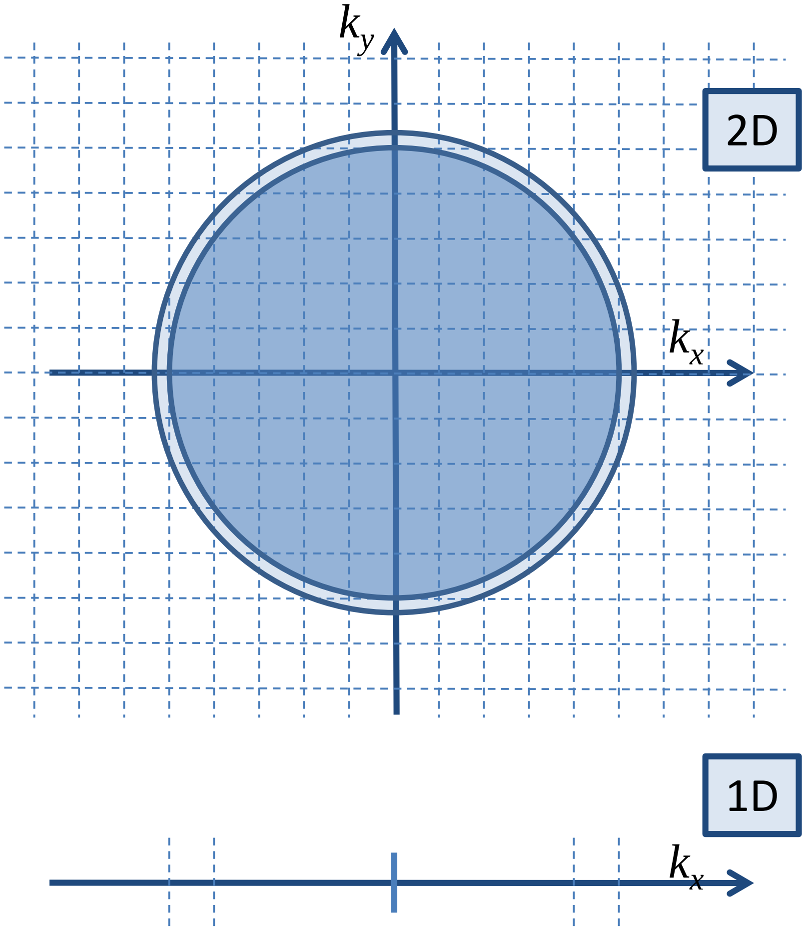




Density of states

Inside the well:

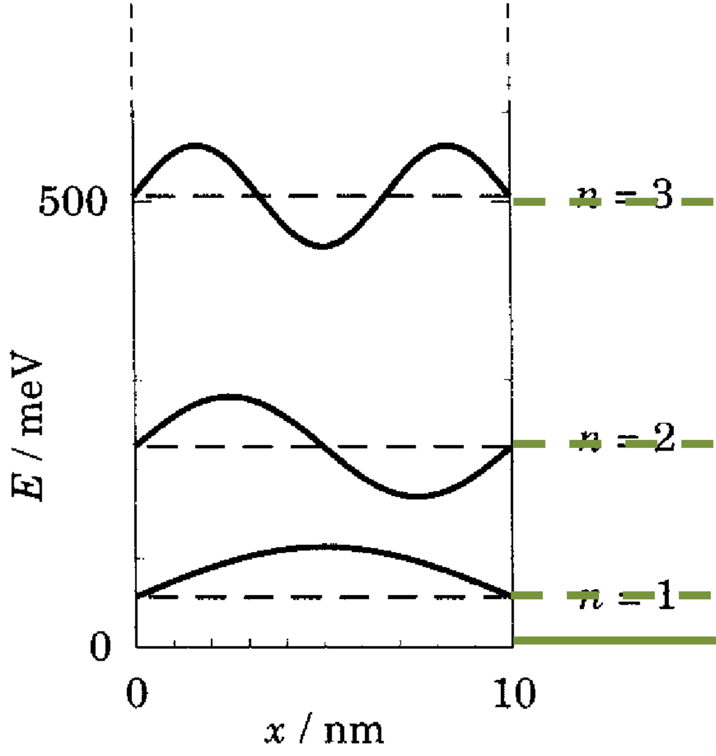
$$\psi(x,t) = \sqrt{\frac{2}{L}}\sin(k_n x\ )\, e^{-i\omega t} \qquad k_n = \frac{n\pi}{L}$$

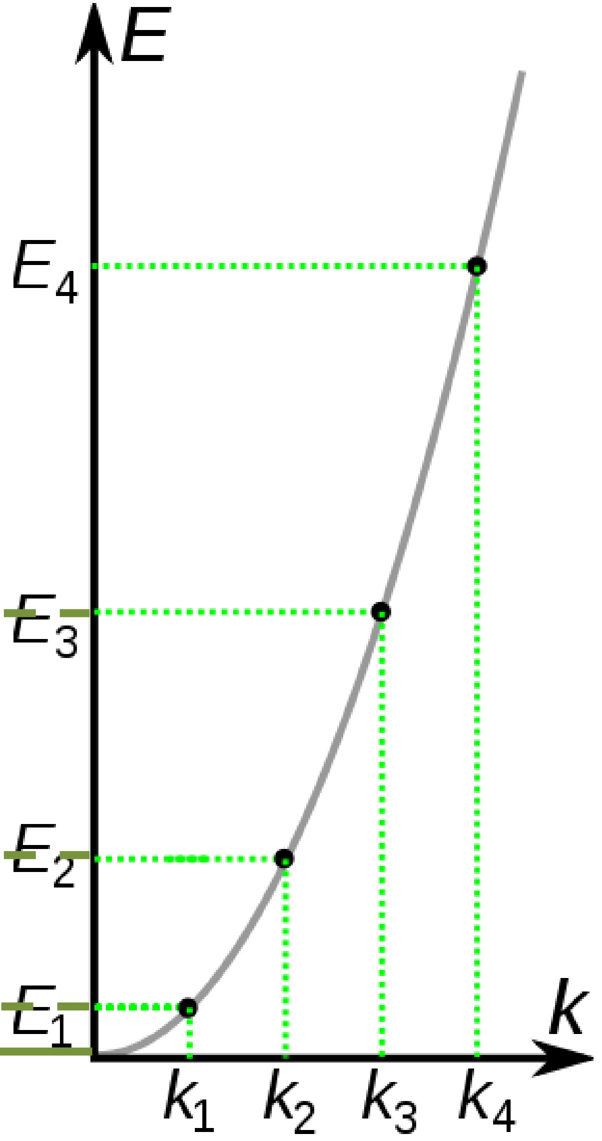
$$\varepsilon_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$

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

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

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





Density of states

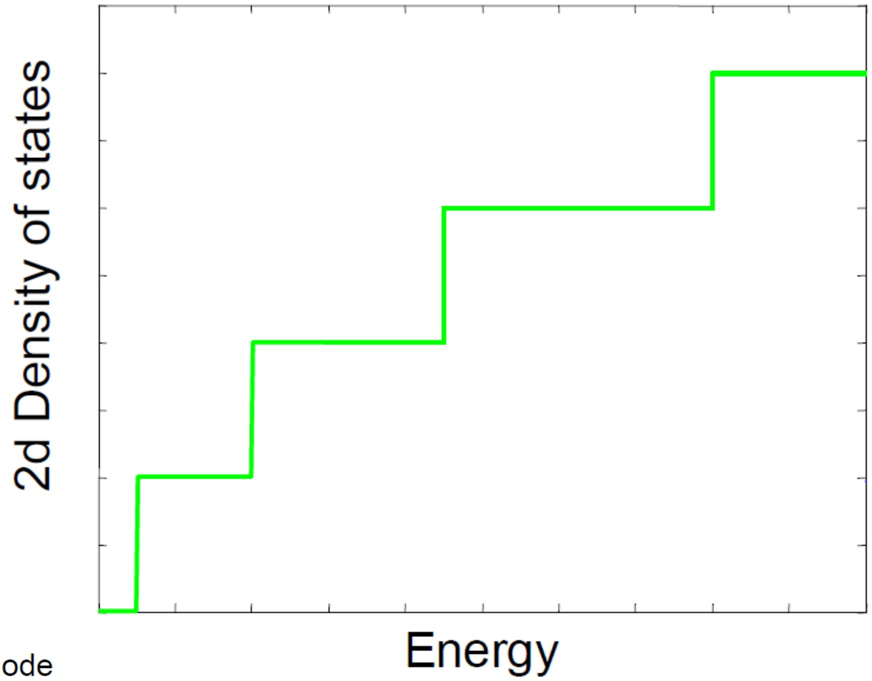
2D density of states for a spherical and parabolic band:

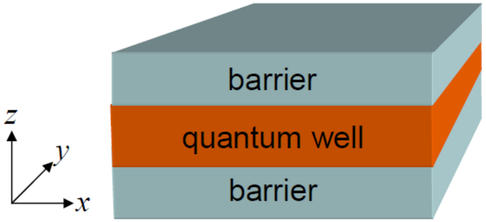
$$\rho^{2D}(E)dE = \rho_k^{2D}\, d\vec{k} = 2\left(\frac{1}{2\pi}\right)^2 2\pi k\, dk$$

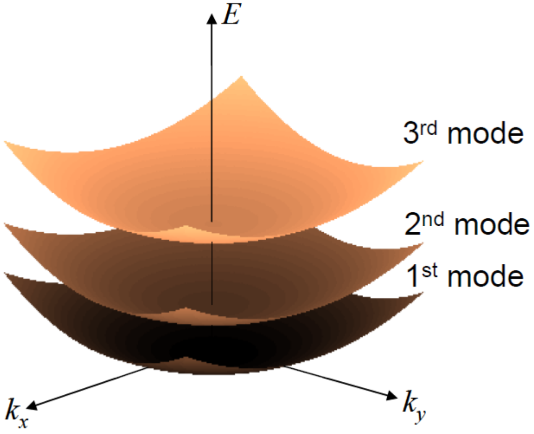
$$\rho_a^{2D}(E)dE = \frac{m_0 m^*}{\pi\hbar^2}\theta(E - E_a)\, dE$$

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

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

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

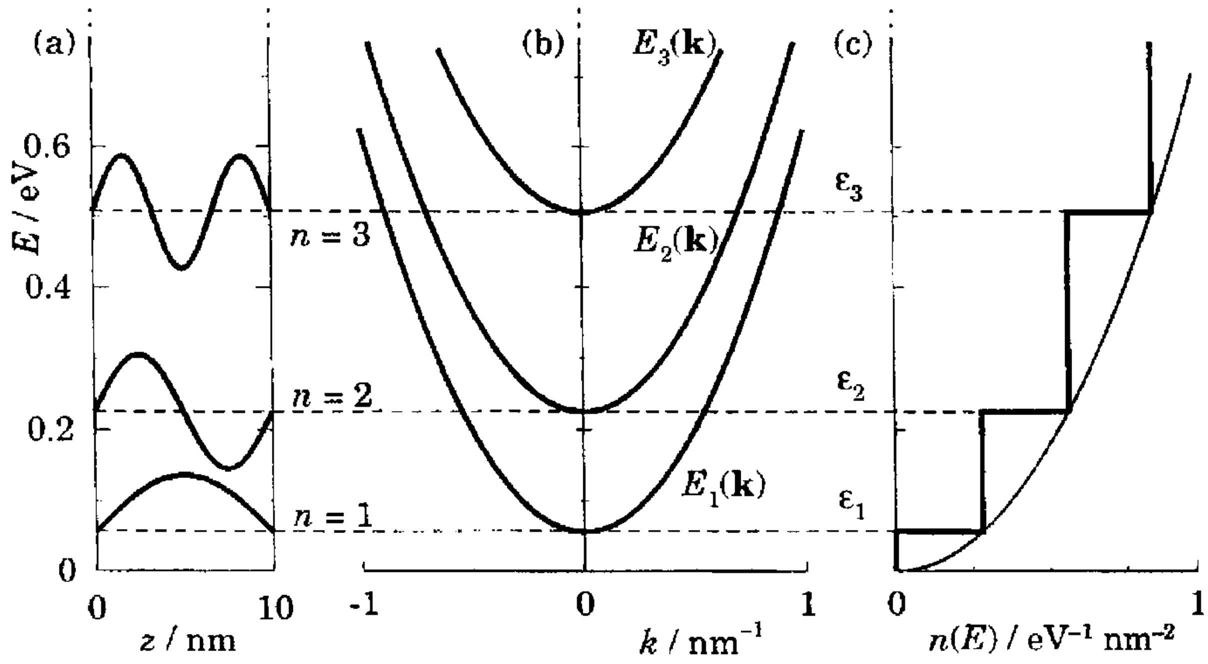


FIGURE 4.7. (a) Potential well with energy levels, (b) total energy including the transverse kinetic energy for each subband, and (c) steplike density of states of a quasi-two-dimensional system. The example is an infinitely deep square well in GaAs of width 10 nm. The thin curve in (c) is the parabolic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

Density of states – 2D

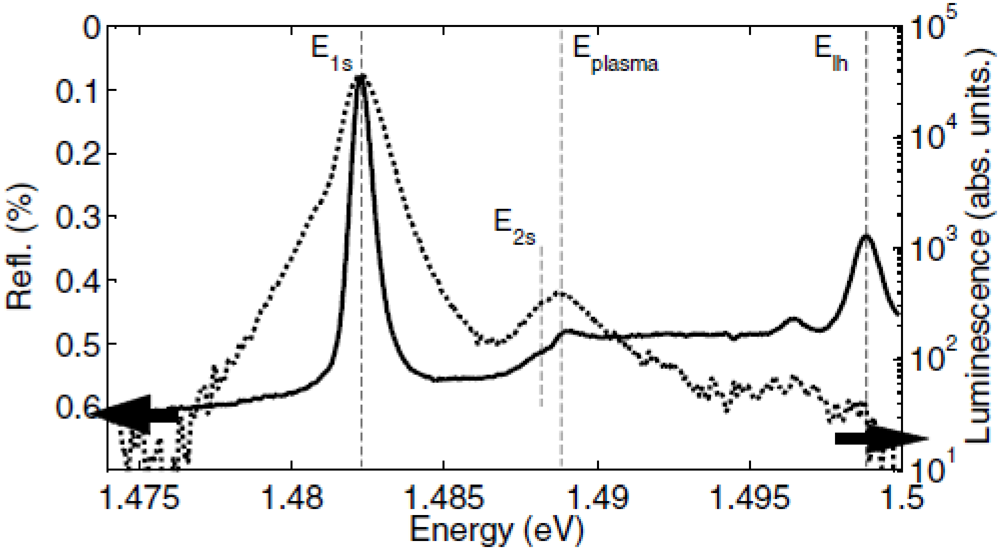


FIG. 1. cw absorption (i.e., 1 − reflectivity; bold line, left axis) and the TR-PL integrated over 1300 ps (logarithmic scale, right) results. $E_{1s} = 1.4823$ eV ($E_{2s} = 1.4882$ eV) is the 1*s* (2*s*) heavy-hole exciton, $E_{\mathrm{plasma}} = 1.4888$ eV, light-hole exciton $E_{\mathrm{lh}} = 1.4988$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

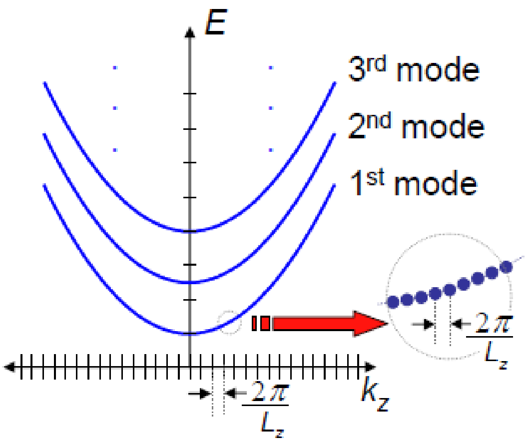
J. Szczytko, et al. Phys. Rev. Lett. 93, 137401 (2004)

Density of states – 1D

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

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

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



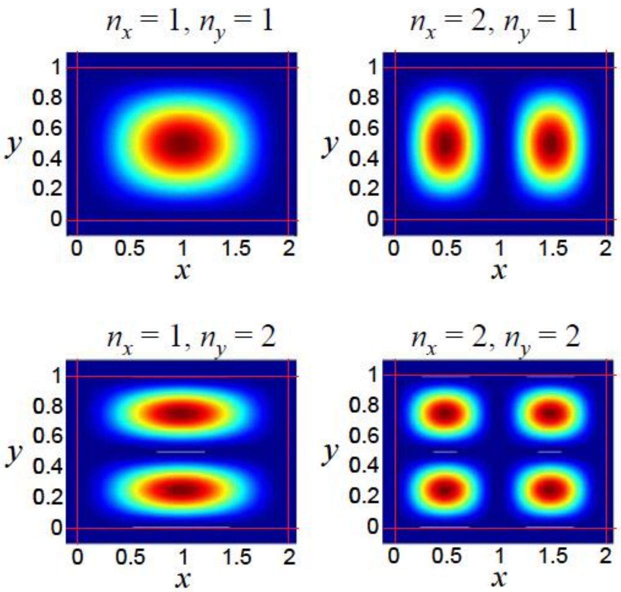
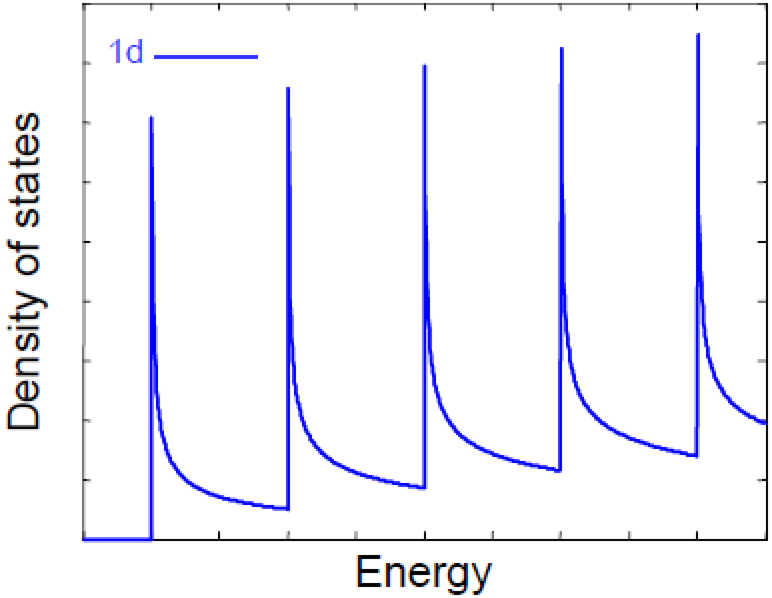


Fig. 2.13. The first four modes of the quantum wire. Since in this example, $L_x > L_y$ the $n_x = 2$, $n_y = 1$ mode has lower energy than the $n_x = 1$, $n_y = 2$ mode.



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Density of states – 1D

0D density of states

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

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

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

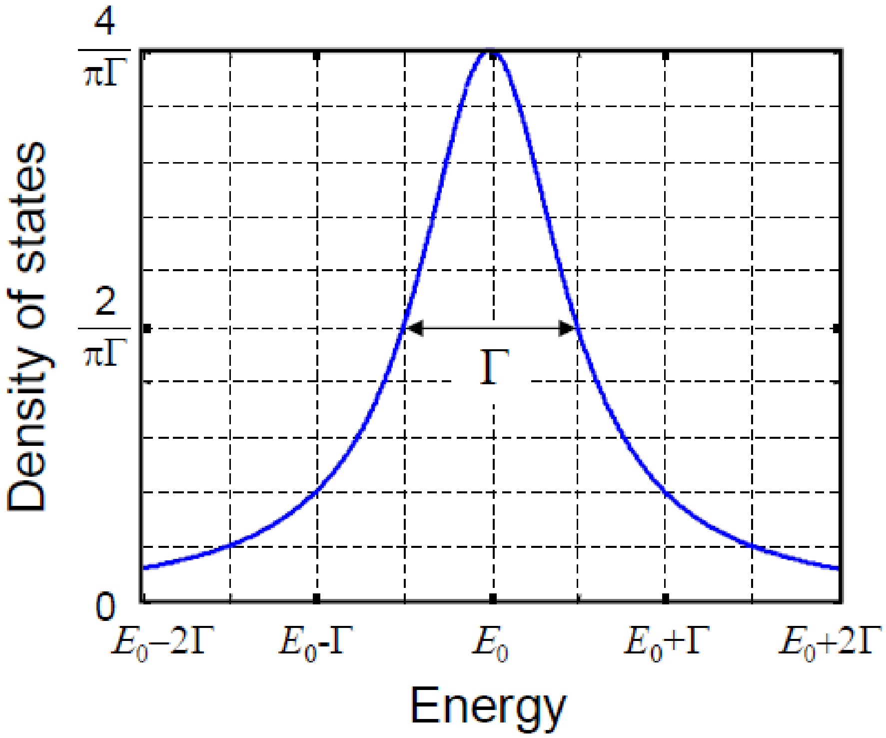
$$\psi(t) = \mathrm{A} \exp\left(-i\frac{E_0 t}{\hbar} - \frac{t}{2\tau}\right), \qquad t > 0$$

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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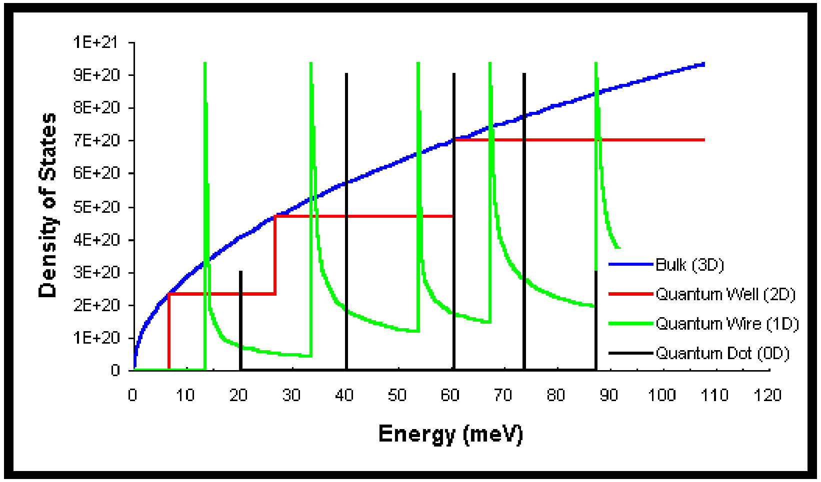
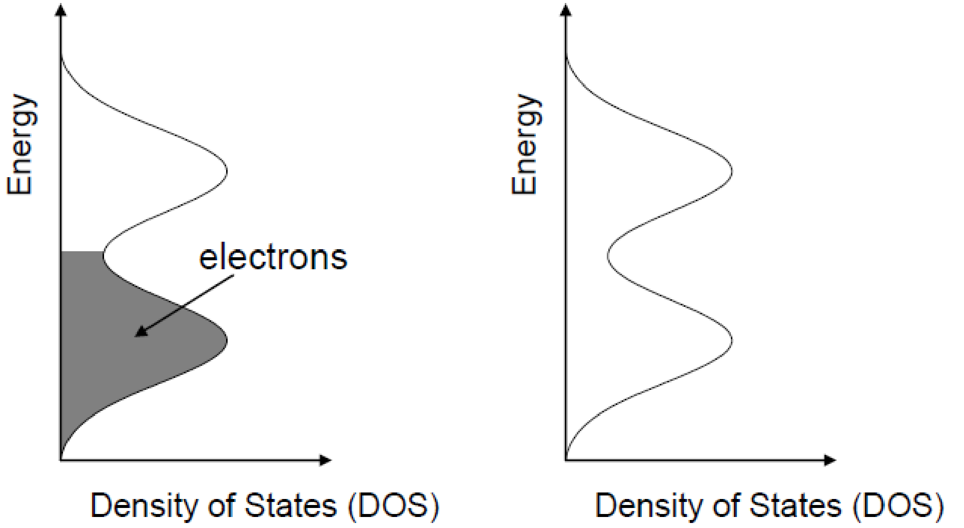
Density of states – the summary

Density of states





(a) Partly filled = metal

(b) Completely filled or empty = insulator or semiconductor

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Electrons statistics in crystals

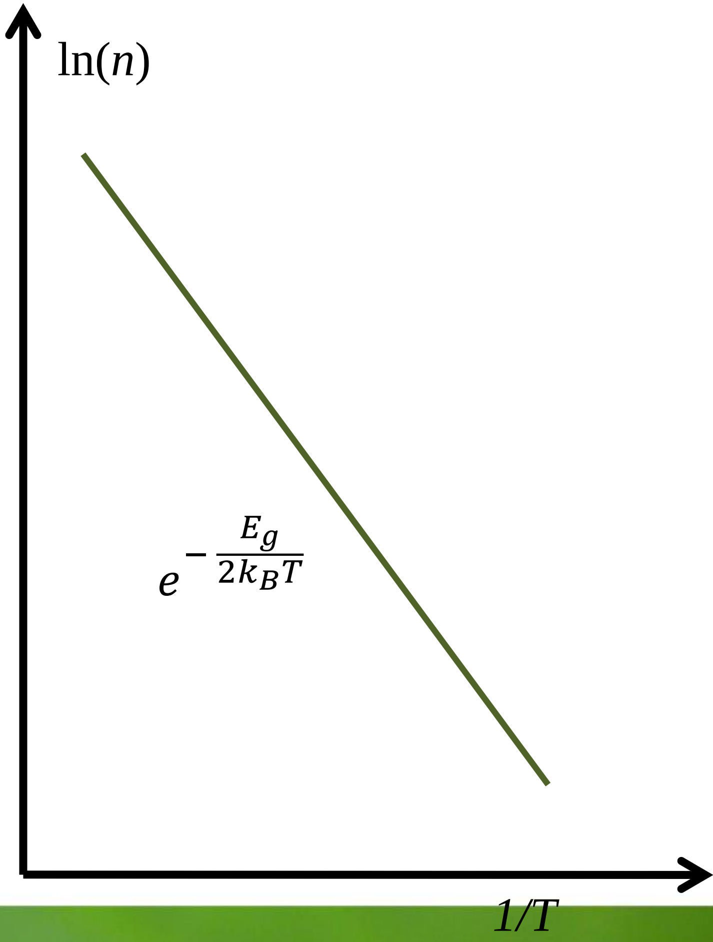
What is the concentration of carriers for T>0?

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?

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).

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

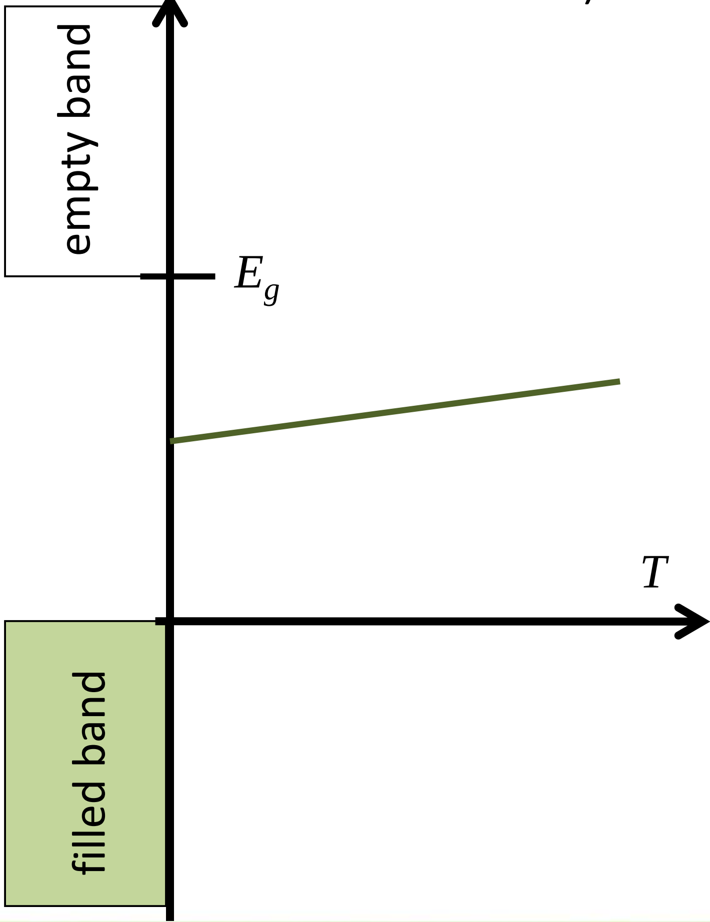
(general formula)

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

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

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

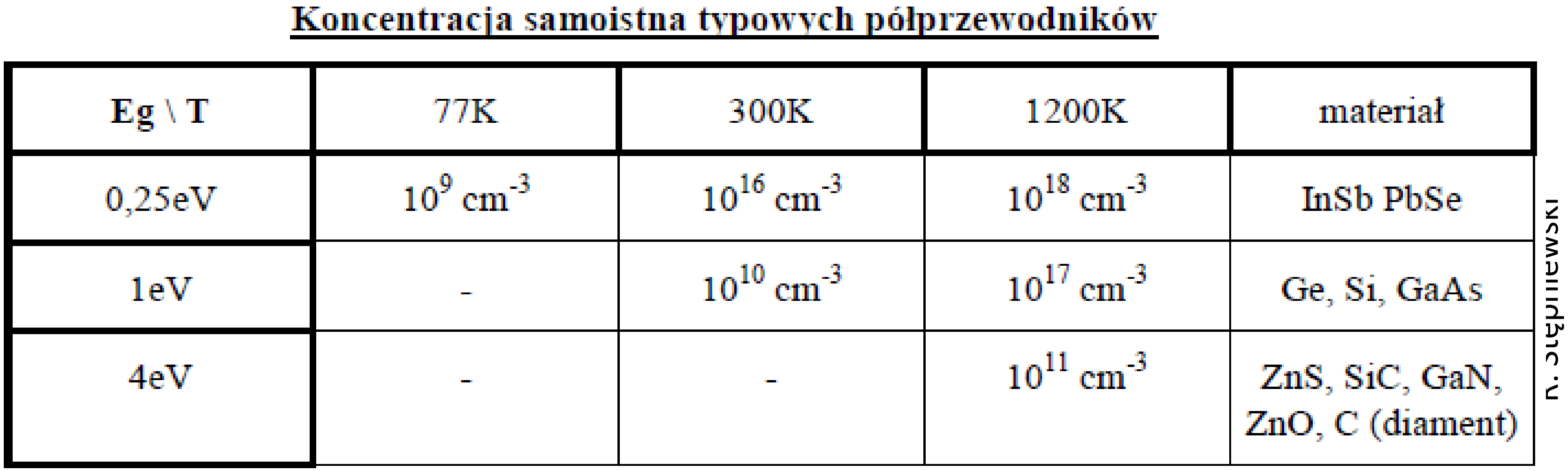
in our notation the middle of the band is 0



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)

K. 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

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

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

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

Domieszkowanie półprzewodników

Carriers:

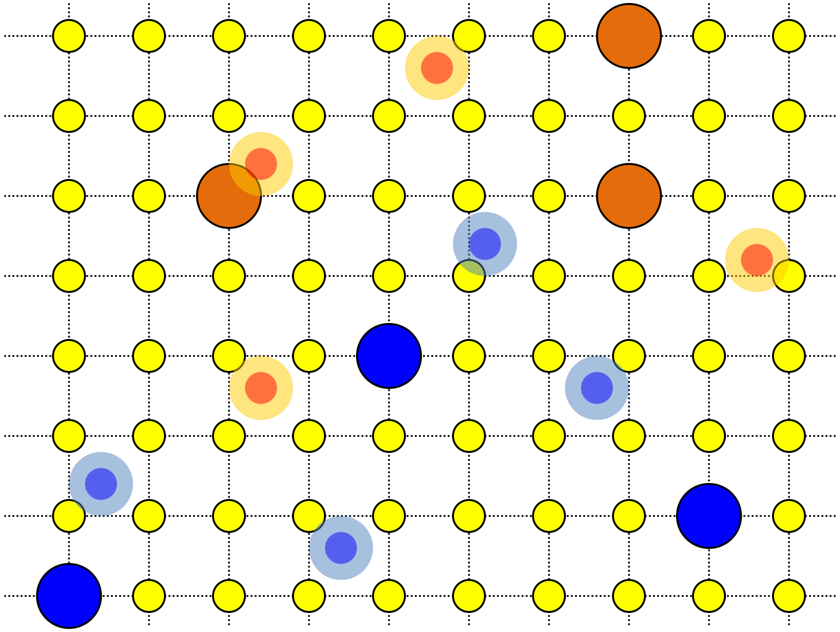
holes ● +

electrons ● -

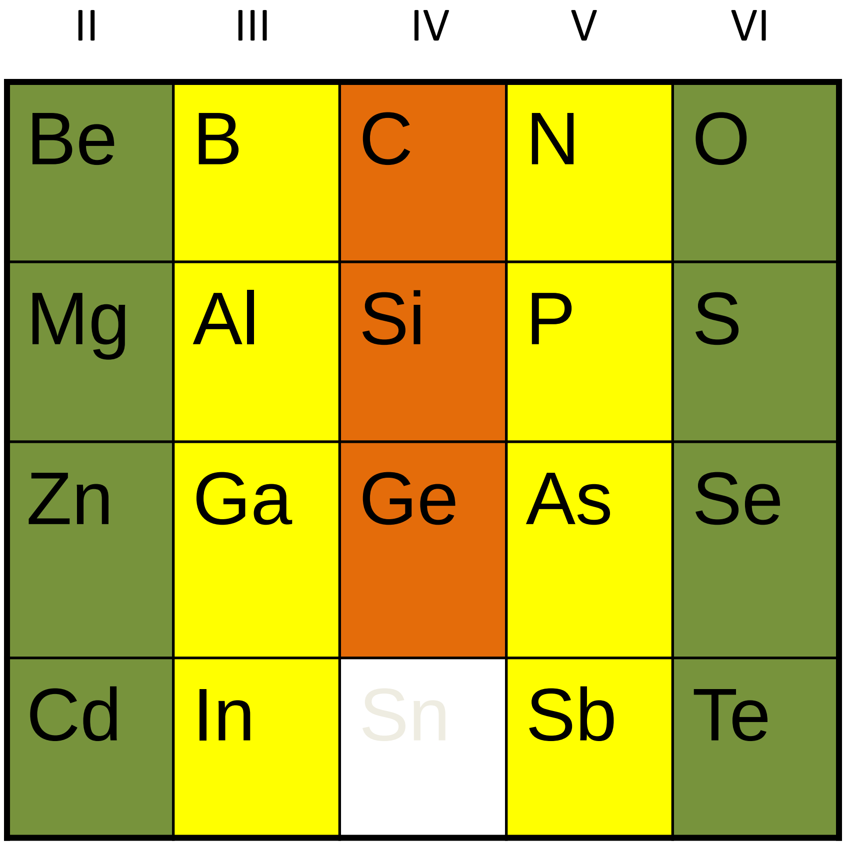
Dopants:

● 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

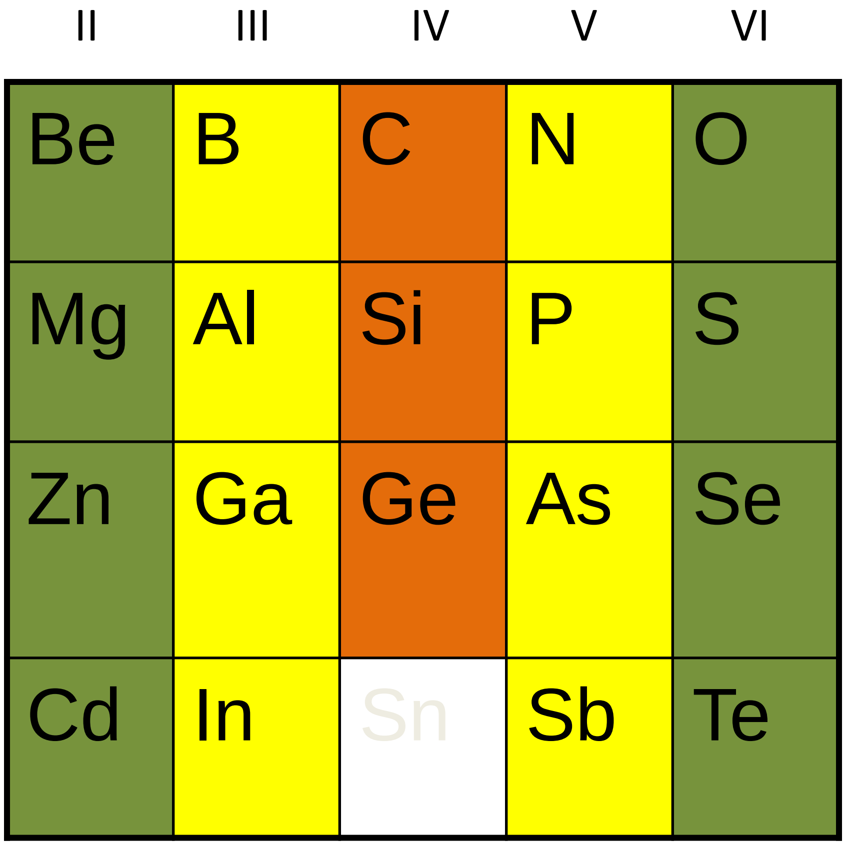
Dopants, impurities and defects

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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Group IV: diamond, Si, Ge
Group III-V: GaAs, AlAs, InSb, InAs...
Group II-VI: ZnSe, CdTe, ZnO, SdS...

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.

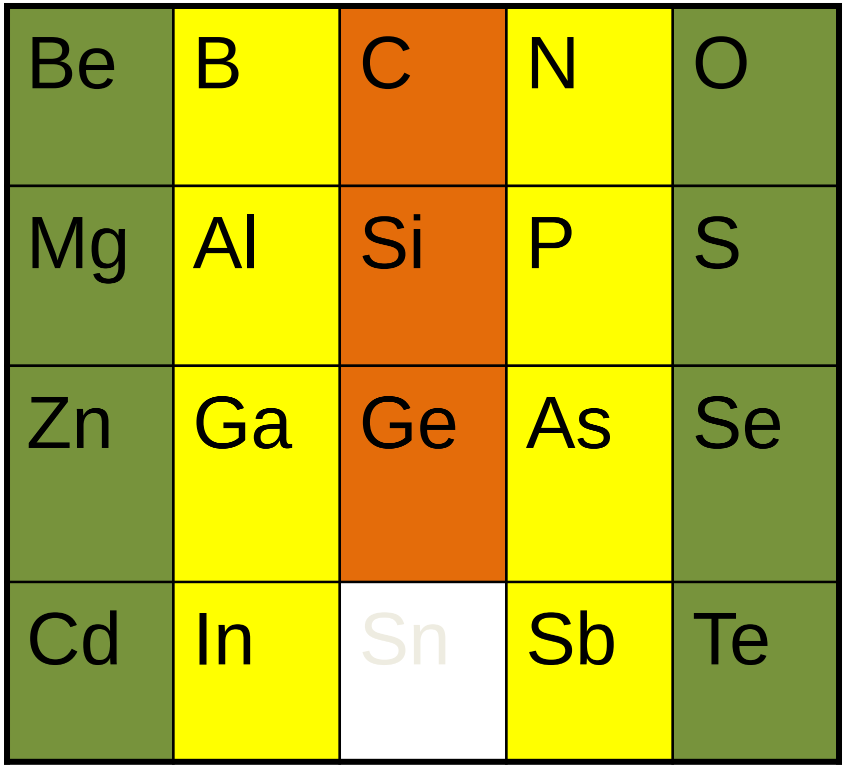
$$E_n = -\left(\frac{m^*}{m_0}\right)\frac{1}{\varepsilon_r^2}Ry\frac{1}{n^2}$$

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



II	III	IV	V	VI
Be	B	C	N	O
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Group IV: diamond, Si, Ge
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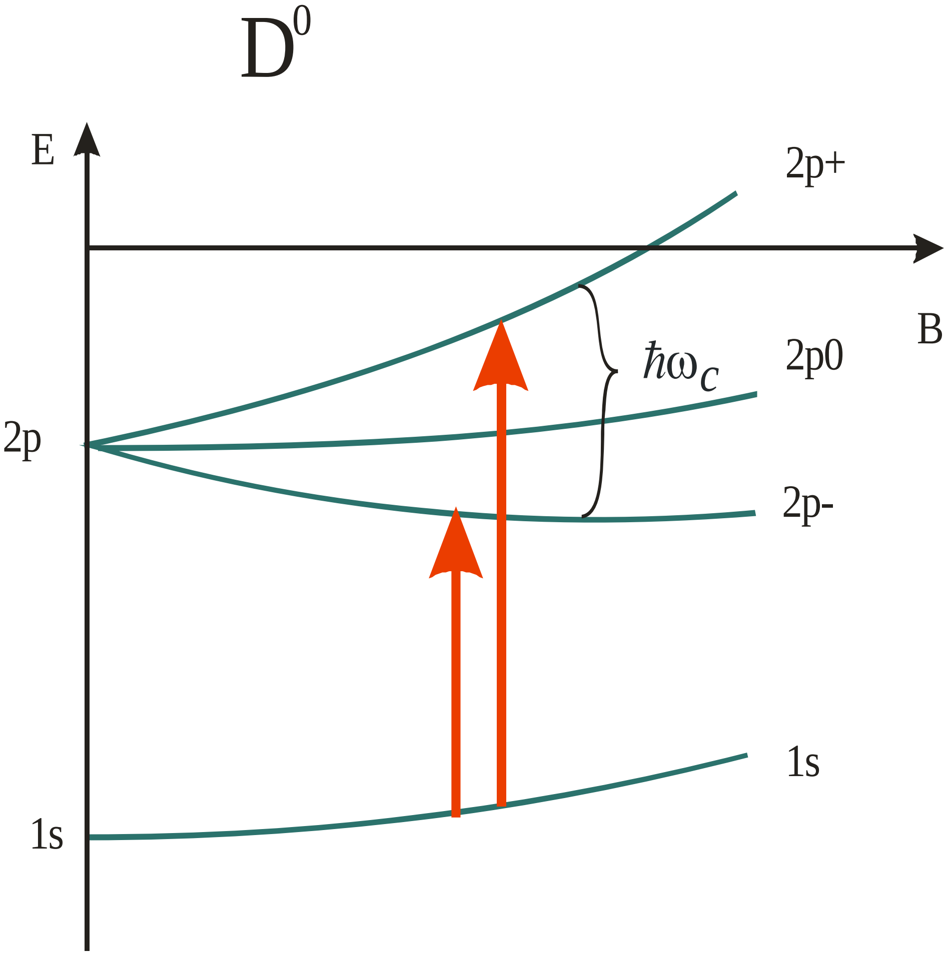
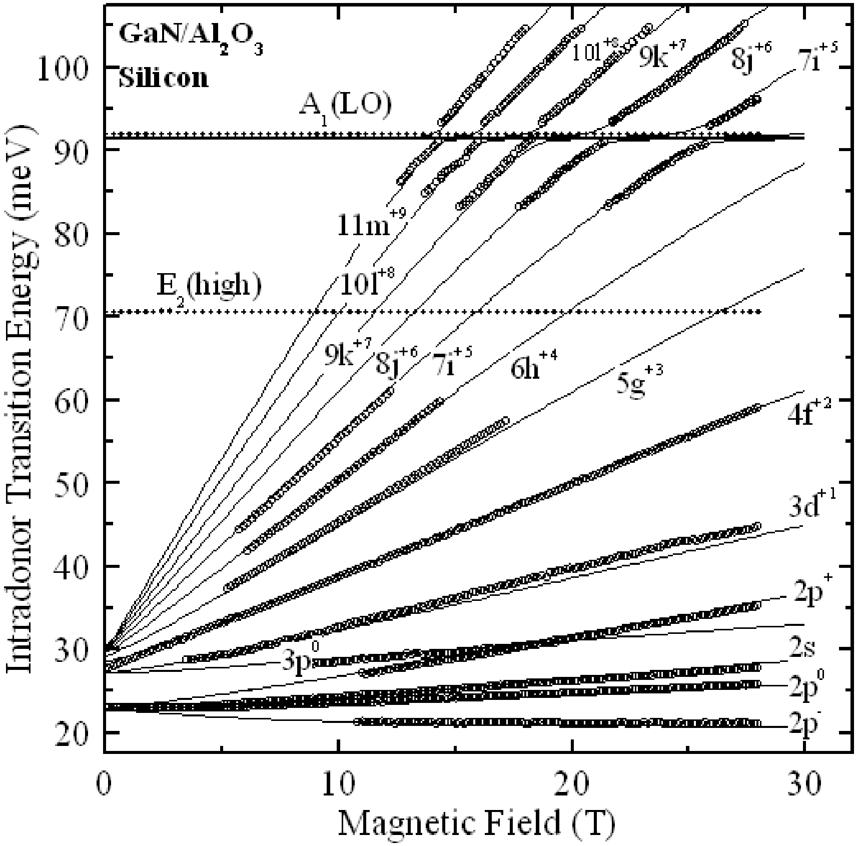
Far infrared spectroscopy

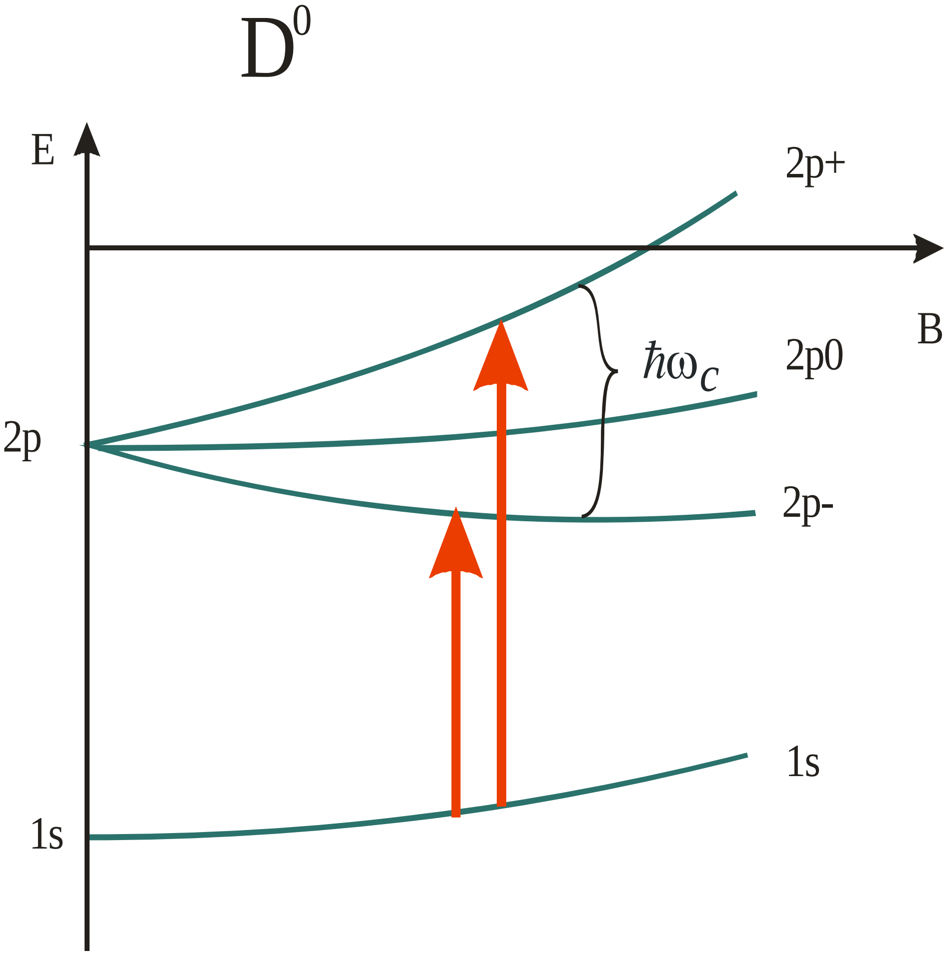


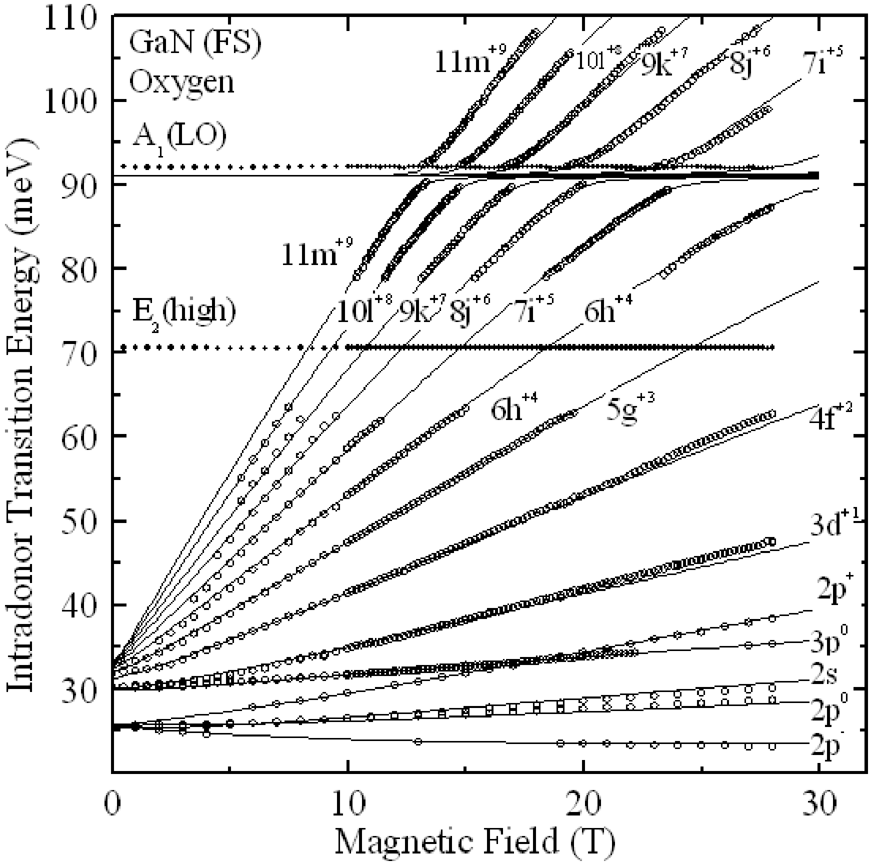


Silicon

R$_y$=30.28(5) meV

Far infrared spectroscopy



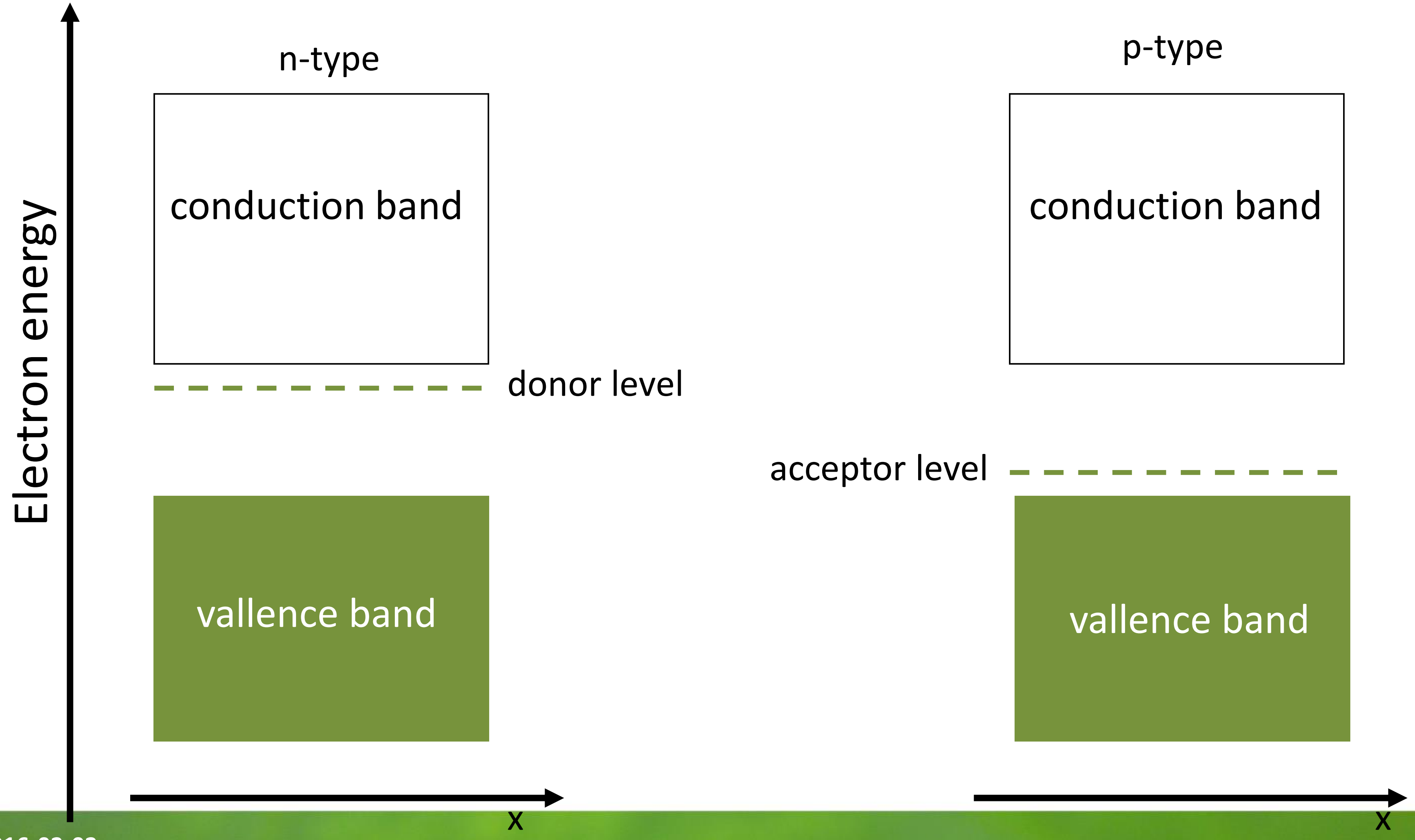


Oxygen

R_y=30.28(5) meV

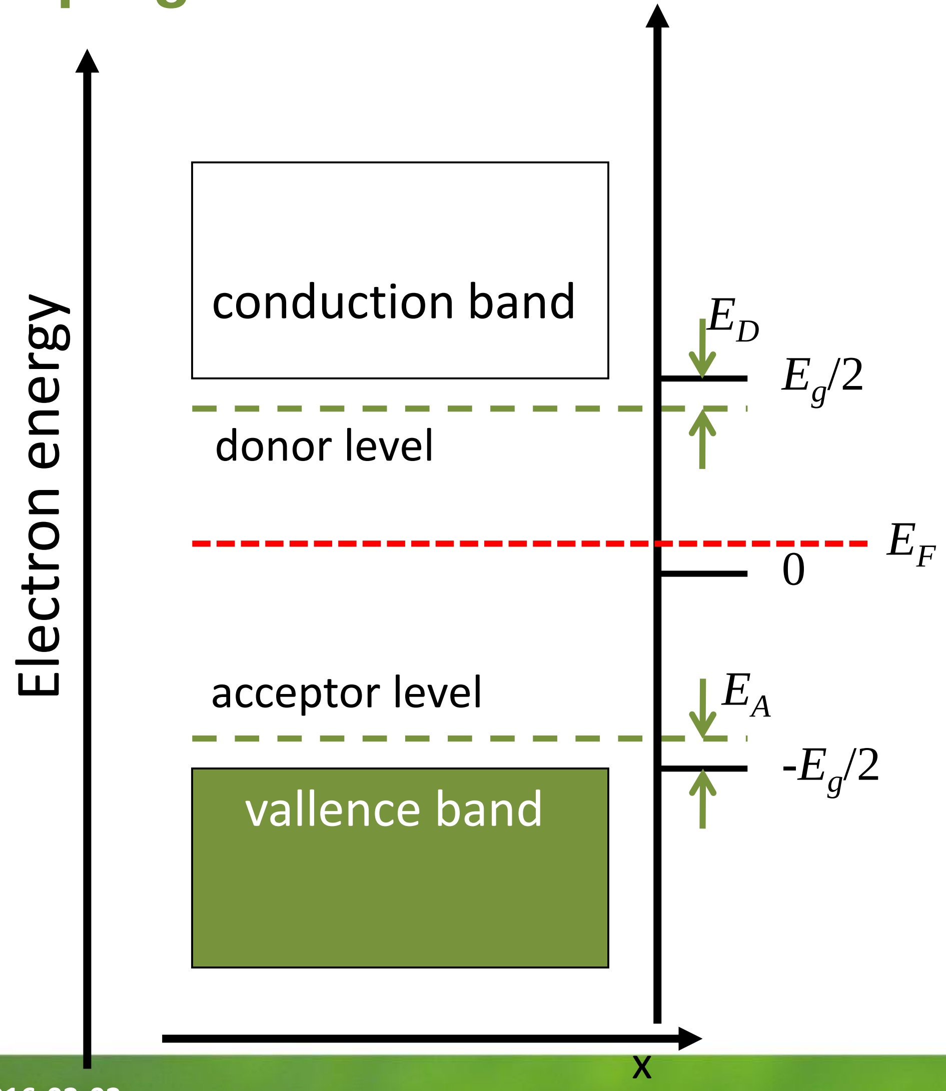
Dopants, impurities and defects

Hydrogen-like model – ionization of the dopant



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

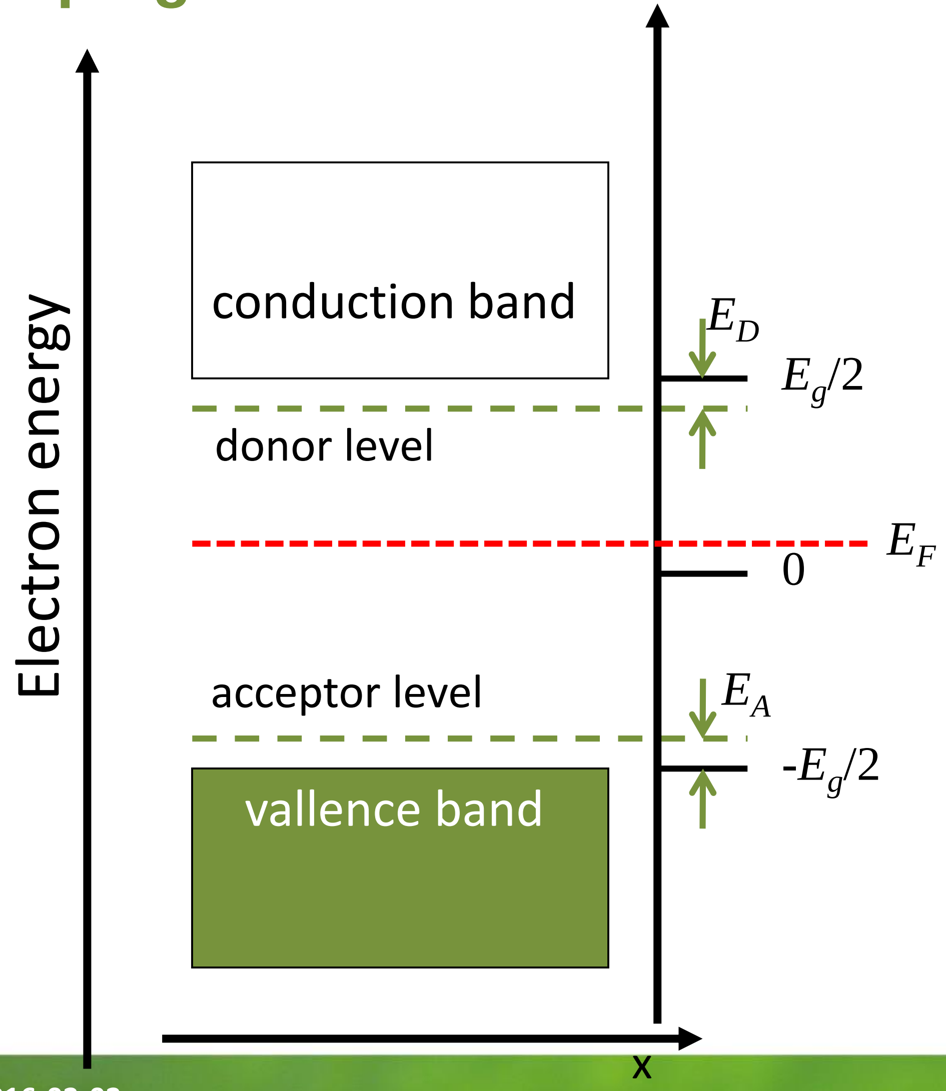
p_v – concentration of holes in valence band

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:

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

The electronic band structure

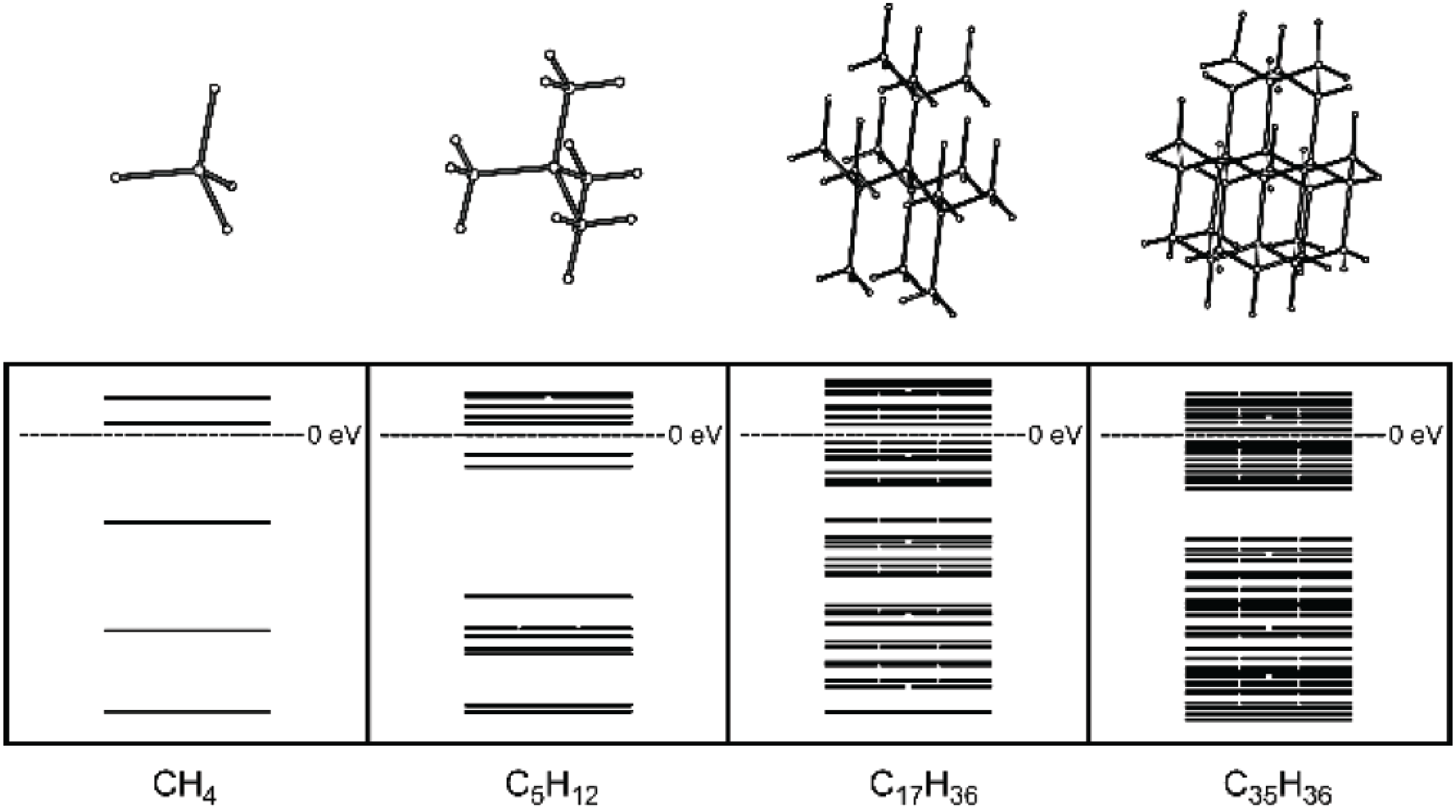


Fig. 2.3 Development of the diamond band gap

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

The electronic band structure

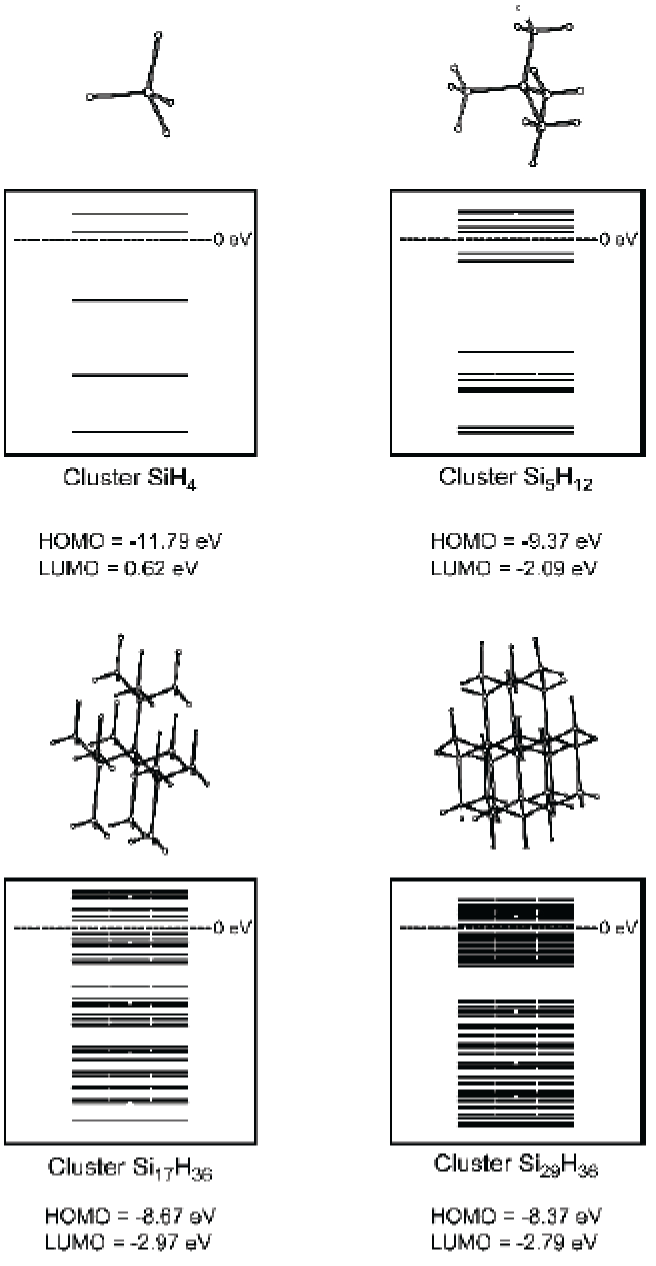


Fig. 2.4 Development of the Si band gap

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Tight-Binding Approximation

We describe the crystal electrons in terms of a linear superposition of atomic eigenfunctions (LCAO – Linear Combination of Atomic Orbitals) $H = H_A + V'$:

$$H_A(\vec{r} - \vec{R}_n)\varphi_j(\vec{r} - \vec{R}_n) = E_j\varphi_j(\vec{r} - \vec{R}_n)$$

Equation for the free atoms that form the crystal

$$H_A = -\frac{\hbar^2}{2m}\Delta + V_A(\vec{r} - \vec{R}_n)$$

j-th state e

Atom in position $\vec{R}_n$

$$H = H_A + V' = -\frac{\hbar^2}{2m}\Delta + V_A(\vec{r} - \vec{R}_n) + \sum_{m \neq n} V_A\left(\vec{r} - \vec{R}_m\right)$$

Perturbation: the influence of atoms in the neighborhood of $\vec{R}_m$:

$$V'(\vec{r} - \vec{R}_n) = \sum_{m \neq n} V_A\left(\vec{r} - \vec{R}_m\right)$$

Good for valence band of covalent crystals, d-orbital bands etc.

Tight-Binding Approximation

Approximate solution in the form of the Bloch function:

$$\Phi_{j,\vec{k}}(\vec{r}) = \sum_n a_n \varphi_j(\vec{r}-\vec{R}_n) = \sum_n \exp(i\,\vec{k}\vec{R}_n)\,\varphi_j(\vec{r}-\vec{R}_n)$$

Check:

blackboard

$$\Phi_{j,\vec{k}+\vec{G}}(\vec{r}) = \Phi_{j,\vec{k}}(\vec{r})$$

$$\Phi_{j,\vec{k}}(\vec{r}+\vec{T}) = \exp(i\,\vec{k}\vec{T})\,\Phi_{j,\vec{k}}(\vec{r})$$

Energies determined by the variational method:

$$E(\vec{k}) \le \frac{\left\langle \Phi_{j,\vec{k}}(\vec{r}) \middle| H \middle| \Phi_{j,\vec{k}}(\vec{r}) \right\rangle}{\left\langle \Phi_{j,\vec{k}}(\vec{r}) \middle| \Phi_{j,\vec{k}}(\vec{r}) \right\rangle}$$

Expression

$$\left\langle \Phi_{j,\vec{k}}(\vec{r}) \middle| \Phi_{j,\vec{k}}(\vec{r}) \right\rangle = \sum_{n,m} \exp[i\vec{k}(\vec{R}_n - \vec{R}_m)] \int \varphi_j^*(\vec{r}-\vec{R}_m)\varphi_j(\vec{r}-\vec{R}_n)\,dV$$

can be easily simplify assuming a small overlap of wave functions for $n \neq m$

$$\left\langle \Phi_{j,\vec{k}}(\vec{r}) \middle| \Phi_{j,\vec{k}}(\vec{r}) \right\rangle = \sum_n \int \varphi_j^*(\vec{r}-\vec{R}_n)\varphi_j(\vec{r}-\vec{R}_n)\,dV = \cdots$$

How many?

Tight-Binding Approximation

Approximate solution in the form of the Bloch function:

$$\Phi_{j,\vec{k}}(\vec{r}) = \sum_n a_n \varphi_j(\vec{r}-\vec{R}_n) = \sum_n \exp\left(i\,\vec{k}\vec{R}_n\right)\varphi_j(\vec{r}-\vec{R}_n)$$

Check:

$$\Phi_{j,\vec{k}+\vec{G}}(\vec{r}) = \Phi_{j,\vec{k}}(\vec{r})$$

$$\Phi_{j,\vec{k}}(\vec{r}+\vec{T}) = \exp\left(i\,\vec{k}\vec{T}\right)\Phi_{j,\vec{k}}(\vec{r})$$

Energies determined by the variational method:

$$E(\vec{k}) \le \frac{\left\langle \Phi_{j,\vec{k}}(\vec{r}) \middle| H \middle| \Phi_{j,\vec{k}}(\vec{r}) \right\rangle}{\left\langle \Phi_{j,\vec{k}}(\vec{r}) \middle| \Phi_{j,\vec{k}}(\vec{r}) \right\rangle}$$

$$E(\vec{k}) \approx \frac{1}{N}\left\langle \Phi_{j,\vec{k}}(\vec{r}) \middle| H \middle| \Phi_{j,\vec{k}}(\vec{r}) \right\rangle =$$

$$= \sum_{n,m} \exp\left[i\vec{k}\left(\vec{R}_n - \vec{R}_m\right)\right] \int \varphi_j^*(\vec{r}-\vec{R}_m)\left[E_j + V'(\vec{r}-\vec{R}_n)\right]\varphi_j(\vec{r}-\vec{R}_n)\, dV$$

Tight-Binding Approximation

Approximate solution in the form of the Bloch function:

$$\Phi_{j,\vec{k}}(\vec{r}) = \sum_n a_n \varphi_j(\vec{r} - \vec{R}_n) = \sum_n \exp(i\,\vec{k}\vec{R}_n)\,\varphi_j(\vec{r} - \vec{R}_n)$$

Check:

$$\Phi_{j,\vec{k}+\vec{G}}(\vec{r}) = \Phi_{j,\vec{k}}(\vec{r})$$

$$\Phi_{j,\vec{k}}(\vec{r} + \vec{T}) = \exp(i\,\vec{k}\vec{T})\,\Phi_{j,\vec{k}}(\vec{r})$$

Energies determined by the variational method:

$$E(\vec{k}) \le \frac{\left\langle \Phi_{j,\vec{k}}(\vec{r}) \middle| H \middle| \Phi_{j,\vec{k}}(\vec{r}) \right\rangle}{\left\langle \Phi_{j,\vec{k}}(\vec{r}) \middle| \Phi_{j,\vec{k}}(\vec{r}) \right\rangle}$$

$$E(\vec{k}) \approx \frac{1}{N}\left\langle \Phi_{j,\vec{k}}(\vec{r}) \middle| H \middle| \Phi_{j,\vec{k}}(\vec{r}) \right\rangle =$$

Only the vicinity of $\vec{R}$_n

$$= \sum_{n,m} \exp[i\vec{k}(\vec{R}_n - \vec{R}_m)] \int \varphi_j^*(\vec{r} - \vec{R}_m)[E_j + V'(\vec{r} - \vec{R}_n)]\varphi_j(\vec{r} - \vec{R}_n)\,dV$$

Only diagonal terms $\vec{R}_n = \vec{R}_m$ in E_j

Tight-Binding Approximation

$$E(\vec{k}) \approx \frac{1}{N}\left\langle \Phi_{j,\vec{k}}(\vec{r}) \middle| H \middle| \Phi_{j,\vec{k}}(\vec{r}) \right\rangle =$$

Only the vicinity of $\vec{R}$_n

$$= \sum_{n,m} \exp[i\vec{k}(\vec{R}_n - \vec{R}_m)] \int \varphi_j^*(\vec{r}-\vec{R}_m)[E_j + V'(\vec{r}-\vec{R}_n)]\varphi_j(\vec{r}-\vec{R}_n)\, dV$$

Only diagonal terms $\vec{R}_n = \vec{R}_m$ in E_j

When the atomic states $\varphi_j(\vec{r}-\vec{R}_n)$ are spherically symmetric (s-states), then overlap integrals depend only on the distance between atoms:

$$E_n(\vec{k}) \approx E_j - A_j - B_j \sum_{m} \exp[i\vec{k}(\vec{R}_n - \vec{R}_m)]$$

$$A_j = -\int \varphi_j^*(\vec{r}-\vec{R}_n)[V'(\vec{r}-\vec{R}_n)]\varphi_j(\vec{r}-\vec{R}_n)\, dV$$

$$B_j = -\int \varphi_j^*(\vec{r}-\vec{R}_m)[V'(\vec{r}-\vec{R}_n)]\varphi_j(\vec{r}-\vec{R}_n)\, dV$$

Restricted to only the nearest neighbours of $\vec{R}_n$

Tight-Binding Approximation

When the atomic states $\varphi_j(\vec{r}-\vec{R}_n)$ are spherically symmetric (s-states), then overlap integrals depend only on the distance between atoms:

$$E_n(\vec{k}) \approx E_j - A_j - B_j \sum_m \exp\left[i\vec{k}(\vec{R}_n - \vec{R}_m)\right]$$

$$A_j = -\int \varphi_j^*(\vec{r}-\vec{R}_n)[V'(\vec{r}-\vec{R}_n)]\varphi_j(\vec{r}-\vec{R}_n)\, dV$$

$$B_j = -\int \varphi_j^*(\vec{r}-\vec{R}_m)[V'(\vec{r}-\vec{R}_n)]\varphi_j(\vec{r}-\vec{R}_n)\, dV$$

The result of the summation depends on the symmetry of the lattice:

For sc structure: $\vec{R}_n - \vec{R}_m = (\pm a, 0{,}0); (0, \pm a, 0); (0{,}0, \pm a);$

$$E_n(\vec{k}) \approx E_j - A_j - 2B_j\left[\cos k_x a + \cos k_y a + \cos k_z a\right]$$

For bcc structure :

$$E_n(\vec{k}) \approx E_j - A_j - 8B_j \cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right)\cos\left(\frac{k_z a}{2}\right)$$

For fcc structure :

$$E_n(\vec{k}) \approx E_j - A_j - 4B_j\left[\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right) + c.p.\right]$$

Tight-Binding Approximation

For *sc* structure: $\vec{R}_n - \vec{R}_m = (\pm a, 0{,}0); (0, \pm a, 0); (0{,}0, \pm a);$

$$E_n(\vec{k}) \approx E_j - A_j - 2B_j\left[\cos k_x a + \cos k_y a + \cos k_z a\right]$$

$$B_j = -\int \varphi_j^*(\vec{r} - \vec{R}_m)\left[V'(\vec{r} - \vec{R}_n)\right]\varphi_j(\vec{r} - \vec{R}_n)\, dV$$

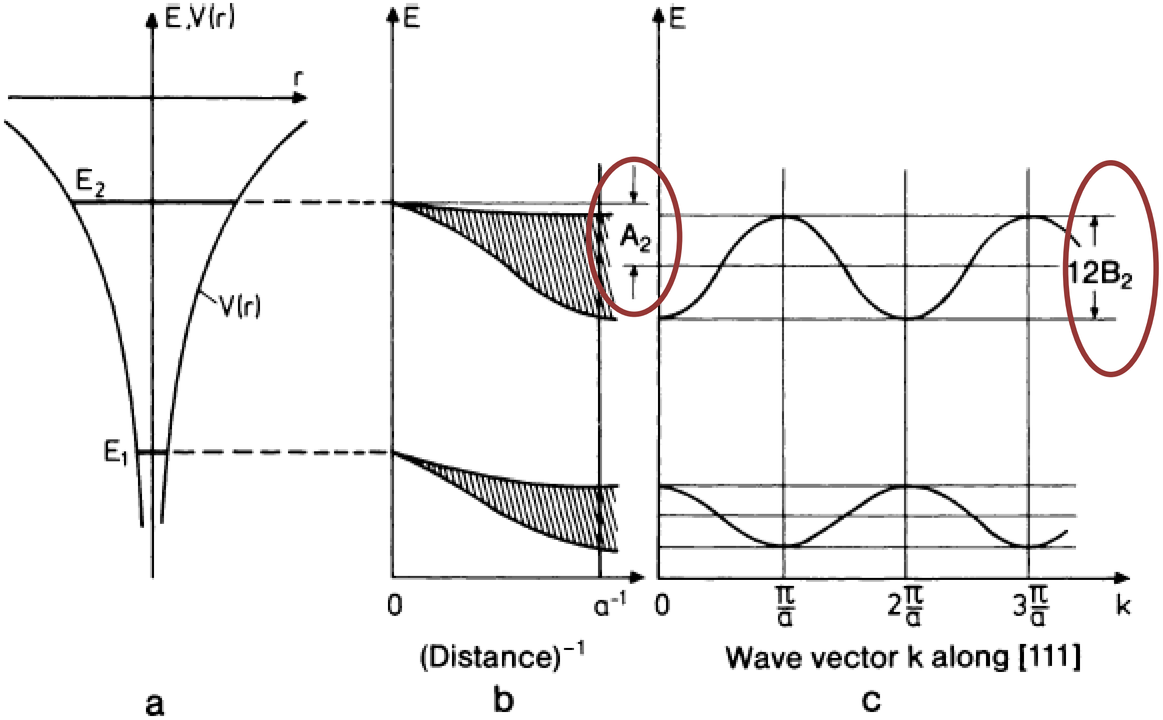

Fig. 7.8 a–c. Qualitative illustration of the result of a tight-binding calculation for a primitive cubic lattice with lattice constant a. (**a**) Position of the energy levels E_1 and E_2 in the potential $V(\mathbf{r})$ of the free atom. (**b**) Reduction and broadening of the levels E_1 and E_2 as a function of the reciprocal atomic separation r^{-1}. At the equilibrium separation a the mean energy decrease is A and the width of the band is $12B$. (**c**) Dependence of the one-electron energy E on the wave vector $k(1,1,1)$ in the direction of the main diagonal [111]

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

Tight-Binding Approximation

For sc structure: $\vec{R}_n - \vec{R}_m = (\pm a, 0,0); (0, \pm a, 0); (0,0, \pm a);$

$$E_n(\vec{k}) \approx E_j - A_j - 2B_j[\cos k_x a + \cos k_y a + \cos k_z a]$$

$$B_j = -\int \varphi_j^*(\vec{r} - \vec{R}_m)[V'(\vec{r} - \vec{R}_n)]\varphi_j(\vec{r} - \vec{R}_n)\, dV$$

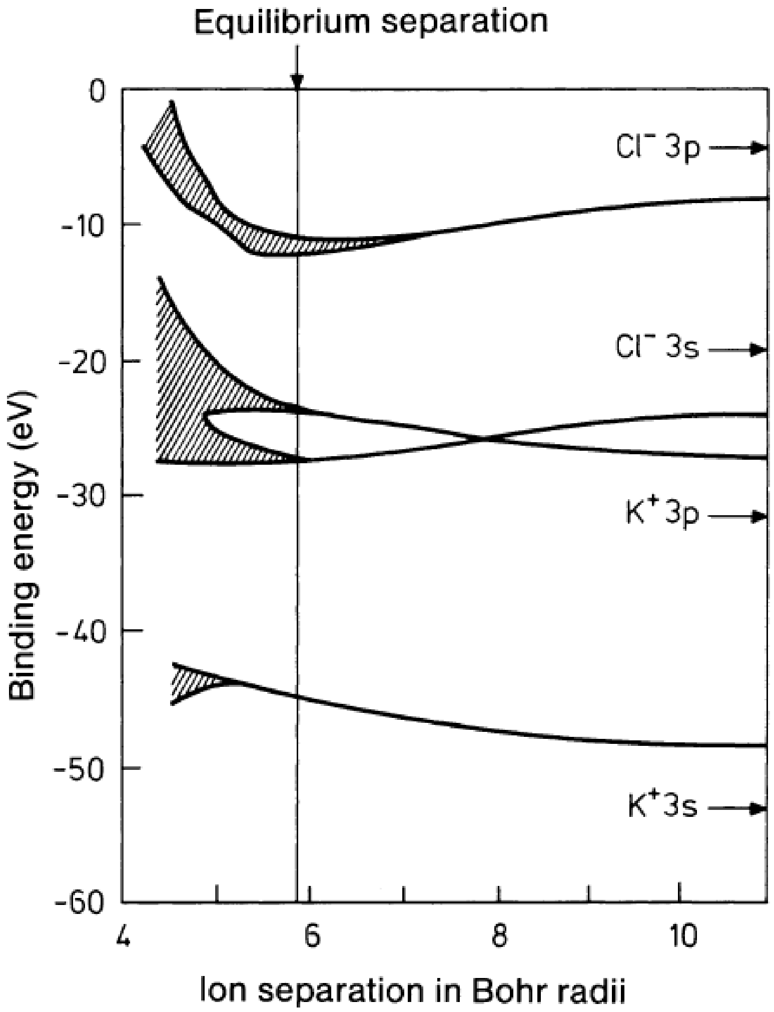

Fig. 7.10. The four highest occupied energy bands of KCl calculated as a function of the ionic separation in Bohr radii ($a_0 = 5.29 \times 10^{-9}$ cm). The energy levels in the free ions are indicated by arrows. (After [7.2])

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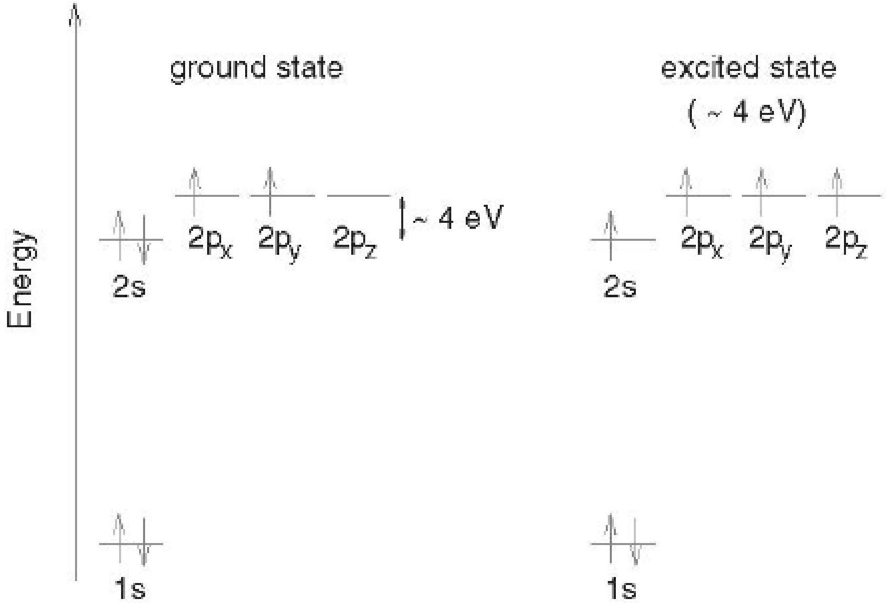
Tight-Binding Approximation

Linear dispersion relation in graphene:

Tight binding approach with the only nearest neighbors interaction [P. R. Wallace, „The Band Theory of Graphite”, Physical Review 71, 622 (1947).] gives:

$$E(\vec{k}) = \pm\sqrt{\gamma_0^2\left(1 + 4\cos^2\frac{k_y a}{2} + 4\cos\frac{k_y a}{2}\cdot\cos\frac{k_x\sqrt{3}a}{2}\right)} \approx \hbar\tilde{c}\left|\vec{k} - \vec{k}_i\right|$$



$$|\phi_1\rangle = \frac{1}{\sqrt{3}}|2s\rangle + \sqrt{\frac{2}{3}}|2p_x\rangle$$

$$|\phi_2\rangle = \frac{1}{\sqrt{3}}|2s\rangle - \frac{1}{\sqrt{6}}|2p_x\rangle + \frac{1}{\sqrt{2}}|2p_y\rangle$$

$$|\phi_2\rangle = \frac{1}{\sqrt{3}}|2s\rangle - \frac{1}{\sqrt{6}}|2p_x\rangle - \frac{1}{\sqrt{2}}|2p_y\rangle$$

Tight-Binding Approximation

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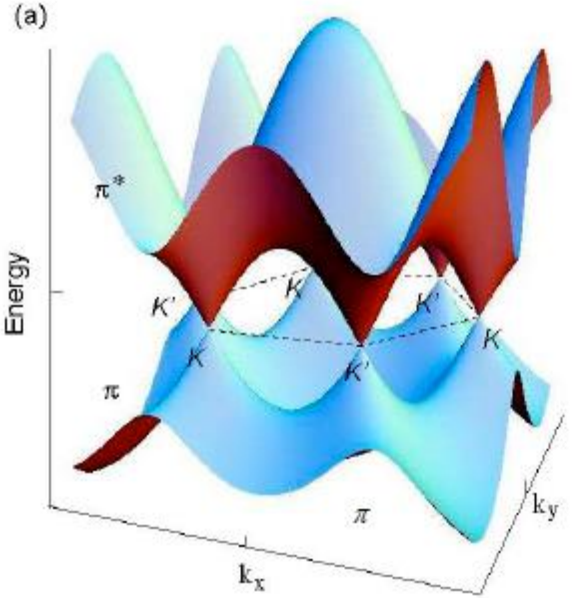

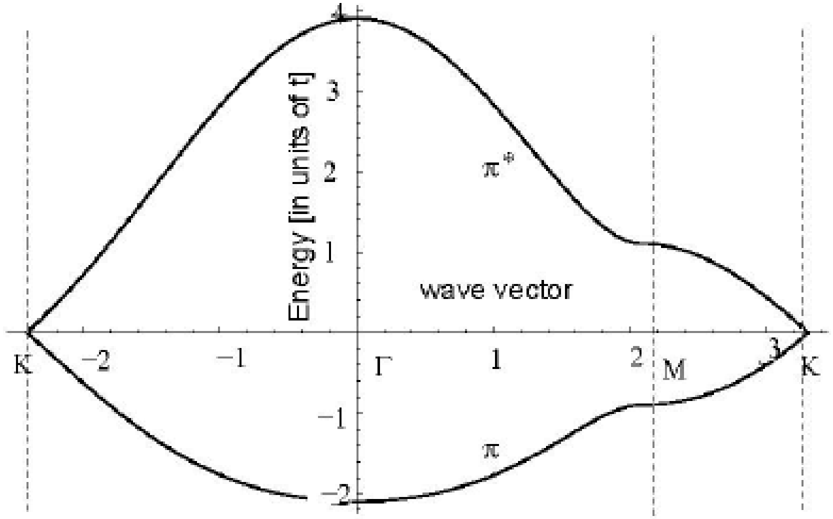

Tight-Binding Approximation

Linear dispersion relation in graphene:

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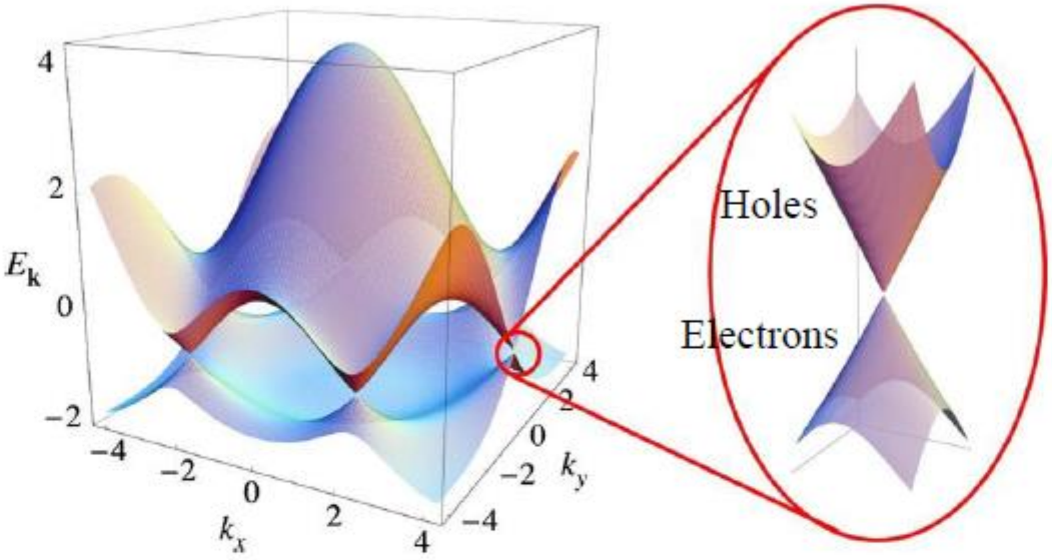

Tight-Binding Approximation

Linear dispersion relation in graphene:

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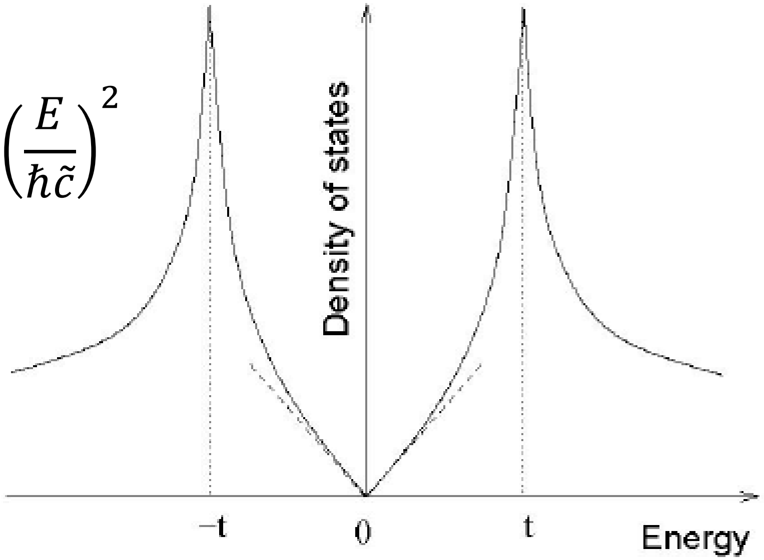
The number of states in the volume of πk^2:

$$N(E) = \frac{2}{(2\pi)^2}\,\pi k^2 = \frac{2}{(2\pi)^2}\,\pi\left(\vec{k}-\vec{k}_i\right)^2 = \frac{2}{(2\pi)^2}\,\pi\left(\frac{E}{\hbar\tilde{c}}\right)^2$$

$$\rho(E) = \frac{\partial N(E)}{\partial E} = \frac{E}{\pi(\hbar\tilde{c})^2}$$



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.

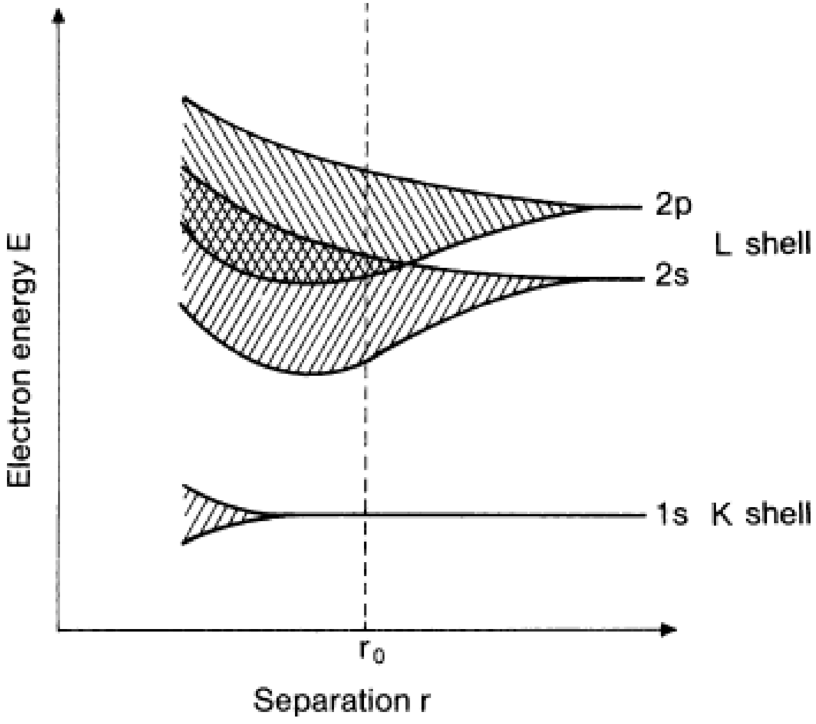


Fig. 1.1. Broadening of the energy levels as a large number of identical atoms from the first row of the periodic table approach one another (schematic). The separation r_0 corresponds to the approximate equilibrium separation of chemically bound atoms. Due to the overlap of the $2s$ and $2p$ bands, 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

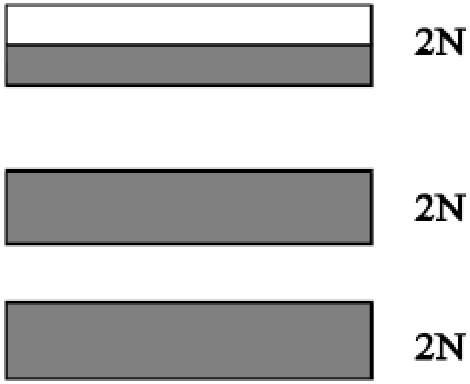
The existence of a forbidden gap is not tied to the periodicity of the lattice! Amorphous materials can also display a band gap.

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).

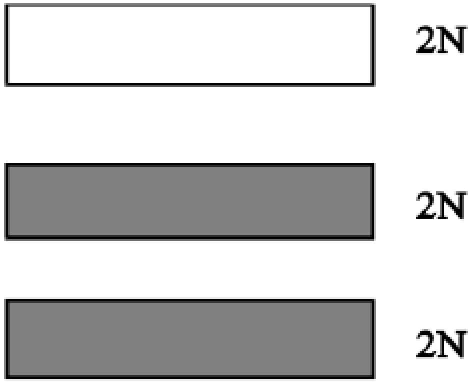
Each band can be occupied by $2N$ electrons.

Tight-Binding Approximation

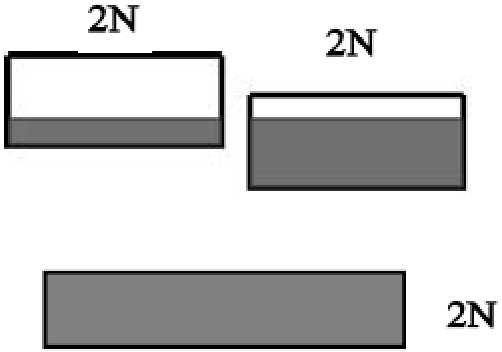
If a crystal with a primitive cubic lattice contains N atoms and thus N primitive unit cells, then an **atomic energy level $\boldsymbol{E_i}$** of the free atom will split into N states (due to the interaction with the rest of $N-1$ atoms). **Each band can be occupied by $\boldsymbol{2N}$ electrons**.



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!)

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Tight-Binding Approximation

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

Be

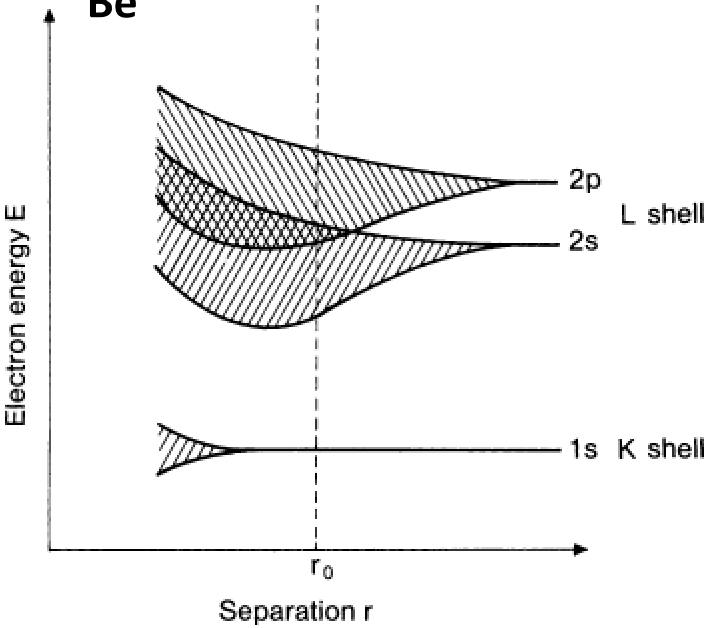

Fig. 1.1. Broadening of the energy levels as a large number of identical atoms from the first row of the periodic table approach one another (schematic). The separation r_0 corresponds to the approximate equilibrium separation of chemically bound atoms. Due to the overlap of the $2s$ and $2p$ bands, 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

C, Si, Ge

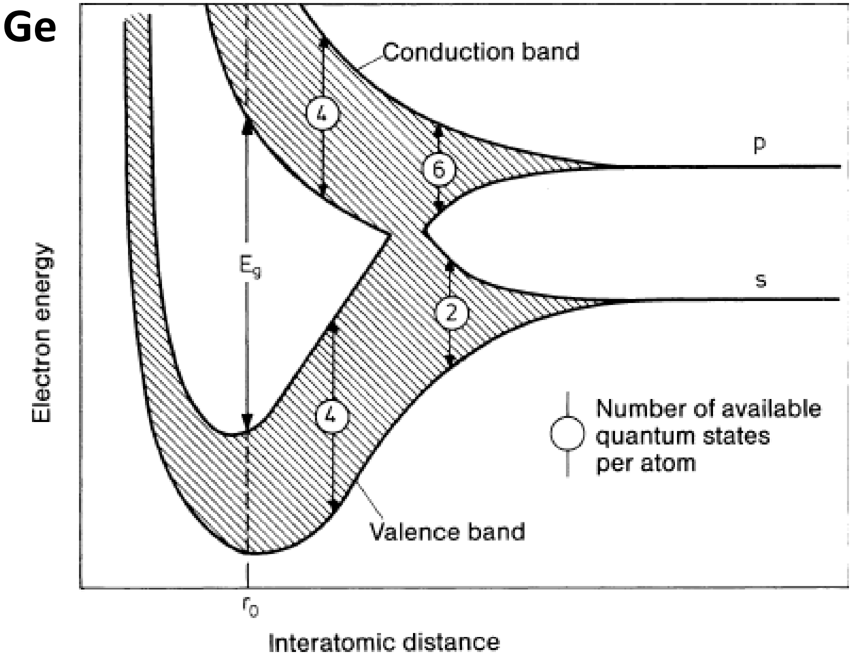

Fig. 7.9. Schematic behavior of the energy bands as a function of atomic separation for the tetrahedrally bound semiconductors diamond (C), Si, and Ge. At the equilibrium separation r_0 there is a forbidden energy gap of width E_g between the occupied and unoccupied bands that result from the sp^3 hybrid 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])

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Tight-Binding Approximation

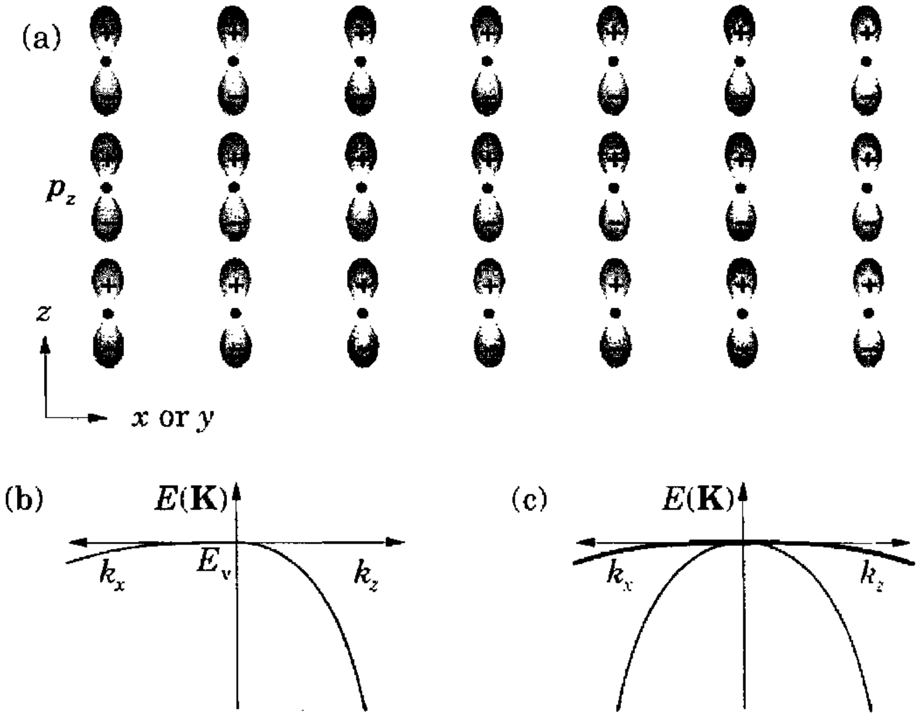


FIGURE 2.17. Valence bands constructed from p orbitals. (a) Lattice of p_z orbitals. (b) Band structure of the p_z orbitals only; the band is 'light' along k_z to the right and 'heavy' along k_x (or k_y) to the left. (c) Total bands from all three p orbitals, showing a doubly degenerate 'heavy' band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

Tight-Binding Approximation

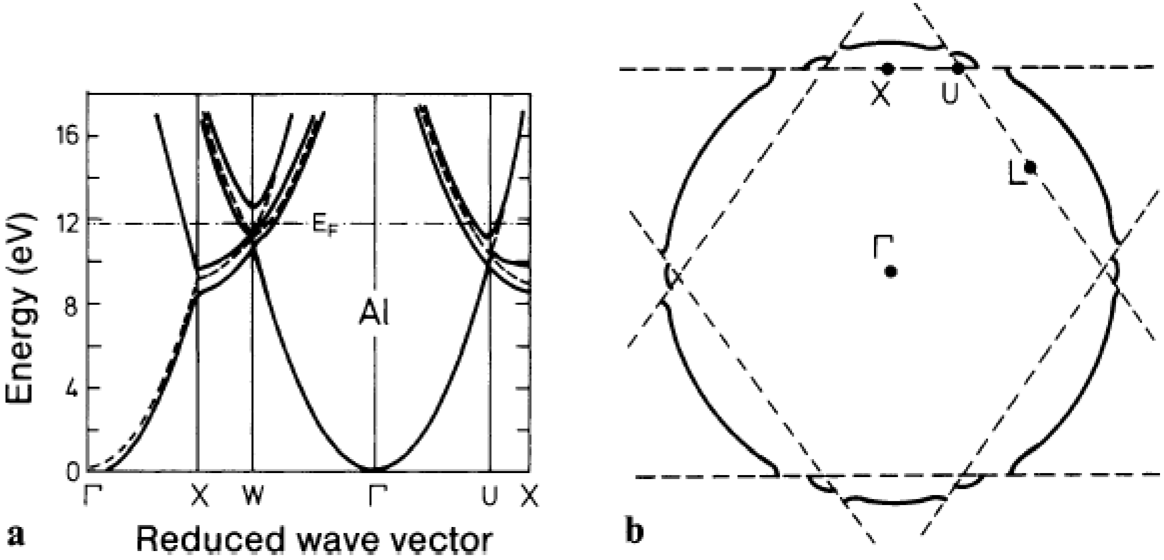


Fig. 7.11. (a) Theoretical bandstructure $E(\boldsymbol{k})$ for Al along directions of high symmetry (Γ is the center of the Brillouin zone). The dotted lines are the energy bands that one would obtain if the *s*- and *p*-electrons in Al were completely free ("empty" lattice). After [7.3]. (b) Cross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

Fermi surfaces of metals

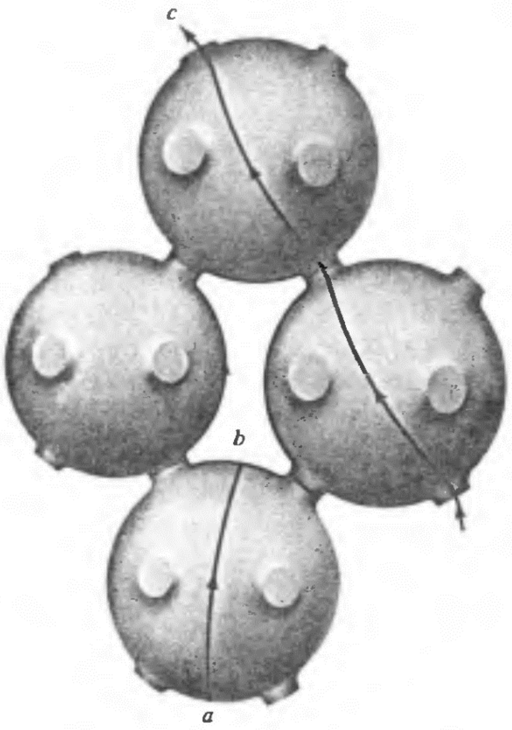


Figure 15.7
Indicating only a few of the surprisingly many types of orbits an electron can pursue in k-space when a uniform magnetic field is applied to a noble metal. (Recall that the orbits are given by slicing the Fermi surface with planes perpendicular to the field.) The figure displays (a) a closed particle orbit; (b) a closed hole orbit; (c) an open orbit, which continues in the same general direction indefinitely in the repeated-zone scheme.

Cu

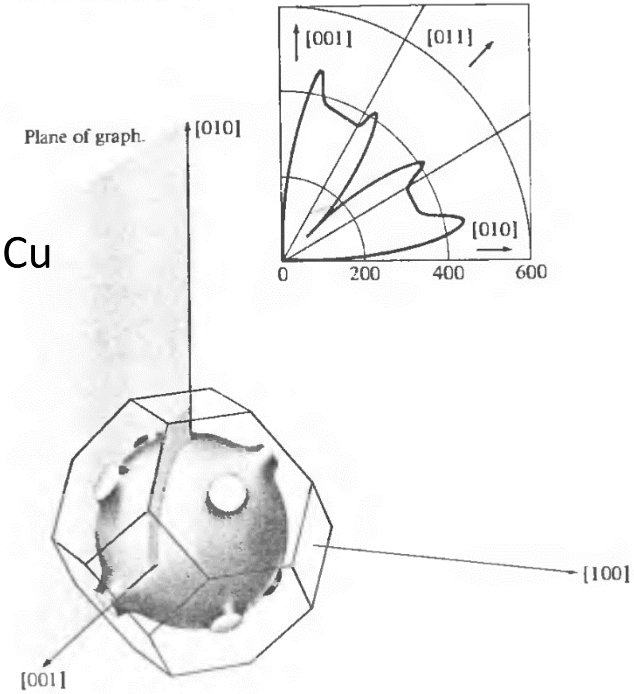


Figure 15.8
The spectacular direction dependence of the high-field magnetoresistance in copper that is characteristic of a Fermi surface supporting open orbits. The [001] and [010] directions of the copper crystal are as indicated in the figure, and the current flows in the [100] direction perpendicular to the graph. The magnetic field is in the plane of the graph. Its magnitude is fixed at 18 kilogauss, and its direction varied continuously from [001] to [010]. The graph is a polar plot of

$$\frac{\rho(H)-\rho(0)}{\rho(0)}$$

vs. orientation of the field. The sample is very pure and the temperature very low (4.2 K—the temperature of liquid helium) to insure the highest possible value for $\omega_c\tau$. (J. R. Klauder and J. E. Kunzler, *The Fermi Surface*, Harrison and Webb, eds., Wiley, New York, 1960.)

Ashcroft, Mermin

Fermi surfaces of metals

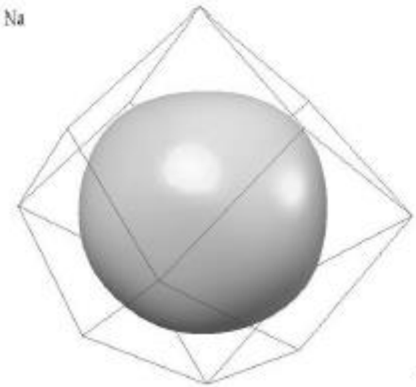


Fig.10 Fermi surface of sodium.

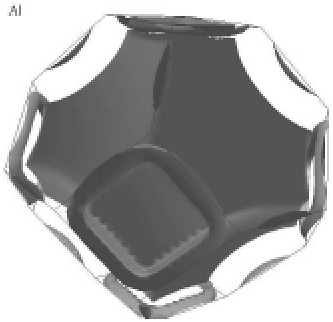


Fig.13 Fermi surface of aluminum

Fig.12 Fermi surface of calcium

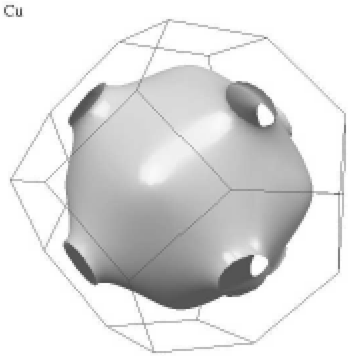


Fig. 11 In the three noble metals the free electron sphere bulges out in the [111] directions to make contact with the hexagonal zone faces.

http://physics.unl.edu/tsymbal/teaching/SSP-927/Section%2010_Metals-Electron_dynamics_and_Fermi_surfaces.pdf

Fermi surfaces of metals

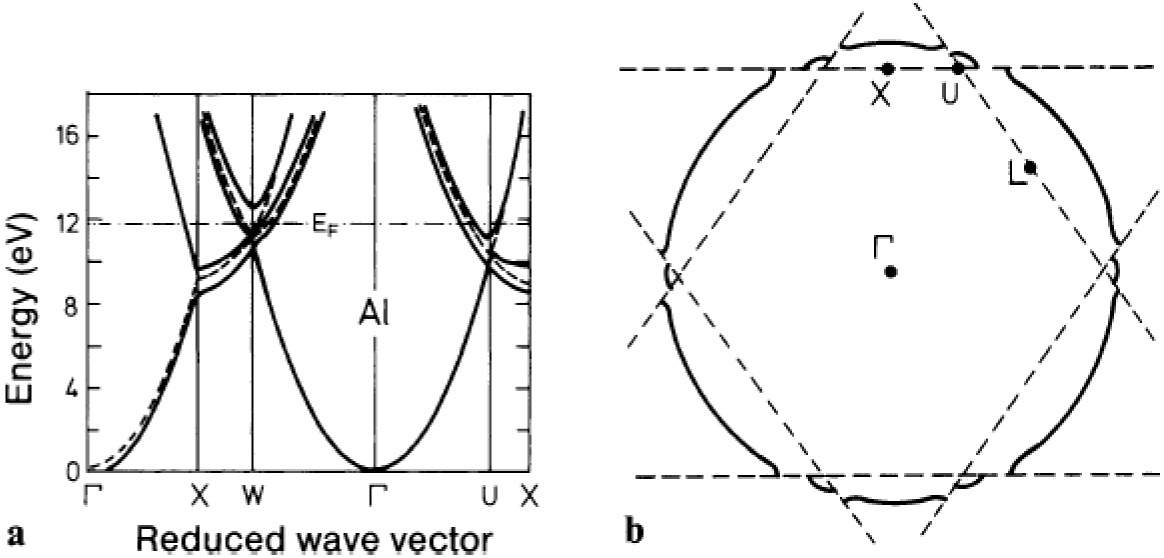
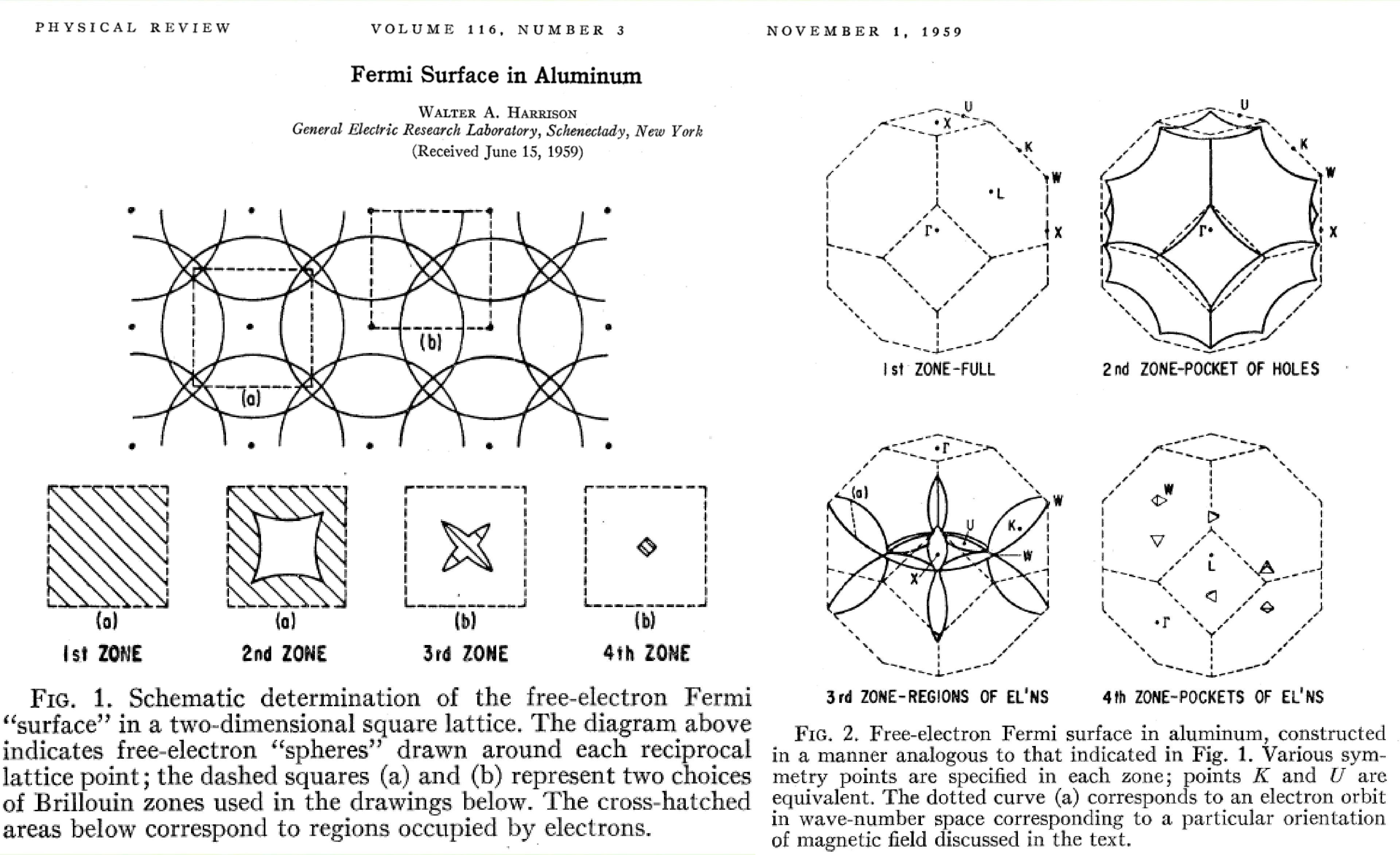


Fig. 7.11. **(a)** Theoretical bandstructure $E(\boldsymbol{k})$ for Al along directions of high symmetry (Γ is the center of the Brillouin zone). The dotted lines are the energy bands that one would obtain if the *s*- and *p*-electrons in Al were completely free ("empty" lattice). After [7.3]. **(b)**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

Tight-Binding Approximation



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Fermi Surface in Aluminum

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(Received June 15, 1959)

FIG. 1. Schematic determination of the free-electron Fermi "surface" in a two-dimensional square lattice. The diagram above indicates free-electron "spheres" drawn around each reciprocal lattice point; the dashed squares (a) and (b) represent two choices of Brillouin zones used in the drawings below. The cross-hatched areas below correspond to regions occupied by electrons.

FIG. 2. Free-electron Fermi surface in aluminum, constructed in a manner analogous to that indicated in Fig. 1. Various symmetry points are specified in each zone; points *K* and *U* are equivalent. The dotted curve (a) corresponds to an electron orbit in wave-number space corresponding to a particular orientation of magnetic field discussed in the text.